

Introduction To Python Programming

I: The Python language

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Python is High Level, Interpreted and Dynamic

- No memory management
- No system programming needed
- Complex data structures
- Extensive library of modules (“batteries included”)
- Standalone programs
- Scripting language
- Interactive use
- Embeddable into applications
- OS and system agnostic

Useful *everywhere*

Written in or Extends Python:

PyMOL	TensorFlow
NEST	NEURON
Blender	Qiime
HTSeq	BUSCO

...

...

Run Python on:

Windows	Supercomputers
Linux	Desktops
OSX	Microcontrollers
Android	

Focus on your problem, not your code

Example: Replace text strings
in a list of files

- Python version below

Python

```
import fileinput

files=["test1.txt", "test2.txt", "test3.txt"]

for line in fileinput.input(files, inplace=True):
    print(line.replace('Goodbye!', 'Hello!'), end='')
```

Focus on your problem, not your code

Example: Replace text strings in a list of files

- Python version below
- C to the right

Python

```
import fileinput

files=["test1.txt", "test2.txt", "test3.txt"]

for line in fileinput.input(files, inplace=True):
    print(line.replace('Goodbye!', 'Hello!'), end='')
```

C

```
#include <stdio.h>
#include <stdlib.h>
#include <stddef.h>
#include <string.h>
#include <sys/types.h>
#include <fcntl.h>
#include <sys/stat.h>
#include <unistd.h>
#include <err.h>
#include <string.h>

char * find_match(const char *buf, const char * buf_end, const char *pat, size_t len)
{
    ptrdiff_t i;
    char *start = buf;
    while (start + len < buf_end) {
        for (i = 0; i < len; i++)
            if (start[i] != pat[i]) break;

        if (i == len) return (char *)start;
        start++;
    }
    return 0;
}

int replace(const char *from, const char *to, const char *fname)
{
#define bail(msg) { warn(msg " '%s'", fname); goto done; }
    struct stat st;
    int ret = 0;
    char *buf = 0, *start, *end;
    size_t len = strlen(from), nlen = strlen(to);
    int fd = open(fname, O_RDWR);

    if (fd == -1) bail("Can't open");
    if (fstat(fd, &st) == -1) bail("Can't stat");
    if (!(buf = malloc(st.st_size))) bail("Can't alloc");
    if (read(fd, buf, st.st_size) != st.st_size) bail("Bad read");

    start = buf;
    end = find_match(start, buf + st.st_size, from, len);
    if (!end) goto done; /* no match found, don't change file */

    ftruncate(fd, 0);
    lseek(fd, 0, 0);
    do {
        write(fd, start, end - start); /* write content before match */
        write(fd, to, nlen); /* write replacement of match */
        start = end + len; /* skip to end of match */
        end = find_match(start, buf + st.st_size, from, len); /* find match again */
    } while (end);

    /* write leftover after last match */
    if (start < buf + st.st_size)
        write(fd, start, buf + st.st_size - start);

done:
    if (fd != -1) close(fd);
    if (buf) free(buf);
    return ret;
}

int main()
{
    const char * files[] = { "test1.txt", "test2.txt", "test3.txt" };
    for (int i = 0; i < sizeof(files)/sizeof(char*); i++)
        replace("Goodbye!", "Hello!", files[i]);

    return 0;
}
```

Let's Run some Python

We will use “ipython” for an interactive shell

- Log in to Deigo
- load Python 3
- start iPython

```
ssh -X <your-name>@deigo.oist.jp  
module load python/3.7.3  
ipython3
```

History Of Python

— or —

Why are there two of them?!

```
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module load python/3.7.3  
ipython3
```

Python 2

- Named after Monty Python
- released in 2000
- Huge success; many users, lots of packages
- **End of life 2020**
→ never use it any longer

Python 3

- first released in 2008
- 3.5 onwards is now stable, complete, supported
- **We Recommend Python 3 for all future Python projects.**

