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CENTER FOR SYSTEMS BIOLOGY DRESDEN

Python Algorithms

conditions, loops, functions

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Using material from Benoit Lombardot, Scientific Computing Facility, MPI CBG

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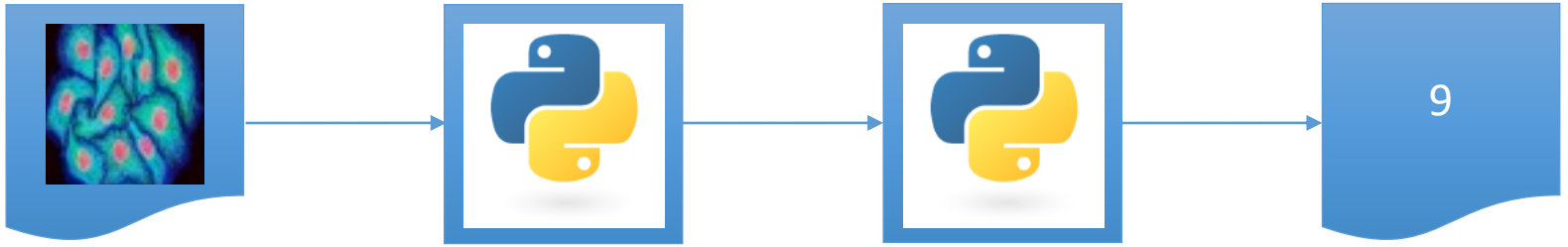
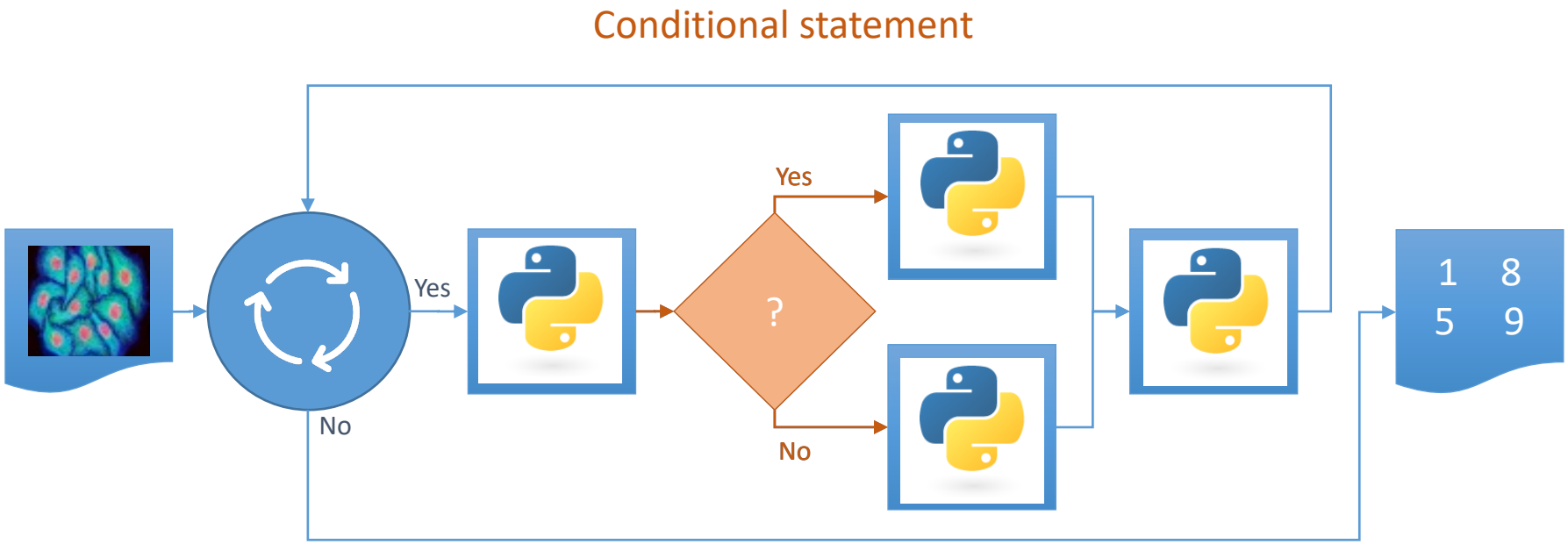
Data science workflows *rarely* look like this

