

# Lecture 3:

# While, Dictionaries, Modules, Reproducibility

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# Overview

- List functions (range, zip, lazy evaluation)
- While loops
- Dictionaries
- Modules, Packages, and Import
- Namespaces
- Reproducibility/Clean Notebook

Handy loop/list related functions

# Generating a list of numbers with “range”

```
>>> list(range(4))
```

```
[0, 1, 2, 3]
```

```
>>> list(range(5, 10))
```

```
[5, 6, 7, 8, 9]
```

```
>>> list(range(2, 9, 2))
```

```
[2, 4, 6, 8]
```

- Same syntax as indexing/slices:
  - start, stop, increment
- `range(4) == range(0, 4, 1)`

# Many list-related functions use “lazy evaluation”

```
x = enumerate(['a', 'b', 'c'])  
  
x  
  
<enumerate at 0x738dcf5156c0>  
  
list(x)  
  
[(0, 'a'), (1, 'b'), (2, 'c')]  
  
for ix, value in enumerate(['a', 'b', 'c']):  
    print(value)  
    if ix == 1:  
        break  
  
'a'  
'b'
```

- Enumerate gives us a list of tuples with the (index, value) pairs
- Imagine x is very very big
- What if we only needed to enumerate the first couple of items in the list?
- Lazy evaluation means only doing calculations when (and therefore **IF**) they are actually needed

# Zip efficiently combines equal length lists and/or tuples

```
>>> x = [10, 50, 100]
>>> y = ['a', 'b', 'c']
>>> zipped = zip(x, y)
>>> zipped
<zip at 0x738dce007ec0>
>>> list(zipped)
[(10, 'a'), (50, 'b'), (100, 'c')]
```

- Zip takes lists/tuples of equal length and (lazily) returns a list of tuples of each position across input

```
[(11_v1, 12_v1, 13_v1),
 (12_v1, 12_v2, 13_v3)]
```

- Works for >2 lists/tuples
- Lazily evaluated
- Will stop when any input ends:

```
list(zip(['a', 'b'], [1]))
```

```
[('a', 1)]
```

## Range is often used to generate indices for strings

```
for x in range(5, 15, 3):  
    print(x)
```

```
5  
8  
11  
14
```

```
a = 'abc'
```

```
b = '123'
```

```
for i in range(len(a)):
```

```
    print(a[i] + b[i])
```

```
a1
```

```
b2
```

```
c3
```

We can iterate over more than 1 list with zip/enumerate

```
list1 = ['a', 'b', 'c']  
list2 = ['1', '2', '3']  
for a,b in zip(list1, list2):  
    print(a + b)
```

a1

b2

c3



Doing a loop until something is True

# Don't always know how many times we need to loop

```
curr_temp, room_temp, minutes = 50, 25, 0

for i in range(1000000000):
    temp_diff = curr_temp - room_temp

    if abs(temp_diff) <= 0.5:
        break

    curr_temp = curr_temp - (0.1 * temp_diff)
    minutes += 1
```

```
curr_temp, room_temp, minutes = 50, 25, 0

while abs(curr_temp - room_temp) > 0.5:
    temp_diff = curr_temp - room_temp
    curr_temp = curr_temp - (0.1 * temp_diff)
    minutes += 1
```

```
while CONDITION:
    repeat BODY
```

# Beware - Infinite Loops

```
while False:
```

```
    print("Never execute")
```

```
while True:
```

```
    print("Will never end")
```

```
x = 50
```