Example

Code comes in *blocks*

- marked by indentation, not "{","}" or "begin", "end"

if, while, function defs etc. end with ":", followed by a block

you don't need to declare variable types

starts a comment

```
# an example python program

def greeting(name, age):
    print("Hi {}".format(name))
    if age>45:
        print("You must be very wise!")

# here the main program starts
while True:
    name = input('your name (or quit) :')
    if name=='quit':
        break
    age = input("what's your age :")
    greeting(name, int(age))

print('Bye now!')
```

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print('Bye now!')
```

Numbers

Integers

- arbitrarily large

Floating point numbers

- 64 bit

- **Complex numbers**

- pair of floats
- use 'j' for imaginary part

```
1+1          # integers
2
1.5*2.5      # floating point
3.75
5/3          # division
1.6666666666666667
5//3         # integer division
1
5%3          # remainder
2
2.5**4       # exponentiation
39.0625
4+3j         # complex numbers
(4+3j)
int(3.5)     # convert types
3
float(4)
4.0
```

Variables

Variables

- stores a value
- don't need to declare the type
 - can force a type with type functions:

```
x = 1                # x is an int
type(x)              # x is an int
int
y = float(x)         # y is a float
type(y)
float
y
1.0
```

```
x = 1                # x is now an int
y = 1.5              # y is a float
z = 3+1j             # z is a complex
res = x+y*z          # res is complex

print("res:", res)   # print the value
res: (5.5+1.5j)

x = x+2              # increase x
x += 2               # same thing
```

Variables

Variables

- stores a value
- don't need to declare the type
 - can force a type with type functions
- most things (“objects”) in Python have *attributes* and *methods*
 - **attribute:** an associated value
 - **method:** object-specific function

```
x = 1                # x is now an int
y = 1.5              # y is a float
z = 3+1j              # z is a complex
res = x+y*z           # res is complex

print("res:", res)    # print the value
res: (5.5+1.5j)

x = x+2               # increase x
x += 2                # same thing

res.real              # an attribute
5.5

res.conjugate()        # a method
(5.5-1.5j)
```

Booleans and comparisons

comparison operators

- all comparisons return **True** or **False**.
- "bool" is the type for **True** and **False**
- (**True** is 1, **False** is 0)
- "and", "or" and "not" combine boolean values:
 - a and b : true if a and b are true
 - a or b : true if either a or b is true
 - not a : true if a is false, false if a is true

```
x = 5
y = 3

x > y           # greater than?
True

x == y          # Equal? Note: two '=='
False

x != y          # Not equal?
True

x <= y          # smaller or equal?
False

x==y or y>0     # either or
True

x>0 and x<10   # both
True

x = y<0         # can store booleans
print(x)
False
```

the "if" statement

Do something only "if" true:

```
if <boolean> :  
    <something>  
    <something>
```



code block
indentation

- a code *block* is a group of code lines with the same indentation
 - be careful that you use the exact same number of spaces! Usually 4 per level.
- if the boolean condition is true: run the code in the block

the "if" statement

Do something only "if" true:

```
if <boolean> :  
    <something>  
    <something>
```



code block
indentation

```
else:  
    <something else>  
    <something else>
```

- a code *block* is a group of code lines with the same indentation
 - be careful that you use the exact same number of spaces! Usually 4 per level.
- if the boolean condition is true: run the code in the block
- "else:" optional
 - runs the "else" block if condition failed

the "if" statement

Do something only "if" true:

```
if <boolean> :  
    <something>  
    <something>
```



code block
indentation

```
elif <boolean> :  
    <something>  
    <something>
```

```
else:  
    <something else>  
    <something else>
```

- a code *block* is a group of code lines with the same indentation
 - be careful that you use the exact same number of spaces! Usually 4 per level.
- if the boolean condition is true: run the code in the block
- "else:" optional
 - runs the "else" block if all conditions failed
- "elif:" optional, and short for "else if".
 - only tested if the previous test fails
 - can have as many as you want

the "if" statement

Do something only "if" true:

```
x = -3

if x>0:
    print("positive")

elif x<0:
    print("negative")

else:
    print("zero")
```

- a code *block* is a group of code lines with the same indentation
 - be careful that you use the exact same number of spaces! Usually 4 per level.
- if the boolean condition is true: run the code in the block
- "else:" optional
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the "if" statement

Exercise: How do you test if a value is odd?

- Hint: '%' the remainder operator
 - gives the remainder of a division

the "if" statement

Exercise: How do you test if a value is odd?

