Introduction to Python with Application in Bioinformatics

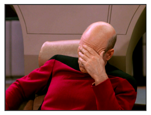
Nanjiang Shu

2024-07-15 (Day 1)

Why programming?

Typical workflow

1. Get data
2. Clean, transform data in spreadsheet
3. Copy-paste, copy-paste, copy-paste
4. Run analysis & export results
5. Realise the columns were not sorted correctly
6. Go back to step 2, Repeat



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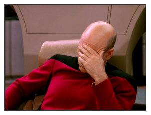

With programming, you can automate some manual procesures

Why Python?

- Readability and simplicity

In [ ]:
```
# In Python
print("Hi, Python!")
```

Why Python?

- Readability and simplicity

In [ ]:
```
# In Python
print("Hi, Python!")
```

In [ ]:
```
/* In C++ */
#include <iostream>

int main() {
    std::cout << "Hi, Python!" << std::endl;
    return 0;
}
```

- Integration with C.
    - Numpy, which builds the fundatation for the popular deep learning package - Tensorflow
- `pandas` to read, manipulate and write Excel files programmtically

In [ ]:
```python
print(1 + 1)
print("Hello Python")
```

In [ ]:
```python
a = 1 + 1
print(a)
a = "Hello Python"
print(a)
```

```
In [ ]: print(1 + 1)
        print("Hello Python")
```

```
In [ ]: a = 1 + 1
        print(a)
        a = "Hello Python"
        print(a)
```

- Fixed values, e.g. `1` and `Hello Python` , in the Python code are called `literals`
- Liternals are immutable
- The name `a` that holds the value is called a `variable`

In [ ]:
```
a = 1
a = "ATCG"
a = True
a = None
```

In [ ]:
```
# Can you tell the types of them?
sequence_length = 200
scale = 2.5
gene_id = "ABC12345"
is_DNA = False
```

Use `type()` function to determine the type of a variable

In [ ]:
```
```

In [ ]:

```
sequence_length = 200
print(sequence_length)
```

In [ ]:

```
seq_len = 200
seq_lens = [100, 150, 200] # a list
print(seq_lens[1])
```

List and Tuple

- List and tuple are ordered collection of elements

```
In [ ]: seq_len = 200
        seq_lens = [100, 150, 200] # a list
        print(seq_lens[1])
```

```
In [ ]: seq_lens = (100, 150, 200) # a tuple
        print(seq_lens[1])
```

In [ ]:

```
li = [100, 150, None, "ATCG", 3.1415, seq_len, seq_lens]
li
```

Difference of List and Tuple

- List is mutable
- Tuple is immutable

In [ ]:
```
li_seqlens = [100, 150, 200]
tu_seqlens = (100, 150, 200)
```

Difference of List and Tuple

- List is mutable
- Tuple is immutable

In [ ]:

```
li_seqlens = [100, 150, 200]
tu_seqlens = (100, 150, 200)
```

In [ ]:

```
li_seqlens[1] = 500
print(li_seqlens)
```

Difference of List and Tuple

- List is mutable
- Tuple is immutable

In [ ]:
```
li_seqlens = [100, 150, 200]
tu_seqlens = (100, 150, 200)
```

In [ ]:
```
li_seqlens[1] = 500
print(li_seqlens)
```

In [ ]:
```
tu_seqlens[1] = 500
```

Set

- Set is an unordered collection of unique elements

In [ ]:
```
gene_ids = {"TP53", "COX2", "EGFR", "MTOR"} # a set
gene_ids
```

Set

- Set is an unordered collection of unique elements

```
In [ ]: gene_ids = {"TP53", "COX2", "EGFR", "MTOR"} # a set
        gene_ids
```

```
In [ ]: # set is unordered
        gene_ids = {"1", "2", "3", "4", "5"}
        for e in seq_lens:
            print(e)
```

Set

- Set is an unordered collection of unique elements

```
In [ ]: gene_ids = {"TP53", "COX2", "EGFR", "MTOR"} # a set
        gene_ids
```

```
In [ ]: # set is unordered
        gene_ids = {"1", "2", "3", "4", "5"}
        for e in seq_lens:
            print(e)
```

```
In [ ]: # set has unique element
        gene_ids = {"1", "1", "2", "2", "3"}
        print(gene_ids)
```

In [ ]:
```python
sequence_info = {  # a dictionary
    "gene": "TP53",
    "species": "Homo sapiens",
    "length": 2000
}
```

```
In [ ]: 8/2
In [ ]: 1 + 1.5
In [ ]: result = 0.1 + 0.2 - 0.3
        print(result)
```

```
In [ ]: print(result == 0.0)
```

Warning: keep in mind the precision limitations of floating-point arithmetic.