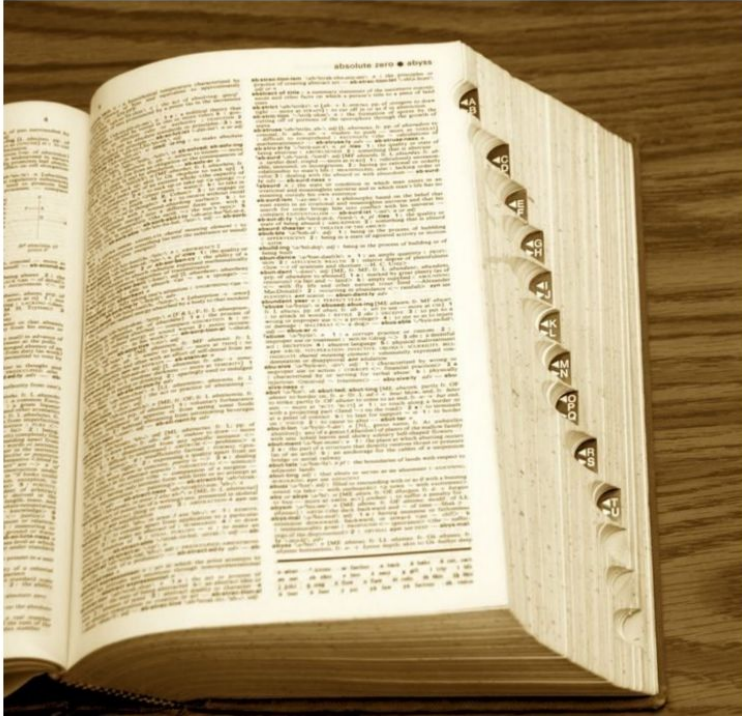
```
while x < 100:
```

```
    x = 5
```

- If condition is **False** at beginning loop body will not run
- If condition can never be made **False** loop body will repeat until python crashes ("infinite loop")
  - Make sure variables in conditional are actually changed during the loop
  - Be careful with direction of inequalities
  - Be careful using "while True:"

Indexes are great, but what if we don't want  
to use (only) integers?

# Dictionaries (aka hashmaps, maps, hash...)



the *key*

Each *word* in a dictionary  
has a *definition*

the *value*

Words are stored in a way  
that enables easy look-up.

# Dictionaries store sets of links between keys and values

```
d = {} # create an empty dictionary
d["key"] = "value" # map key -> value
d["any number/string"] = 10
d[42] = "any variable"
d["even list"] = [1, 2, 3, (4, 5)]

x = 5
y = {x: x+1, x-5: x/2} # variables
```

```
d
{'key': 'value',
 'any number/string': 10,
 42: 'any variable',
 "even_list": [1, 2, 3, (4, 5)]}

y
{5: 6, 0: 2.5}
```

# Get values in dictionary using keys (or special methods)

```
d = {'key1': 'value1',  
     'key2': ['value2a', 'value2b']}  
  
d['key1']      # 'value1'  
  
d['key2'][1]   # 'value2b'  
  
d.get('key2')  # ['value2a', 'value2b']  
  
d.keys() # dict_keys(['key1', 'key2'])  
  
d.values()  
  
# dict_values(['value1',  
#             ['value2a', 'value2b']])
```

- You can access specific values in dictionary with key in [] or with the .get() method
- d.keys() will provide list of all keys in a dictionary
- d.values() will provide list of all values in a dictionary
- d.items() will provide:
  - zip(d.keys(), d.values())

[('key1', 'value1'), ('key2', ['value2a', 'value2b'])]

# Testing for keys in dictionary

```
d = {'foo': 'bar'}  
  
'foo' in d  # True  
  
'bar' in d  # False (only checks keys)  
  
  
'key1' in d # False  
  
D['key1']  
  
KeyError: 'key1'
```



# Get can be used to return default value if key missing

```
d = dict([[1, 'a'], [10, 'c']])  
  
d.get(50, 'Nope')  
  
'Nope'  
  
d.get(1, 'Nope')  
  
'a'
```

*Note: .setdefault lets you do something similar when adding keys*

## setdefault can be **create** default value if key missing

```
d = {1: ['a', 'b'], 2: ['c']}  
  
d[1].append('d')  
  
{1: ['a', 'b', 'd'], 10: ['c']}
```

```
if 5 in d:  
    d[5].append('e')  
  
else:  
    d[5] = ['e']  
  
{1: ['a', 'b', 'd'], 10: ['c'],  
5: ['e']}
```

```
d = {1: ['a', 'b'], 2: ['c']}  
  
d.setdefault(5, []).append('e')  
  
{1: ['a', 'b', 'd'], 10: ['c'],  
5: ['e']}
```

```
d.setdefault(10, []).append('f')  
  
{1: ['a', 'b', 'd'],  
10: ['c', 'f'],  
5: ['e']}
```