```
if x%2 == 1:  
    print("odd")
```

- Hint: '%' the remainder operator
 - the remainder of an integer division by 2 is 1 if the numerator is odd

the "if" statement

Exercise: How do you test if a value is odd?

```
if x%2 == 1:  
    print("odd")
```

— or —

```
if x%2:  
    print("odd")
```

- Hint: '%' the remainder operator
 - the remainder of an integer division by 2 is 1 if the numerator is odd
 - '1' is True, so we don't need the test to see if it's 1.
But it is often better to be explicit.

looping: the "while" statement

```
while <condition>:  
    <code block>  
    <code block>
```

- Repeat a code block
"while" condition is true
 - break jump out of block
 - continue go back to top of block

```
i = 0  
while i < 10:  
    print("val:", i)  
    i += 1
```

- Example: loop from 0 to 9 and
print each value

Work with Python

How do we actually do things?

- **iPython** good for direct experimentation or as a calculator
- **iPython+ code file** Interactive development – run, debug and so on
- **IDE** Whole development environment
- **Jupyter** Interactive notebooks

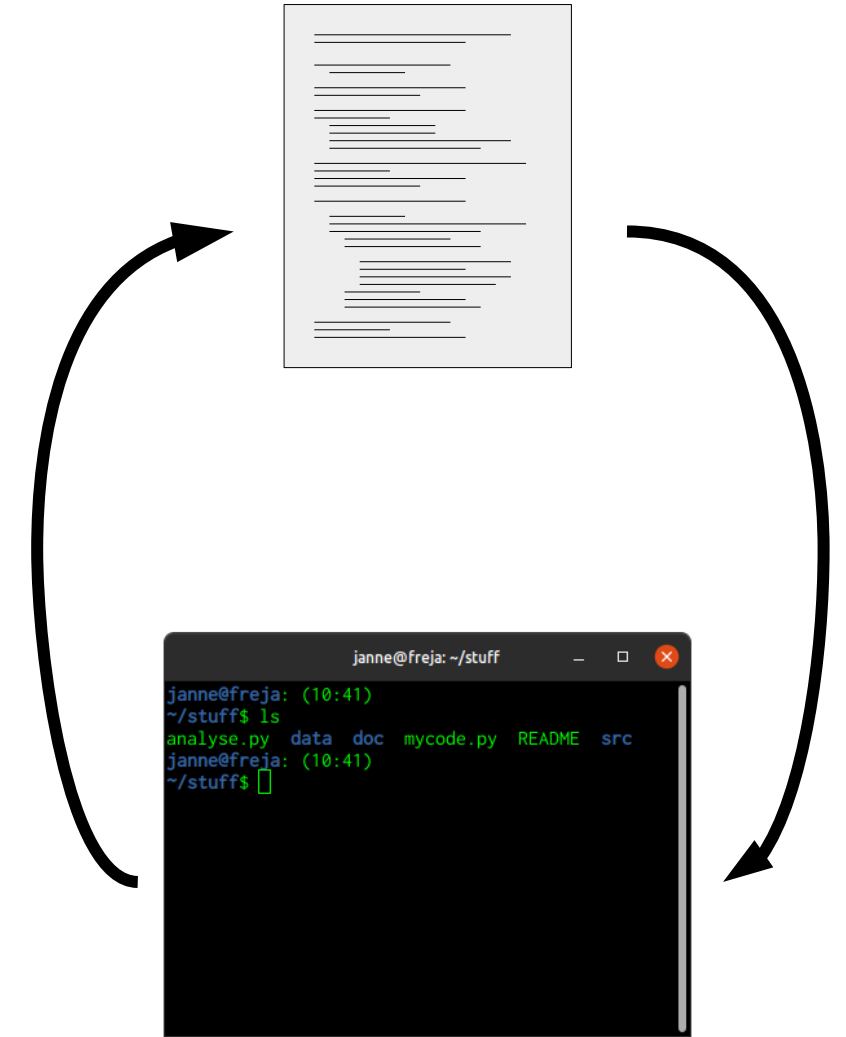
Put your code in a file

Have your code in a file

- Much easier to edit as the code becomes larger
- Can use the code as a regular program

The edit - (compile) - run cycle

1. edit your code in editor
2. run in iPython (or directly in terminal)
3. check results, play around
4. go back to 1.



Put your code in a file

1. Open another terminal

- log in, load python module
- Run either:

```
nano oddloop.py
```

or

```
gedit oddloop.py
```

- Edit your file

gedit:

- Go to preferences->editor, then set:
 - ✓ tab width 4
 - ✓ insert spaces instead of tabs
 - ✓ enable automatic indentation

In general, you want tab width 4 and spaces for tabs in any editor

Put your code in a file

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i = 0
while i<10:
    print("val:", i)
    i += 1
```

Put your code in a file

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- Run either:

```
nano oddloop.py
```

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gedit oddloop.py
```

```
i = 0
while i<10:
    print("val:", i)
    i += 1
```

Run the code:

- Open *another* terminal

log in, load python module

- Run:

```
python3 oddloop.py
```

- Or, in iPython:

```
%run oddloop.py
```

iPython tips:

you can edit multi-line "cells"

- automatically indents blocks
- press enter on last line to run.

```
In [4]: while i<10:  
...:     print("val:", i)  
...:     i += 1
```

Advanced:

- `%edit` edits cells in vim editor
- `%debug` runs code in debugger

`%run` will run a python program

- Will stop at the end, let you examine variables, etc

```
%run oddloop.py
```

`%load` will load a file as if you had typed it in

- Can go back and edit, etc.

```
%load oddloop.py
```

Quick Exercise:

Print out the numbers from 0-9, saying if they're odd or even:

```
even: 0
odd: 1
even: 2
odd: 3
even: 4
odd: 5
even: 6
odd: 7
even: 8
odd: 9
```

- Use "while" and "if"
- remember “%” to test if odd or even

Quick Exercise:

Print out the numbers from 0-9, saying if they're odd or even:

even: 0
odd: 1
even: 2
odd: 3
even: 4
odd: 5
even: 6
odd: 7
even: 8
odd: 9

- Use "while" and "if"
- remember "%" to test if odd or even

```
i = 0

while i < 10:
    if i % 2 == 1:
        print("odd: ", i)
    else:
        print("even:", i)

    i += 1
```

Strings

- quote strings with " or '
 - ''' ... ''' are multi-line strings
- use \ to escape characters
 - \' and \" == " and '
 - \n == new line
 - \t == tab
 - \\ == the \' character itself

```
s = "hi world!"      # a string
s = 'hi world!'      # " or ' both work
print(s)
hi world!
```

```
s = 'I\'m\ na string' # \' escapes
print(s)               # characters
I'm
a string
```

```
# multi-line strings
s = '''first line
second line
'''

print(s)
first line
second line
```

String interpolation

```
greeting = 'Hello {}'.format('World')  
print(greeting)  
Hello World!
```

- You can "fill in" values into a string
- mark places in the string with '{}'
 - use the 'format()' method to set the value.

String interpolation