In [ ]:
```
result = 0.1 + 0.2 - 0.3
print(result)
```

In [ ]:
```
print(result == 0.0)
```

In [ ]:
```
print((result - 0.0) < 1e-6)
```

```
In [ ]: "protein"[1:4]
In [ ]: "a" == "b"
In [ ]:
```

```
In [ ]: 1 + 1.5
```

When you run operations on different data types, an underlying data type conversion has been made

```
In [ ]: 1 + 1.5
```

```
In [ ]: # Guess what will be the result for this?
        1 + True
```

What about `dkfsjdsklut`

- well, this is a valid name, but NOT recommended`

```
In [ ]: global = 5
```

```
In [ ]: # show the type of value with type()
        print(type(result))
```

```
In [ ]: # convert float value to string value with str()
        str(2.5)
```

In [ ]:
```
sequence = "ATGCTACGATaCG"
len(sequence)
```

In [ ]:
```
seq_lens = [100, 200, 300]
len(seq_lens)
```

len()

```
In [ ]: sequence = "ATGCTACGATaCG"
        len(sequence)
```

```
In [ ]: seq_lens = [100, 200, 300]
        len(seq_lens)
```

```
In [ ]: # can you get the length of an integer
        len(3)
```

```
In [ ]: read_counts = [1500, 2000, 1750, 2250, 1900, 2500]
        print("total_reads:", sum(read_counts))
```

```
In [ ]: expression_levels =  [2.5, 3.6, 4.2, 5.0, 3.8, 3.8, 9.5, 100.1]
        print("Max expression level:", max(expression_levels))
        print("Min expression level:", min(expression_levels))
```

```
In [ ]: print("Average expression level: ", sum(expression_levels)/len(expressi
In [ ]: read_counts = [1500, 2000, 1750, 2250, 1900, 2500]
        sorted_read_counts = sorted(read_counts)
        print(sorted_read_counts)
```

In [ ]:
```
seq_len1 = 150
seq_len2 = 181

seq_len1 <= seq_len2
```

In [ ]:

```
freq1 = 0.51
freq2 = 1.5

freq1 > 0.5 and freq2 > 0.5
```

```
In [ ]: gene_ids = ["TP53", "COX2", "EGFR", "MTOR"] # a set

        "TP53" in gene_ids
```

In [ ]:

```python
length = 500
species = "Mouse"
read_count = 100
# I want to evaluate the condition that length is larger than 300 or sp
# and read_count is larger than 200
# Expected value: False
length > 300 or species == "Mouse" and read_count > 200
```

A word of caution when using operators

```
In [ ]: length = 500
        species = "Mouse"
        read_count = 100
        # I want to evaluate the condition that length is larger than 300 or sp
        # and read_count is larger than 200
        # Expected value: False
        length > 300 or species == "Mouse" and read_count > 200
```

```
In [ ]: (length > 300 or species == "Mouse") and read_count > 200
```

A word of caution when using operators

In [ ]:

```python
length = 500
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read_count = 100
# I want to evaluate the condition that length is larger than 300 or sp
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# Expected value: False
length > 300 or species == "Mouse" and read_count > 200
```

In [ ]:

```python
(length > 300 or species == "Mouse") and read_count > 200
```

- Always remember that **and** takes precedence over **or** in logical expressions.
- Use parentheses `()` to make your intended grouping explicit and improve readability.

```
In [ ]: mylist[1:3]
```

```
In [ ]: mylist[0:9:2] # [start, stop, step]
```

```
In [ ]: mylist[3:] # from 4th position to the end
```

```
In [ ]: mylist[:5] # from the beginning to the 5th position
```

```
In [ ]: mylist[:] # the same as mylist[::], mylist[::1]
In [ ]: mylist[-1] # return the last element, equivalent to mylist[8]
```

```
In [ ]: # What will be the result for this?
        mylist[::-1]
```