**Dictionary of lists - very common data structure**

# Modules

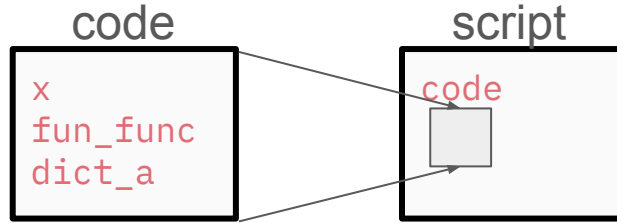
# Folder containing multiple python scripts

```
CSCI_2202/
```

- script.py
- code.py
- my\_module/
  - stats.py
  - micro.py
  - physics/
    - code.py
    - answers.py

# import lets us access functions (and objects) in other files

```
# code.py  
  
x = 10  
  
def fun_func(y):  
    z = y + 10  
  
    return z  
  
dict_a = {x: x + 1}
```



```
# script.py (or notebook)  
  
import code  
  
print(code.x)  
  
print(code.fun_func(30))  
  
print(code.dict_a[code.x])  
  
10  
  
40  
  
11
```

Import to .ipynb is easy but importing FROM a .ipynb is more complicated

# import lets us access functions (and objects) in other files

```
# code.py

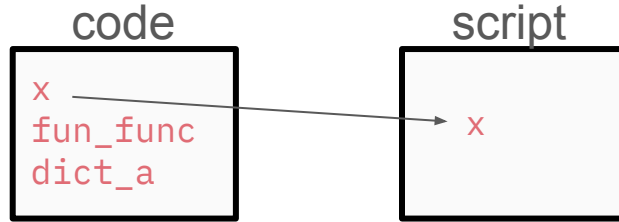
x = 10

def fun_func(y):

    z = y + 10

    return z

dict_a = {x: x + 1}
```



```
# script.py (or notebook)

from code import x

print(x)

print(code.x)

print(code.fun_func(10))

10

Error

Error
```

# import lets us access functions (and objects) in other files

```
# code.py

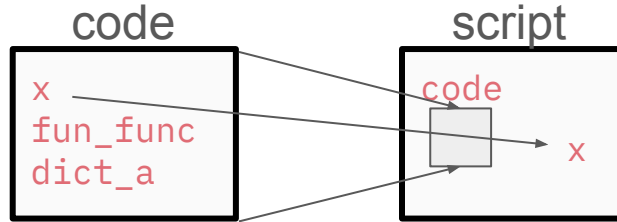
x = 10

def fun_func(y):

    z = y + 10

    return z

dict_a = {x: x + 1}
```



```
# script.py (or notebook)

from code import x

import code

print(x)

print(code.x)

print(code.fun_func(30))

print(code.dict_a[code.x])
```

10

10

40

11

# import lets us access functions (and objects) in other files

```
# code.py

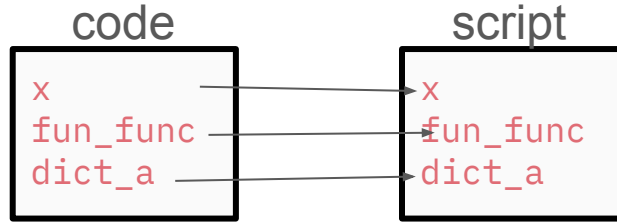
x = 10

def fun_func(y):

    z = y + 10

    return z

dict_a = {x: x + 1}
```



```
# script.py (or notebook)

from code import *

print(x)

print(fun_func(30))

print(dict_a[x])

print(code.x)
```

10

40

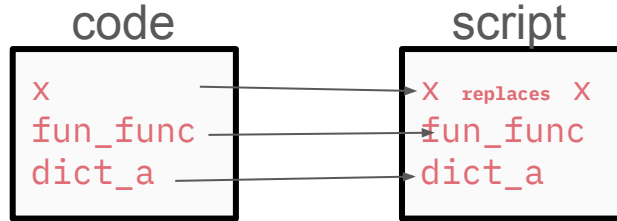
11

ERROR



# import lets us access functions (and objects) in other files

```
# code.py  
  
x = 10  
  
def fun_func(y):  
    z = y + 10  
  
    return z  
  
dict_a = {x: x + 1}
```



```
# script.py (or notebook)  
  
x = 50  
  
from code import *  
  
print(x)  
  
10
```