```
'one: {} two: {}'.format(1,2)  
one: 1 two: 2
```

```
'two: {1} onetwo: {0} {1}'.format(1,2)  
two: 2 onetwo: 1 2
```

```
'int: {0:5d} int: {0:05d}'.format(123)  
int:    123 int: 00123
```

```
'f: {0:8.2f} {0:8.3e}'.format(1234.567)  
float:  1234.57 1.23e+03
```

You can "fill in" values into a string

- mark places in the string with '{}'
- use the 'format()' method to set the value.
- {0} = use first argument to format()
- { : something } - format specifier
 - num - field width
 - .num - decimals
 - g, d, f, e, s... - data type

String-related functions and methods

- use `input()` to ask for user input
- Many functions work on strings:
 - `len(s)` length of string
 - `int(s)` convert string to int
 - `float(s)` convert to float
- Strings have a lot of methods:
 - convert text
 - test what kind of text it is
 - find substrings
 - split strings

```
s = input("name: ") # get user input
print("Hi", s)
Hi Janne

len(s)                # string length
5

s.isalpha()           # lots of methods
True

s.find('nn')           # find substring
2

'nn' in s              # test substring
True                  # inclusion

int("42")              # convert to other
42                   # types
```

Substrings and indexing

```
s = "hi world!"

print(s[3])           # get character
'w'                  # at pos 3
print(s[3:6])         # from pos 3 to
'wor'                # before 6
print(s[-2])          # index from end
'd'

s[3] = 'W'         # Error!

s=s[:3]+'W'+s[4:]     # create new string
                     # instead
```

- get substrings with "[...]"
 - index starts at 0
 - [-x] index from end:
 - [-1] == last character
 - [x:y] == "from x to y-1"
 - [:y] == [0:y]
 - [x:] == "from x to end"
 - [:] == the entire string
- can't change strings ("immutable")
 - create copy instead

Lists

- a list of elements
 - elements can be any type, including lists.
 - you can mix different types in a single list
- `append()`, `pop()` adds and removes elements to the end. Fast.
 - `insert(i)` and `pop(index)` adds and removes from middle or start
 - ***much slower than append***

```
e = []                # an empty list
a = [1, 2, 3]         # a list of ints
b = ['text', [7, 1.3]] # mixed list

a.append(7)           # add an element
[1, 2, 3, 7]          # to the end

elem = a.pop()        # remove and return
print(elem, a)        # last element
7 [1, 2, 3]

a.insert(1, 99)        # add or remove from
[1, 99, 2, 3]         # middle of list

a.pop(1)
[1, 2, 3]
```

Lists

- Index list like with string
 - `[n]`, `[m:n]`, `[n:]` ...

-

```
a = [1,2,3,4,5]
a[0]           # First element
1
a[1:3]         # a[1] and a[2]
[2, 3]

a[2:]          # to end
[3, 4, 5]

a[:3]          # from beginning
[1, 2, 3]

a[-1]          # count from back
5
```

Lists

- Index list like with string
 - `[n]`, `[m:n]`, `[n:]` ...
- Lists are mutable
- Many methods and functions:
 - `max()`, `min()`, `len()`, `sum()` ...
 - `l.sort()`, `l.index()`, `l.count()`
- `n in list` - test for element existence

```
a = [1,2,3,4,5]
a[0]           # First element
1
a[1:3]         # a[1] and a[2]
[2, 3]

a[3] = 99      # lists are mutable

max(a)
99

a.sort()       # sort in place
[1, 2, 3, 5, 99]

5 in a         # is 5 in a?
True
```

Lists: ranges and loops

```
for <var> in <iterable>:  
    <do something with var>
```

```
# example:
```

```
a = [1,2,3,4,5]
```

```
for i in a:  
    print(i)
```

```
# range
```

```
for i in range(1,10):  
    print(i)
```

```
# create a list from a range
```

```
a = list(range(1,10,2))
```

do something with each list element with 'for'

- the index variable is set to each element in the list in turn

range() creates a sequence

range(start, end, step)

- creates sequence
 - start - first element
 - end - last element +1
 - step - step size (optional)

Mini exercise: a list of squares

Create a list of squares of 1 to 10:

[1, 4, 9, 16, 25, 36, 49, 64, 81, 100]

- Hints:
 - `list.append(element)`
 - `range(start, end)`
- write code in a file “squares.py”
- Test either from command line
 - `python3 squares.py`
- or within ipython:
 - `%run squares.py`

Mini exercise: a list of squares

Create a list of squares of 1 to 10:

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```
# Create empty list

# Set i to each value in 1-10

    # calculate i**2, append
    # to the list

# After the loop, print list
```