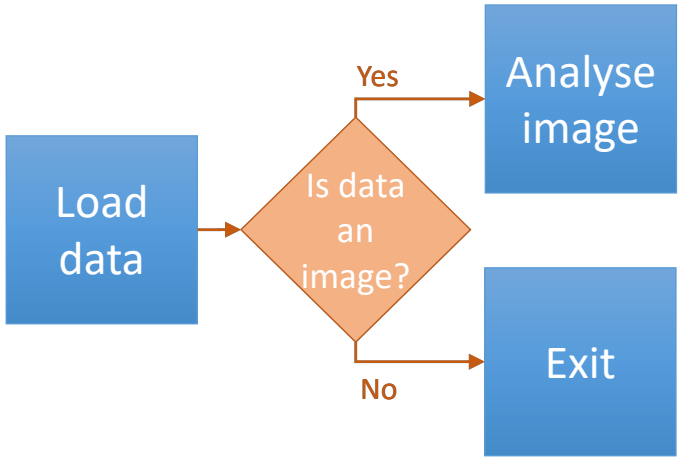


Data science workflows *rather* look like this



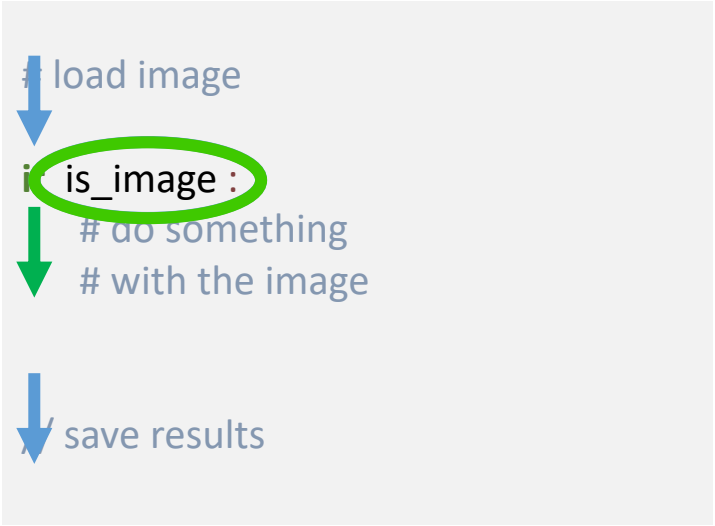
Example use cases for conditional statements

- Check if pre-requisites are met
- Check if data has the right format
- Check if processing results are within an expected range
- Check for errors



Conditionals are implemented with the `if` statement

- Depending on a condition, some lines of code are executed or not.



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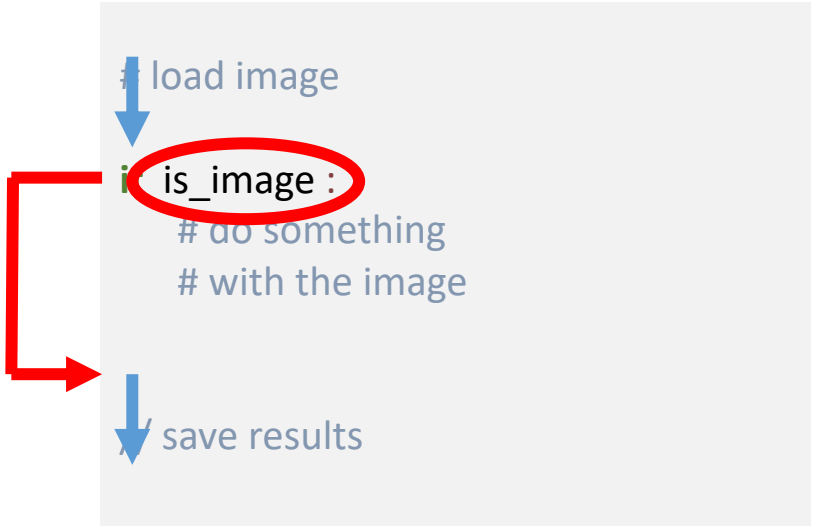