# dir function can be used to see what is in a module

```
# code.py

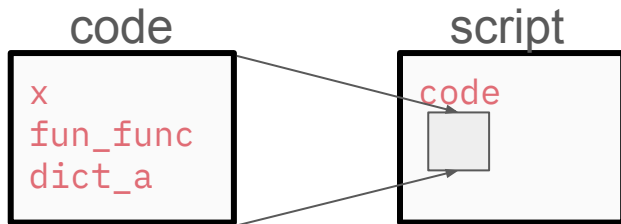
x = 10

def fun_func(y):

    z = y + 10

    return z

dict_a = {x: x + 1}
```



```
# script.py (or notebook)

import code

dir(code)

['__builtins__',
 '__cached__', '__doc__',
 '__file__', '__loader__',
 '__name__', '__package__',
 '__spec__', 'dict_a',
 'fun_func', 'x']
```

# PYTHONPATH - where python looks for modules/packages

```
import sys

print(sys.path)

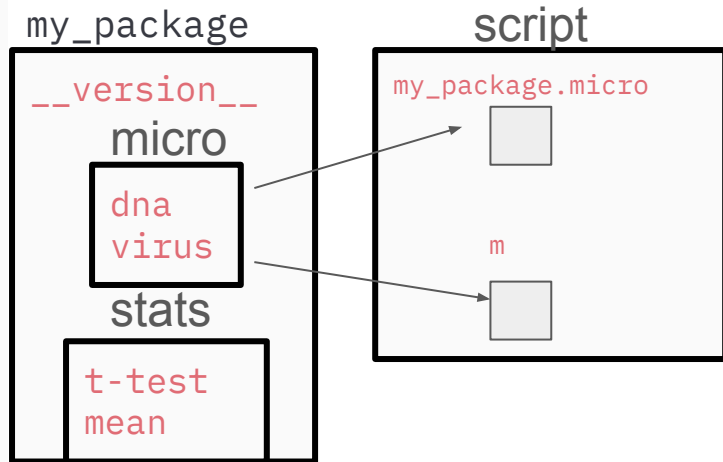
[current_folder, python_library,
python_libdynload,
python_sitepackages...]
```

- System variable that controls where python checks for packages
- Order matters - it will check list in order and stop if it finds the import
  - Our `code.py` will be imported instead of “`code`” in the standard library because it comes first
- Anaconda is managing this for you (via `conda`)
- You can edit this in script using `sys.path` but usually a BAD IDEA!

What if you have lots of modules?

# Packages are made of modules - dotted import

- `script.py`
- `my_package`
  - `__init__.py`
  - `micro.py`
  - `stats.py`



```
# script.py (or notebook)
import my_package.micro
print(my_package.micro.dna)
'agc'

import my_package.micro as m
print(m.is_virus(m.dna))
True
```

# Packages - aliases keep code simpler!

- script.py
- my\_package
  - `__init__.py`
  - `micro.py`
  - `stats.py`
  - `physics/`
    - `__init__.py`
    - `astro.py`

```
# script.py (or notebook)

import my_package.physics.astro

print(my_package.physics.astro.cosmo_const)

import my_package.physics.astro as astro

print(astro.cosmo_const)

from my_package.physics.astro import *

print(cosmo_const)
```

How does python keep track of things?  
Namespaces

# Namespaces map names to objects

```
# code.py

x = 10

def fun_func(y):

    z = y + 10

    return z

dict_a = {x: x + 1}
```

code

```
x
fun_func
dict_a
```

code\_v2

```
x
fun_func
dict_a
```

Namespaces are basically dictionaries

```
code = {'fun_func': fun_func,
        'x': x,
        'Dict_a': dict_a}
```

What is useful is we often have multiple namespaces in our code

```
code_v2 = {'fun_func': fun_func,
           'x': x,
           'Dict_a': dict_a}
```

Namespaces let us use the same variable name to mean different things.



# functions (among others) create new namespaces

```
i = 50  
  
def func(i):  
    i = 10  
    return i
```

```
j = func(i)  
print(i, j)  
  
50, 10
```

```
top_namespace = {'i': obj1, #50  
                 'j': obj2, #10  
                 'func': func}  
  
func_namespace = {'i': obj4} # 10
```

Namespaces form a hierarchy.