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Mini exercise: a list of squares

Create a list of squares of 1 to 10:

[1, 4, 9, 16, 25, 36, 49, 64, 81, 100]

```
# Create empty list
squares = []

# Set i to each value in 1-10
for i in range(1,11):

    # calculate i**2, append
    # to the list
    squares.append(i**2)

# After the loop, print list
print(squares)
```

- Hints:
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 - `range(start, end)`
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List Comprehensions

A common pattern:

```
lst = []  
for x in <iterable>:  
    if <condition>:  
        lst.append(<x comp>)
```

For example, our exercise:

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for x in range(1,11):  
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List Comprehensions

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Write it shorter as:

```
lst = [<x comp> for x in <iter> if <cond>]
```

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lst = []  
for x in <iterable>:  
    if <condition>:  
        lst.append(<x comp>)
```

Write it shorter as:

```
lst = [<x comp> for x in <iter> if <cond>]
```

For example, our exercise:

```
squares = []  
for x in range(1,11):  
    # if <condition>:  
    squares.append(x**2)
```

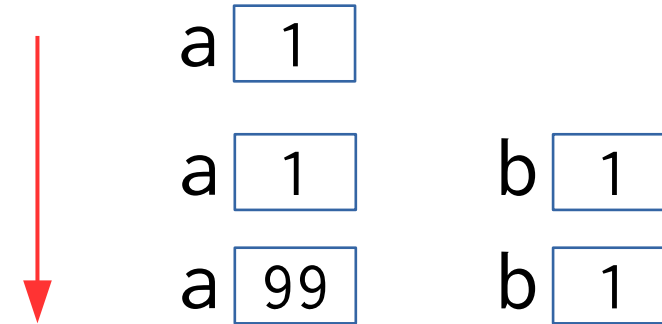
Our exercise again:

```
squares = [x**2 for x in range(1,11)]
```

Lists and simple values

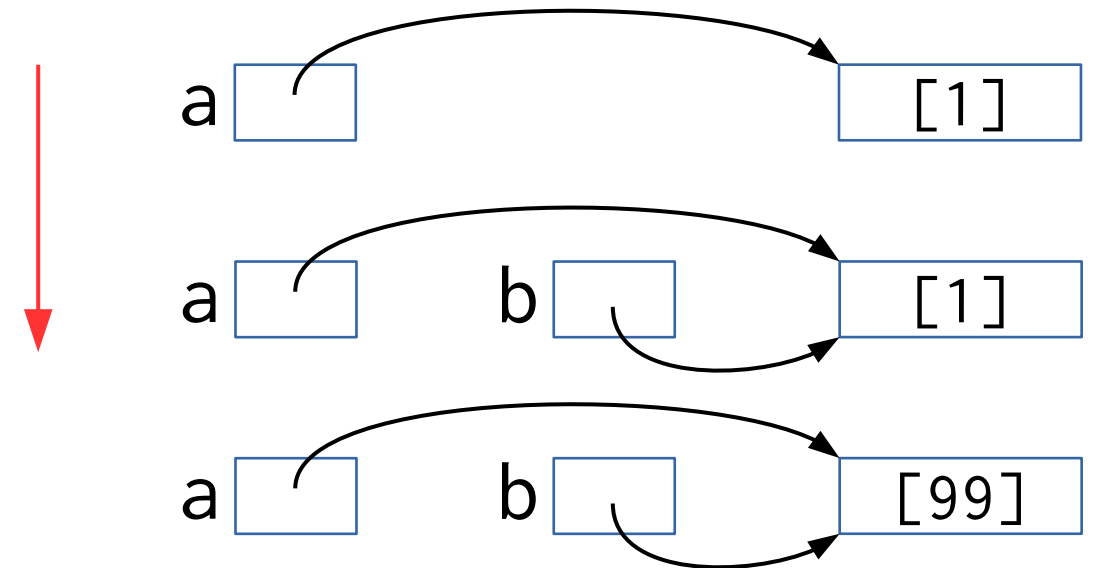
variables *contain* simple values:

```
a = 1          # a == 1
b = a          # b == 1
a = 99         # a == 99, b == 1
print(a,b)
99, 1
```



variables contain *references* to lists:

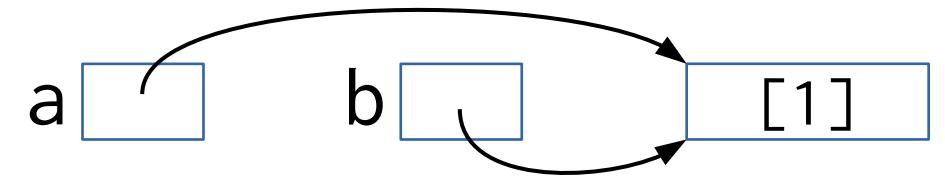
```
a = [1]        # a == [1]
b = a          # b == [1]
a[0] = 99      # a == [99], b == [99]
print(a,b)
[99], [99]
```



Lists and simple values

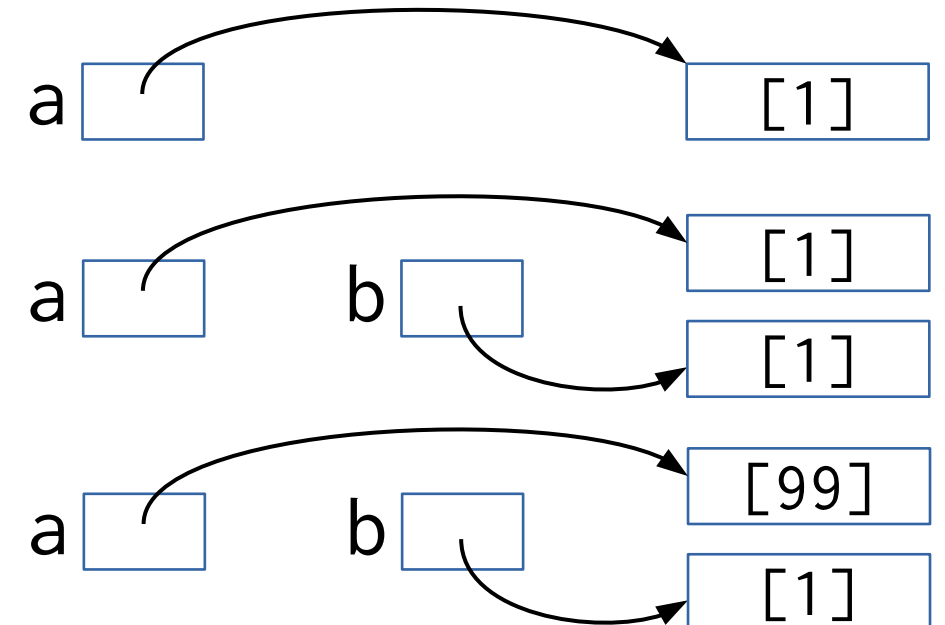
Without using `.copy()`

```
a = [1]          # a == [1]
b = a            # b == [1]
a[0] = 99        # a == [99], b == [99]
print(a,b)
[99], [99]
```



With `.copy()`

```
a = [1]          # a == [1]
b = a.copy()     # b == [1]
a[0] = 99        # a == [99], b == [1]
print(a,b)
[99], [1]
```



Functions

functions *encapsulate* code