`if` / `elif` / `else`: choose from several alternatives

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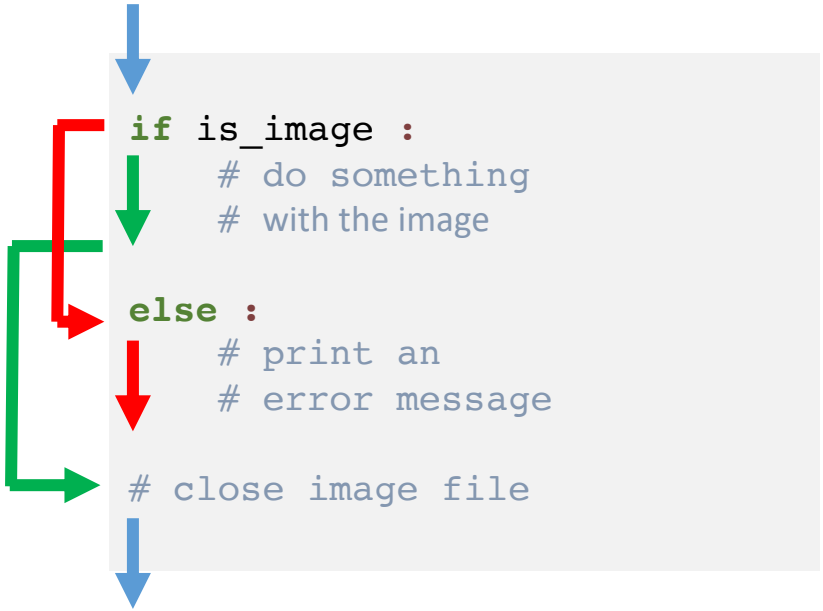
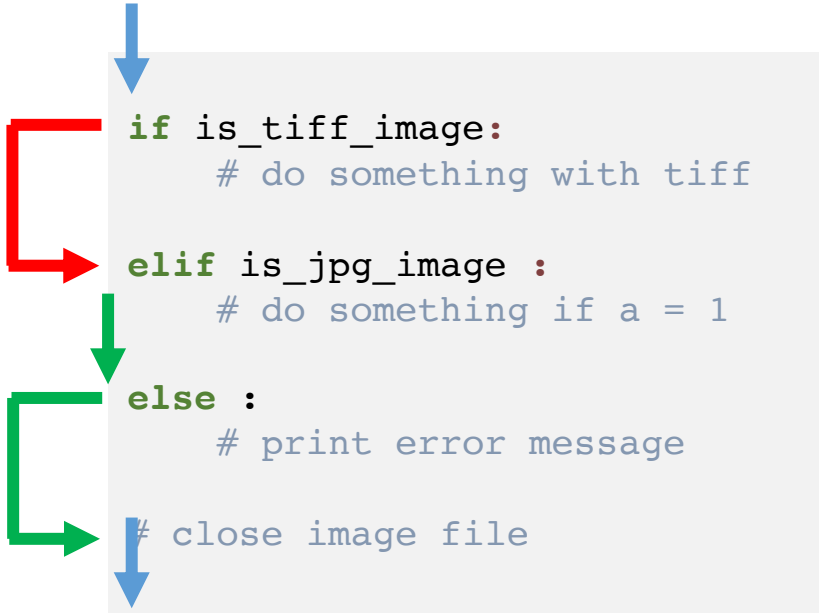
- Depending on conditions, only one of several possible blocks is computed
- Indentation is used to mark where a block starts and ends.
- Indentation helps reading blocks,



```
if is_image :
    # do something
    # with the image

else :
    # print an
    # error message

# close image file
```



```
if is_tiff_image:
    # do something with tiff

elif is_jpg_image :
    # do something if a = 1

else :
    # print error message

# close image file
```