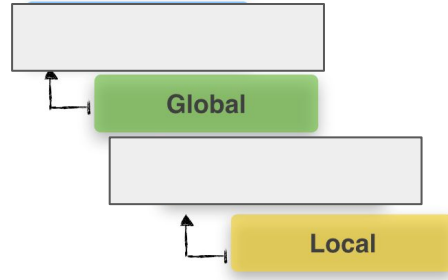
The “Scope” of a bit of code determines which level of this hierarchy it searches for namespace mapping

# Scopes: search hierarchy of namespace: local first

```
i = 50
def func(i):
    i = 10
    return i

j = func(i)
print(i, j)

50, 10
```



```
global = {'i': obj1, #50
          'j': obj2, #10
          'func': func}

local = {'i': obj4} # 10
```

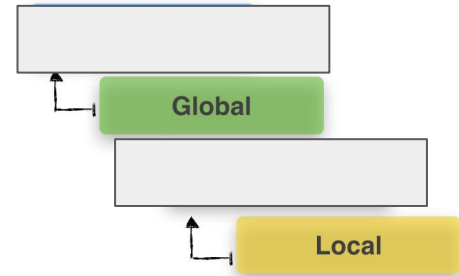
# Error if you try to change a variable in different namespace

```
x = 1

def func():
    x = x - 5
    print(x, '[ x inside func() ]')

func()
```

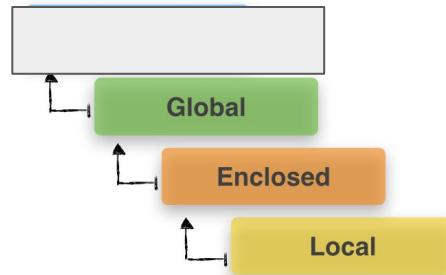
UnboundLocalError: local variable x  
referenced before assignment



**Note:** there are ways to force python to do this but it is usually a bad idea:  
**global, local, nonlocal**

# Nesting can add additional enclosed scopes

```
a_var = 'global value'
def outer():
    a_var = 'enclosed value'
    def inner():
        a_var = 'local value'
        print(a_var)
    inner()
outer()
'local value'
```



```
global = {'a_var': 'global value',
          'outer': outer}
```

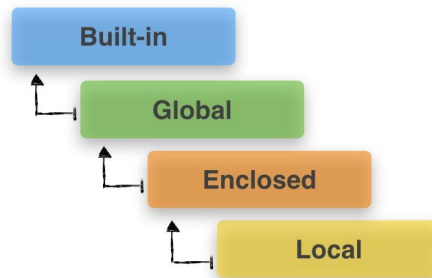
```
enclosed = {'a_var': 'enclosed value',
            'inner': inner}
```

```
local = {'a_var': 'local value'}
```

# Priority list means built-ins can be overwritten

```
def len(in_var):  
    print('my len() function')  
    l = 0  
    for i in in_var:  
        l += 1  
    print(l)  
  
def a_func(in_var):  
    len_in_var = len(in_var)  
    print(len_in_var)  
  
a_func('Hello, World!')  
  
"my len() function"
```

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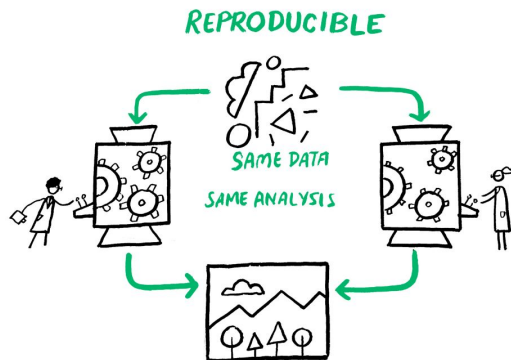


```
Built_in = {'len': len, ...}  
global = {'len': len, 'a_func': a_func}  
local_len = {'l': l, 'i': i, 'in_var':  
in_var}  
local_a_func = {'len_in_var': len_in_var,  
                'In_var': in_var}
```

How do we do good scientific analyses?