```
def <function name>(params):  
    <code block>
```

Docstring

- A string after the function definition with documentation

Parameters

- parameters can have default values
- you can name parameters when calling a function

return sets the return value

```
def line(x, a=0, b=0):  
    '''line(x, a=0, b=0)  
    calculate ax+b'''  
  
    return a*x+b
```

```
line(2, 0.5, 1)    # x=2, a=0.5, b=1  
2.0
```

```
line(2)            # a,b=0 default  
0
```

```
line(2, b=5)       # a=0, b=5  
5
```

Functions

```
def func(x):  
    a = 1          # local a  
    x += 1         # local parameter x  
    print("a:", a, "x:", x)  
  
a=99              # global a  
x=11              # global x  
func(x)  
a: 1 x: 12        # local a and x  
  
print("a:", a, "x:", x)  
a: 99 x: 11        # global a and x
```

Parameters and variables

- parameters and local variables are *local* to the function.
- Parameters copy the value, not the parameter itself

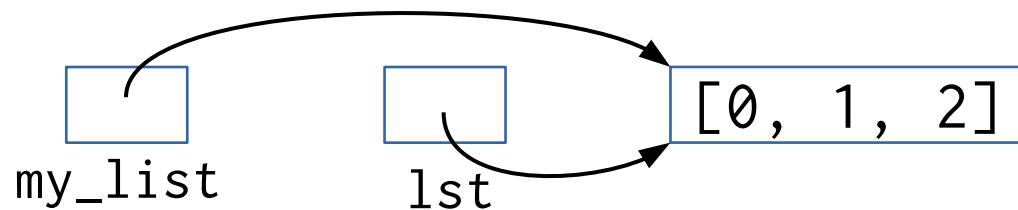
(you *can* use global variables in a function. But please don't.)

Functions

```
def listfunc(lst):  
    lst[0] = 99          # local list  
    print("list:", lst)  
  
my_list = [0,1,2]       # global list  
listfunc(my_list)  
list: [99, 1, 2]  
  
print("list", my_list)  
list: [99, 1, 2]
```

Parameters and variables

- parameters and local variables are *local* to the function.
- Parameters copy the value, not the parameter itself
- you transfer a *reference* to lists
 - functions can change the contents of the list



Functions

Return values

- return any value with 'return'
- can put return anywhere in the code
- A function without return returns None
- You can use 'None' yourself to signify the lack of a value, etc.

```
def print_double(x):  
    print(x, x)  
  
a = print_double(3)  
3 3  
  
print(a)  
None  
  
def print_if_exist(x=None):  
    if x==None:  
        print("no value")  
    else:  
        print(x)
```

Other structures

tuples

- like lists, but immutable
→ faster, take less memory

dictionaries

- key - value pairs.
- key : immutable (string, numeric)
value : any kind of value
- No intrinsic order
- very fast, flexible

```
my_tuple = (1, 2, 3)
my_tuple[1]
2

my_tuple[1] = 99           # Error

my_dict = {'name': 'Janne',
           'age' : 22}

my_dict['name']
Janne

my_dict['numbers']=[1,2,3]
for k,v in my_dict.items():
    print('{}: {}'.format(k,v))
age: 22
numbers: [1, 2, 3]
name: Janne
```

File I/O

open file for reading or writing:

```
with open(<fname>, 'rw') as <var>:  
    <code block>
```

readline() - read one line
readlines() - read list of all lines in file
write(l) - write a string
writelines(l) - write all lines in list

```
# open file for reading  
with open('filename', 'r') as f:  
    # read all lines at once  
    lines = f.readlines()  
  
    # read one line at a time  
    for line in f:  
        # do something w. each line  
  
# write all lines to filename  
with open('filename', 'w') as f:  
    f.writelines(lines)  
  
# f.writeline(l) writes one line
```

Next Session:

We will try out four useful things right on the Deigo cluster:

- Use python modules
- Install python modules for your own use
- write a program that converts a file (a Fasta file) from one format to another
- Write a program that creates a Slurm job script, then submits it as a job.