Comparison operators always have True (1) or False (0) as result

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```
# initialise program
image_size = 99.5

# evaluate quality
if image_size > 99.9 :
    print("Everything is fine.")
else :
    print("We need a larger image!")
```

'We need a larger image!'

```
In [1]: a = 4

        if a = 5:
            print("Hello world")

  File "<ipython-input-1-13fb587c9332>", line 3
    if a = 5:
         ^
SyntaxError: invalid syntax
```

Note: These are two equal signs!

Operator	Description	Example
<, <=	less than, less than or equal to	a < b
>, >=	greater than, greater than or equal to	a > b
==	equal to	a == b
!=	not equal to	a != 1

Conditions can be combined with logic operators

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- Logic operators always take conditions as operands and result in a condition.
  - and
  - or
  - not
- Also combined conditions can be either True (1) or False (0).

```
# initialise program
image_size = 99.9
number_of_images = 3

if image_size >= 99.9 and number_of_images > 5 :
    print("The image is ok.")
```

```
# initialise program
image_size = 99.9

if not image_size < 99.9 :
    print("The image is ok.")
```

```
'The image is ok.'
```

The `in` statement: Checking contents of lists

```
# initialise program
my_list = [1, 5, 7, 8]
item = 3

if item in my_list :
    print("The item is in the list.")
else :
    print("There is no", item, "in", my_list )
```

'There is no 3 in [1, 5, 7, 8]'

- Quite intuitive, isn't it?

```
# initialise program
my_list = [1, 5, 7, 8]
item = 3

if item not in my_list :
    print("There is no", item, "in", my_list )
else :
    print("The item is in the list.")
```

'There is no 3 in [1, 5, 7, 8]'

Rules for readable code

- Every command belongs on its own line

- Insert empty lines to separate important processing steps

- Put spaces between operators and operands, because:

This is easier to read thanthat,orisnt'it?

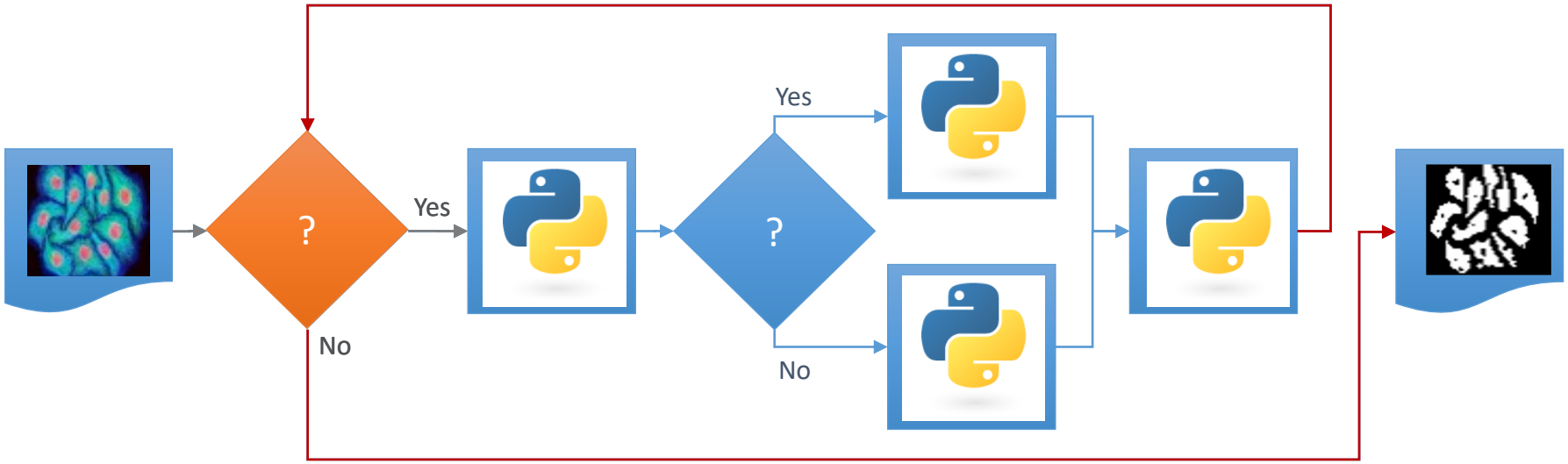
- Indent every conditional block (if/else) using the TAB key
  - Python actually enforces this rule: Indentation *means* combining operations to a block