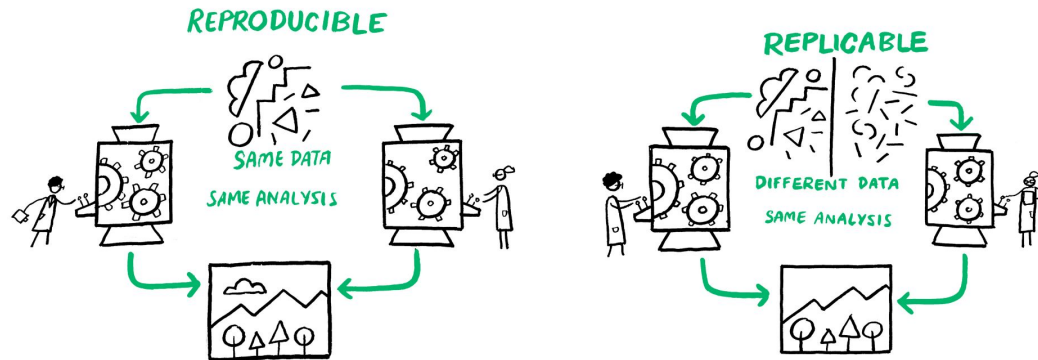
Necessary (but not sufficient) for scientific  
analyses to be reproducible