When the step is negative, it changes the direction

In [ ]:

```
mystr = "123456789"
print("mystr[2] \t= ", mystr[2] )
print("mystr[1:3] \t= ", mystr[1:3])
print("mystr[0:9:2] \t= ", mystr[0:9:2])
print("mystr[3:] \t= ", mystr[3:])
print("mystr[:5] \t= ", mystr[:5])
print("mystr[:] \t= ", mystr[:])
print("mystr[-1] \t= ", mystr[-1])
print("mystr[::-1] \t= ", mystr[::-1])
```

In [ ]:

```
# string is immutable
mystr = "123456789"
mystr[2] = "7"
```

In [ ]:

```
a = 5
print("a=", a)
a = 6
print("a=", a)
```

Are `int`, `float` and `bool` immutable?

In [ ]:
```python
a = 5
print("a=", a)
a = 6
print("a=", a)
```

In [ ]:
```python
# id(var) returns the memory address of var.
a = 5
print("memory address of a = ", id(a), ", value of a = ", a)
a = 6
print("memory address of a = ", id(a), ", value of a = ", a)
```

Are `int`, `float` and `bool` immutable?

In [ ]:
```
a = 5
print("a=", a)
a = 6
print("a=", a)
```

In [ ]:
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# id(var) returns the memory address of var.
a = 5
print("memory address of a = ", id(a), ", value of a = ", a)
a = 6
print("memory address of a = ", id(a), ", value of a = ", a)
```

In [ ]:
```
mylist = [1, 2, 3, 4, 5, 6, 7, 8, 9]
print("memory address of mylist = ", id(mylist), ", value of mylist = "
mylist[2] = 7
print("memory address of mylist = ", id(mylist), ", value of mylist = "
```

In [ ]:
```python
mylist = [1, 2, 3, 4, 5, 6, 7, 8, 9]
mylist.append(15)
print(mylist)
```

In [ ]:
```python
mylist.remove(15)
print(mylist)
```

In [ ]:
```python
del mylist[2]
print(mylist)
```

Session 3: Loops in Python

```
In [ ]: gene_ids = ["TP53", "COX2", "EGFR", "MTOR"]
        # How do we print all IDs, one per line?
```

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```
gene_ids = ["TP53", "COX2", "EGFR", "MTOR"]
# How do we print all IDs, one per line?
```

In [ ]:
```
print(gene_ids[0])
print(gene_ids[1])
print(gene_ids[2])
print(gene_ids[3])
```

Session 3: Loops in Python

In [ ]:

```
gene_ids = ["TP53", "COX2", "EGFR", "MTOR"]
# How do we print all IDs, one per line?
```

In [ ]:

```
print(gene_ids[0])
print(gene_ids[1])
print(gene_ids[2])
print(gene_ids[3])
```

In [ ]:

```
gene_ids = ["TP53", "COX2", "EGFR", "MTOR"]

for gene_id in gene_ids:
    print(gene_id)
```

Note the INDENT of the **for** loop

Indentation is crucial in Python

- Blocks of code are defined by their indentation level.
- Typically, a tab or four spaces are used for each indentation level, but consistency within a block is the key.
- Don't mix tabs and spaces, although it's allowed.

```
In [ ]: for gene_id in gene_ids:
            print(gene_id)
```

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```
In [ ]: for gene_id in gene_ids:
            print(gene_id)
```

```
In [ ]: for gene_id in gene_ids:
            print("==ID==")
            print(gene_id)
```

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- Blocks of code are defined by their indentation level.
- Typically, a tab or four spaces are used for each indentation level, but consistency within a block is the key.
- Don't mix tabs and spaces, although it's allowed.

In [ ]:
```
for gene_id in gene_ids:
    print(gene_id)
```

In [ ]:
```
for gene_id in gene_ids:
    print("==ID==")
    print(gene_id)
```

In [ ]:
```
for gene_id in gene_ids:
        print("==ID==")
        print(gene_id)
```

Types of loops

For loop

```
In [ ]: gene_ids = ["TP53", "COX2", "EGFR", "MTOR"]

        for gene_id in gene_ids:
            print(gene_id)
```

Types of loops

`For` loop