```
# initialise program
a = 5
b = 3
c = 8

# execute algorithm
d = (a + b) / c

# evaluate result
```

```
if a == 5 :
a = 3
print("Yin")
else :
a = 1
print("Yang")
```

```
  Cell In [2], line 3
    print("Yin")
    ^
IndentationError: expected an indented block
```

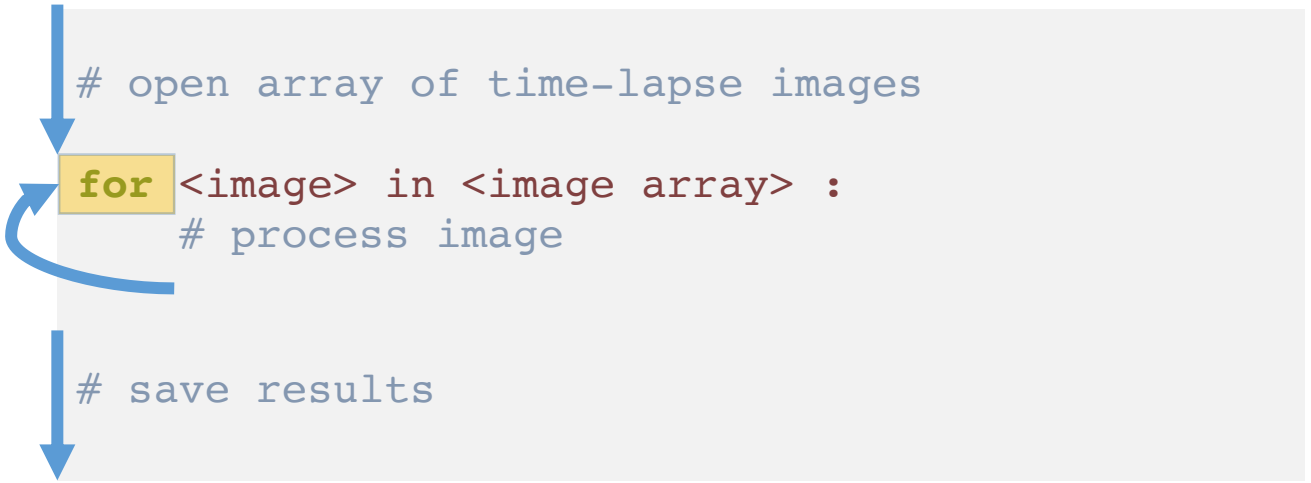
To repeat actions, you run code in **loops**



Loop statement

`for`: execute some lines of code *for* a number of times

- typically for all items in an array-like thing (lists, tuples, images)



`for-in`: Loop over items of a list

- Example list :

```
animal_set = ["Cat", "Dog", "Mouse"]

for animal in animal_set:
    print(animal)
```

```
Cat
Dog
Mouse
```

`range` creates numbers on the fly:

`range(start, stop, step)`

```
# for loops
for i in range(0, 5):
    print(i)
```

```
0
1
2
3
4
```

`for`-loop syntax pitfalls

- Indent the code within the `for` loop
  remember: indentation *means* combining operations to a block