# Reproducibility should be the bare minimum

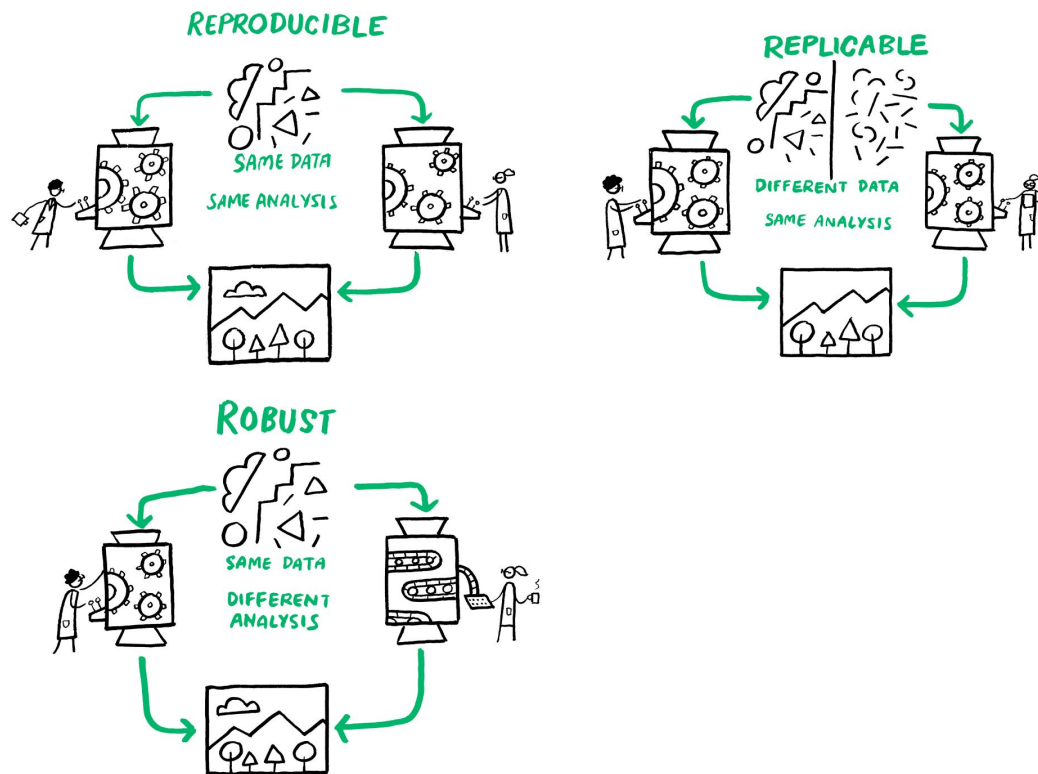




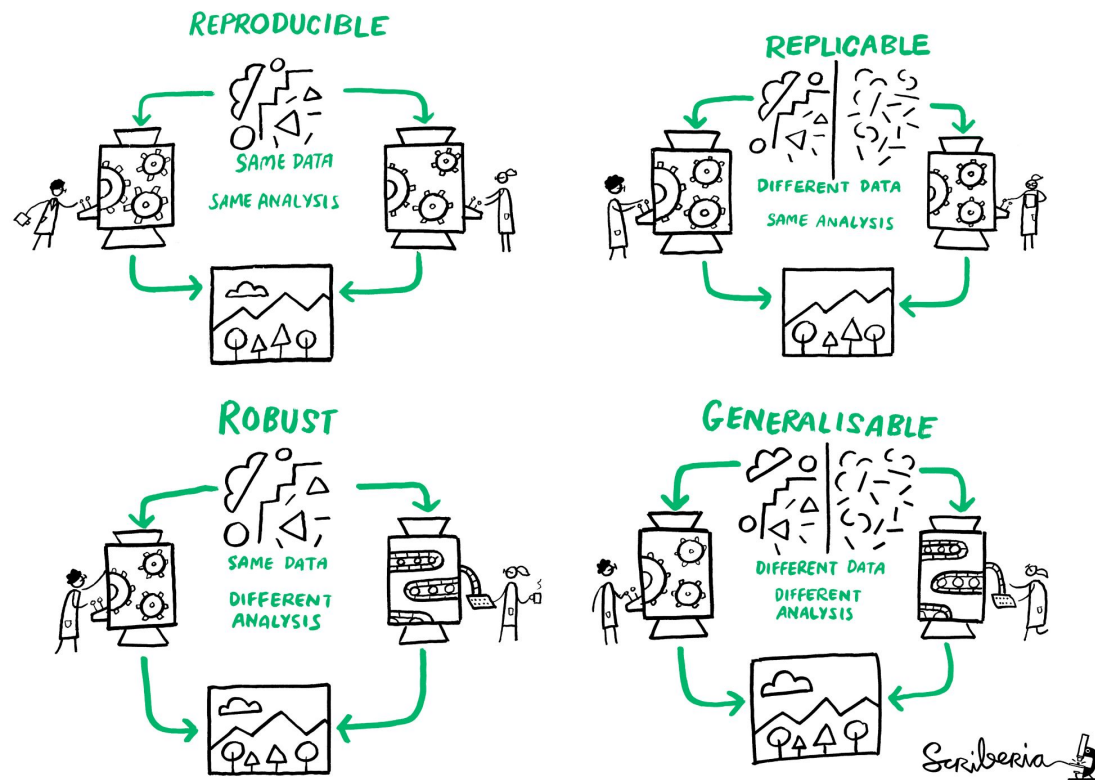
# Reproducibility should be the bare minimum



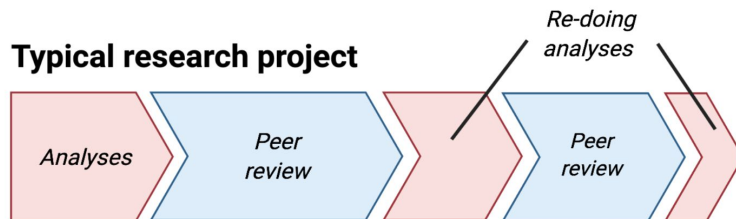
# Reproducibility should be the bare minimum



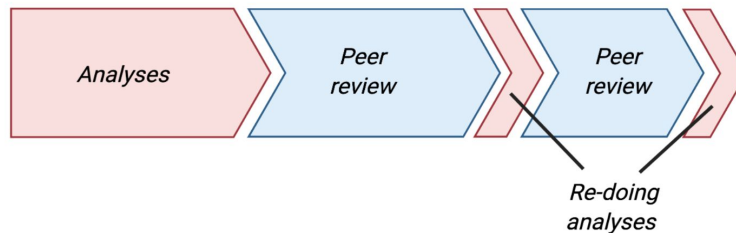
# Reproducibility should be the bare minimum



# Makes your own life easier



**Research project using reproducible practices**



 @dsquintana

[oliviergimenez.github.io/reproducible-science-workshop](https://oliviergimenez.github.io/reproducible-science-workshop)

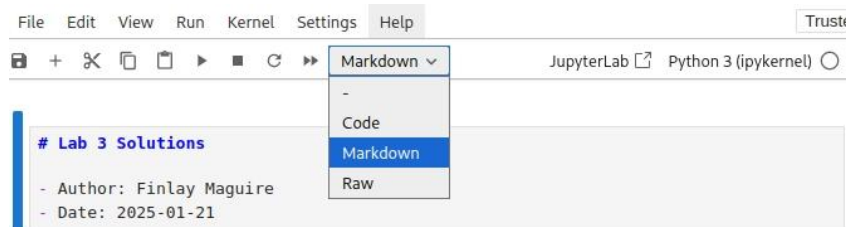
What do we need to do to have reproducible research?