```
In [ ]: gene_ids = ["TP53", "COX2", "EGFR", "MTOR"]

        for gene_id in gene_ids:
            print(gene_id)
```

`While` loop

```
In [ ]: gene_ids = ["TP53", "COX2", "EGFR", "MTOR"]

        i = 0
        while i < len(gene_ids):
            print(gene_ids[i])
            i += 1

        print("== When loop ends, i =", i)
```

In [ ]:
```
gene_ids = ["TP53", "COX2", "EGFR", "MTOR"]

i = 0
while i < len(gene_ids) and not gene_ids[i].startswith("E"):
    print(gene_ids[i])
    i += 1

print("== When loop ends, i =", i)
```

Examples of `while` loop

In [ ]:
```python
gene_ids = ["TP53", "COX2", "EGFR", "MTOR"]

i = 0
while i < len(gene_ids) and not gene_ids[i].startswith("E"):
    print(gene_ids[i])
    i += 1

print("== When loop ends, i =", i)
```

In [ ]:
```python
while True:
    print("yes")
```

Note: there is one built-in function called `range()` which is especially useful for the for loop

In [ ]:
```
for i in range(10):
    print(i)
```

The `range()` function

```
In [ ]: for i in range(10):
            print(i)
```

```
In [ ]: file_basename = "dnaseq"
        for i in range(10):
            seqfile = file_basename + "_" + str(i) + ".fa"
            print("Analyzing " + seqfile)
```

Session 4: Conditional statement

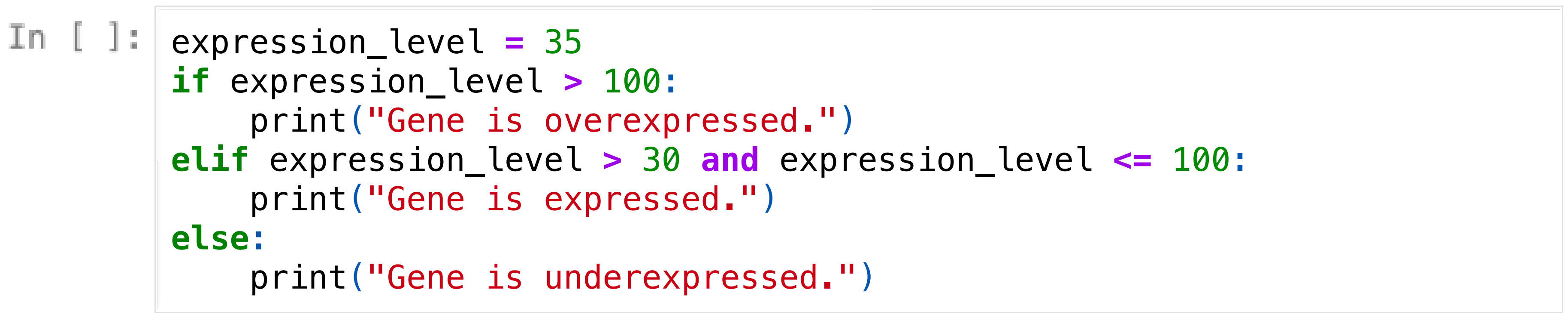
- Conditional statements allow decision-making in a program.
- Python uses `if`, `elif`, and `else` for conditionals.

In [ ]:
```
if condition1:
    # executed if condition1 is True
elif condition2:
    # executed if condition1 is False and condition2 is True
else:
    # executed if both condition1 and condition2 are False
```

In [ ]:
```
dna_sequence = "AGTCTCG"
if 'N' not in dna_sequence:
    print("Valid DNA sequence.")
```

In [ ]:

```python
expression_level = 35
if expression_level > 50:
    print("Gene is overexpressed.")
else:
    print("Gene is not overexpressed.")
```



```
In [ ]: expression_level = 35
        if expression_level > 100:
            print("Gene is overexpressed.")
        elif expression_level > 30 and expression_level <= 100:
            print("Gene is expressed.")
        else:
            print("Gene is underexpressed.")
```

In [ ]:

```python
# Use nested conditionals to categorize genetic variants based on multi
genotype = "AG"
phenotype = "expressed"
if genotype == "AG":
    # Only check phenotype if genotype is "AG"
    if phenotype == "expressed":
        print("Variant " + genotype + " is active and expressed.")
    else:
        print("Variant " + genotype + " is active but not expressed.")
else:
    print("Variant " + genotype + " is a non-target variant.")
```