```
# for loops
for i in range(0, 5):
print(i)
```

```
  File "<ipython-input-15-59c457ae0ac9>", line 3
    print(i)
        ^
IndentationError: expected an indented block
```

Don't forget to indent!

- Colon necessary

```
# for loops
for i in range(0, 5)
    print(i)
```

```
  File "<ipython-input-13-23157c0ed137>", line 2
    for i in range(0, 5)
                       ^
SyntaxError: invalid syntax
```

Don't forget the colon!

Functions

- In case repetitive tasks appear that cannot be handled in a loop, custom functions are the way to go.
- Functions allow to re-use code in different contexts.
- Defined using the `def` keyword
- Indentation is crucial.
- Functions must be defined before called

- Definition

```
def sum_numbers(a, b):
    result = a + b
    return result
```

name (parameters)

body commands

return statement (optional)

- Call

```
c = sum_numbers(4, 5)
print(c)
```

```
9
```

```
sum_numbers(5, 6)
```

```
11
```

```
sum_numbers(3, 4)
```

```
7
```

Functions run a block of code with one command

- In case repetitive tasks appear that cannot be handled in a loop, custom functions are the way to go.
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- Functions must be defined before called

- Definition

```
def sum_numbers(a, b):
    result = a + b
    return result
```

- Call

```
c = sum_numbers(4, 5)
print(c)
```

```
9
```

Keep it short and simple (KISS)

- Let's assume we want to write a function that grades student exams

```
def grade_student_exams(points_achieved: int, total_points_in_exam: int) -> int:
percentage = points_achieved / total_points_in_exam * 100
if percentage > 95:
    grade = 1
elif percentage > 80:
    grade = 2
elif percentage > 60:
    grade = 3
elif percentage > 50:
    grade = 4
else:
    grade = 5
return grade
```

Keep it short and simple (KISS)

- Now we want to extend that function to also grade pass/fail exams

```
def grade_student_exams(points_achieved: int, total_points_in_exam: int ,
pass_fail: bool = True) -> int:
percentage = points_achieved / total_points_in_exam * 100
if percentage > 95:
    grade = 1
elif percentage > 80:
    grade = 2
elif percentage > 60:
    grade = 3
elif percentage > 50:
    grade = 4
else:
    grade = 5
if pass_fail:
    if grade < 5:
        return True
    else:
        return False
else:
    return grade
```

This is rather messy:

It is not clear what the function returns

If `pass_fail` is `False`, we return an integer,

Otherwise a boolean.

Also, reading what the function does is difficult

Keep it short and simple (KISS)

- If we split this into two, we get two nice short and simple functions again

```
def grade_student_exams(points_achieved: int, total_points_in_exam: int) -> int:
percentage = points_achieved / total_points_in_exam * 100
if percentage > 95:
    grade = 1
elif percentage > 80:
    grade = 2
elif percentage > 60:
    grade = 3
elif percentage > 50:
    grade = 4
else:
    grade = 5
return grade

def grade_pass_fail_exam(points_achieved: int, total_points_in_exam: int) -> bool:
grade = grade_student_exams(points_achieved, total_points_in_exam)
if grade < 5:
    return True
else:
    return False
```

Document your functions to keep track of what they do

- Describe what the functions does and what the parameters are meant to be

```
def square(number):
    '''
    Squares a number by multiplying it with itself  and returns its result.
    '''

    return number * number
```

- You can then later print the *documentation* with a ? if you can't recall how a function works.

```
square?
```

```
Signature: square(number)
Docstring: Squares a number by multiplying it with itself and returns its
result.
```

- Hint: most integrated development environments (=coding software) provide automatisms to create a documentation template for your function. Look for *autodocstring* or similar.

Summary

Today, you learned

- Python
  - Conditions: `if` / `elif` / `else`
  - Loops: `for .. in` / `while` / `break` / `continue`
  - Functions: `def`