# Reproducibility checklist

- Don't do anything by hand (even “one-off” tasks)
- Script every interaction with data:
  - Data collection
  - Moving data on your computer
  - Formatting datasets
  - Cleaning data
  - Exploratory data analysis
  - Main analyses
  - Report generation
- Minimise interactivity/point and click interactions
- Keep track of the exact version of every library/program you use
- Version control all data, code, and documentation
- Use a random seed

Notebooks are a key tool for doing this

# Jupyter supports markdown OR code cells



Markdown is a quick way to indicate how to format plaintext

Converts to HTML in background

Supported by many developer tools

# Heading level 1

<h1>Heading level 1</h1>

Heading level 1

Heading

```
# H1
## H2
### H3
```

Bold

```
**bold text**
```

Italic

```
*italicized text*
```

Blockquote

```
> blockquote
```

Ordered List

```
1. First item
2. Second item
3. Third item
```

Unordered List

```
- First item
- Second item
- Third item
```

Code

```
`code`
```

Horizontal Rule

```
---
```

Link

```
[title](https://www.example.com)
```

Image

```
![alt text](image.jpg)
```



# Out of order cell-execution can lead to bugs and errors

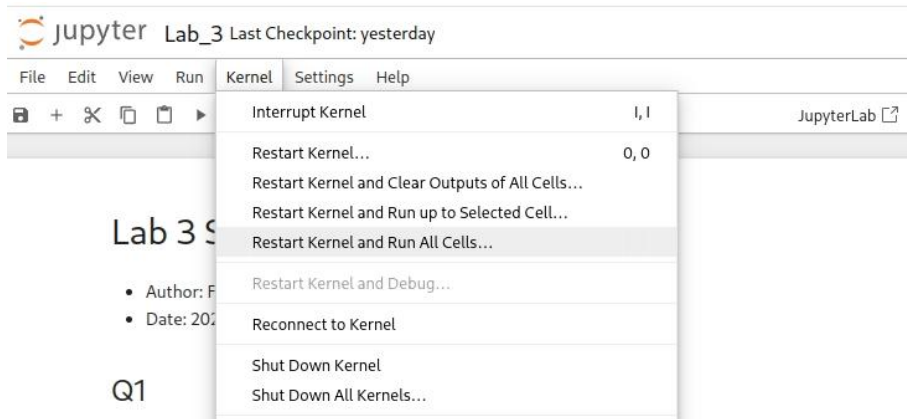
```
[3] y = x(5)
```

```
[1] def x(x):  
    return x * 2
```

```
[2] y = x(100)
```

```
[4] y
```

```
10
```



Always run this at the end of a notebook -  
the notebook on the left will error now!

# Making a good notebook

## Structure your Notebook

- Give your notebook a **title** (H1 header) and a meaningful **preamble** to describe its purpose and contents.
- Use **headings and documentation** in Markdown cells to structure your analysis and explain your steps.

## Refactor & outsource code into modules

- After you've written plain code in cells to get ahead quickly, acquire the habit of **turning stable code into functions** and **move them to a dedicated module**. This makes your notebook more readable and is incredibly helpful when productionizing your workflow. Following is clearer and easier to test than repeating the same code many times in your notebook.

```
import dataprep

df = dataprep.load_and_preprocess_data(filename)
```

- **Stick to the standards of good coding** — Standardise your formatting, use meaningful variable and function names, comment sensibly, modularize your code and don't be too lazy to refactor.

## Restart kernel and run-all cells (and check for errors!)

# Overview

- Several handy list functions (range, zip) use lazy evaluation
- While loops enable easy conditional loops
- Dictionaries store key -> value pairs
- Reusing/organising code can be done using modules & packages
- Namespaces are how python keeps track of variables
- Reproducibility makes for better science
- Creating clean, well-documented, notebooks that run the cells in order is useful for this.