PoL Physics of Life TU Dresden

CENTER FOR SYSTEMS BIOLOGY DRESDEN

jupyter lab

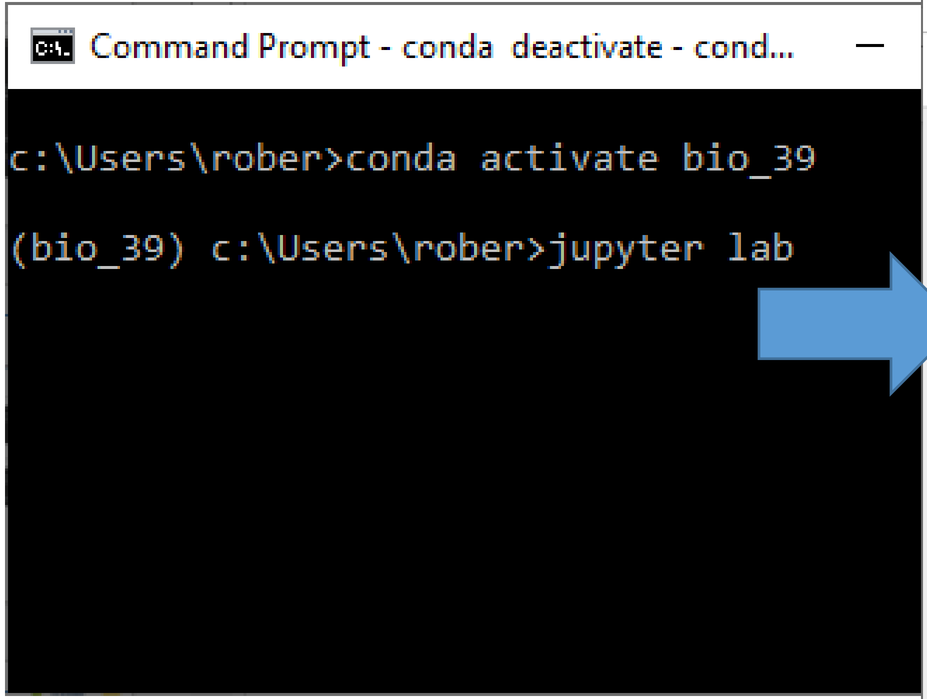
Robert Haase

December 2022

@haesleinhuepf

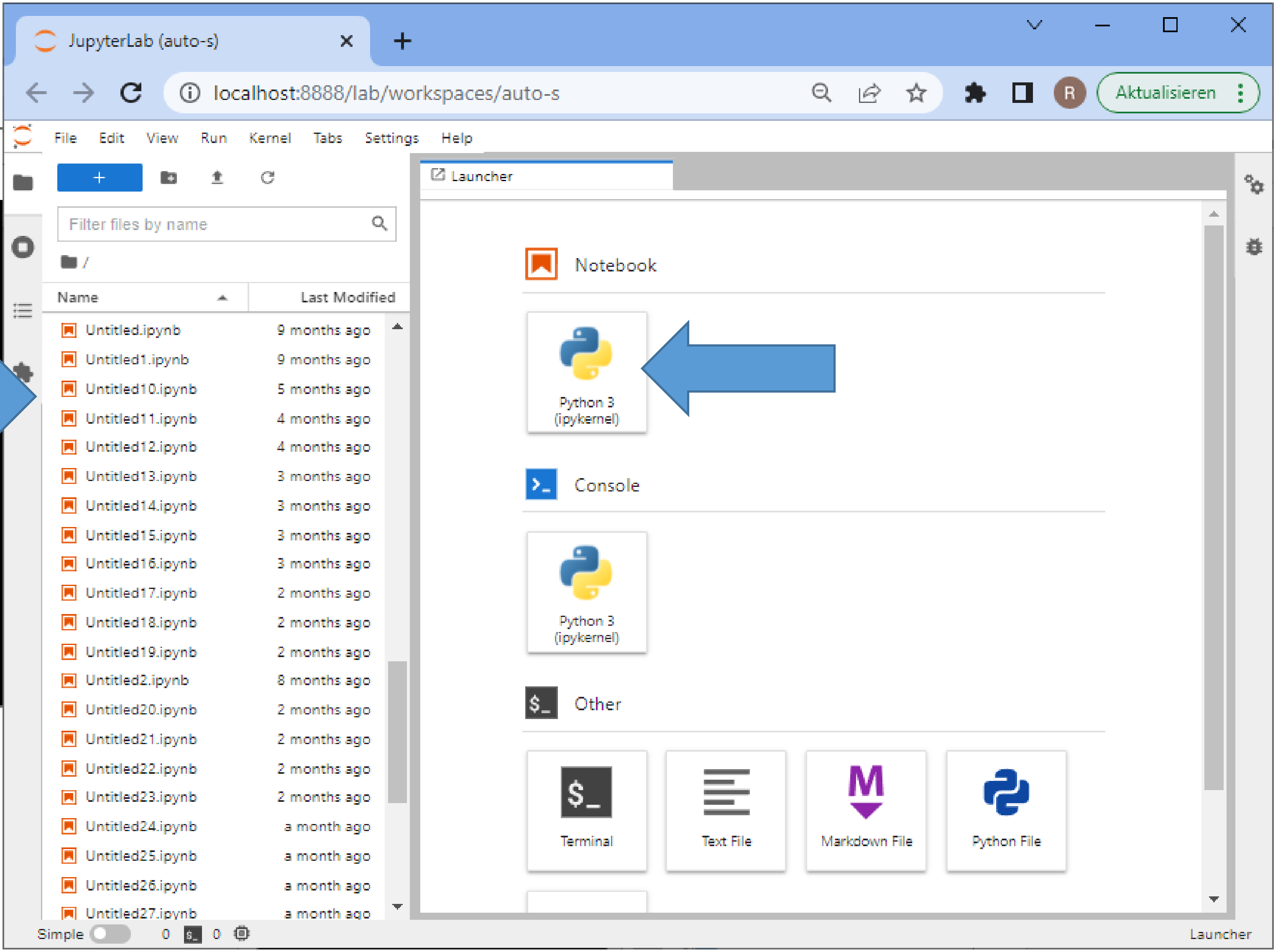
Jupyter lab

- Our programming environment for this course



Command Prompt - conda deactivate - cond...

```
c:\Users\rober>conda activate bio_39

(bio_39) c:\Users\rober>jupyter lab
```



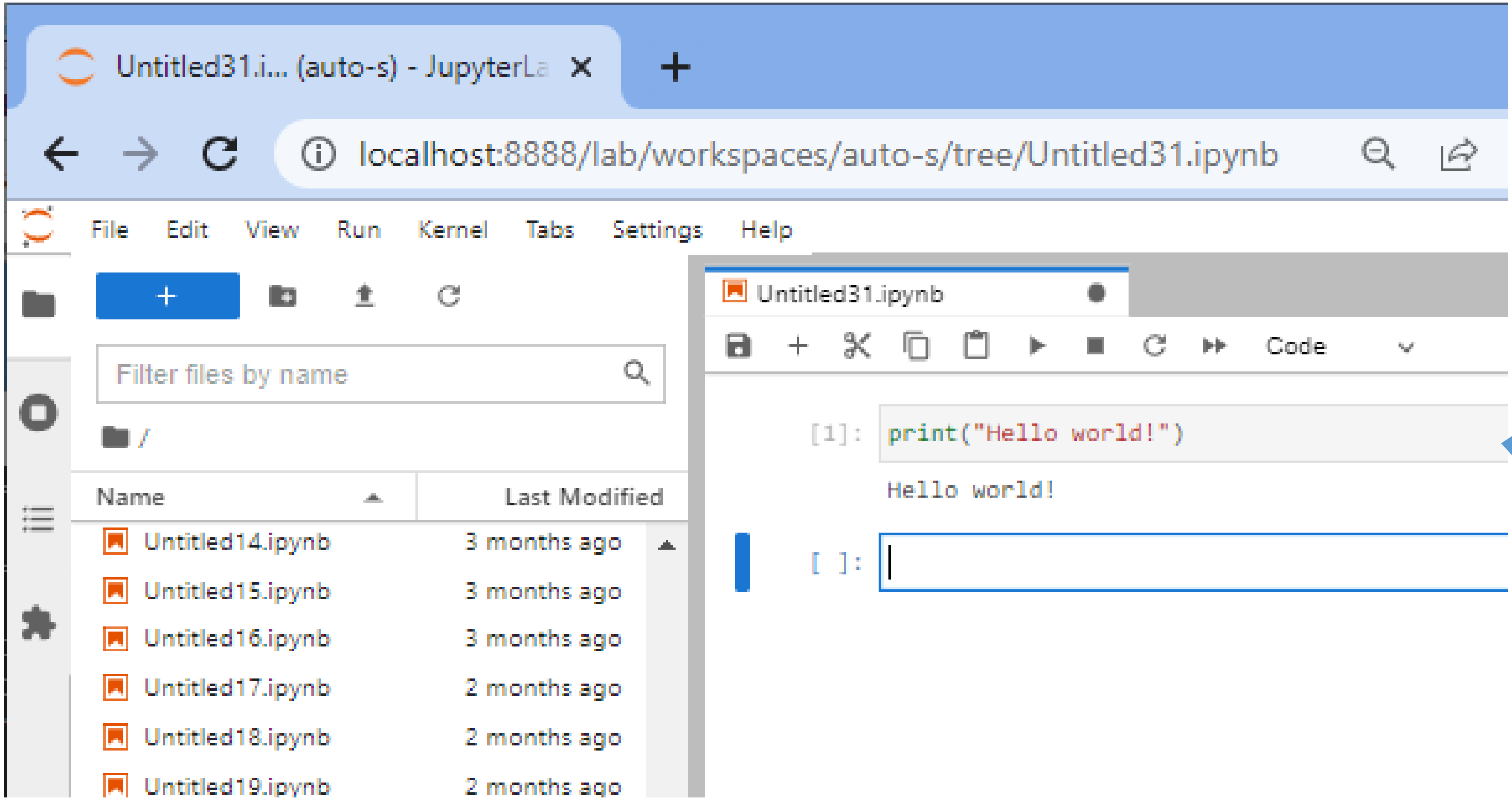
JupyterLab (auto-s)

localhost:8888/lab/workspaces/auto-s

Name	Last Modified
Untitled.ipynb	9 months ago
Untitled1.ipynb	9 months ago
Untitled10.ipynb	5 months ago
Untitled11.ipynb	4 months ago
Untitled12.ipynb	4 months ago
Untitled13.ipynb	3 months ago
Untitled14.ipynb	3 months ago
Untitled15.ipynb	3 months ago
Untitled16.ipynb	3 months ago
Untitled17.ipynb	2 months ago
Untitled18.ipynb	2 months ago
Untitled19.ipynb	2 months ago
Untitled2.ipynb	8 months ago
Untitled20.ipynb	2 months ago
Untitled21.ipynb	2 months ago
Untitled22.ipynb	2 months ago
Untitled23.ipynb	2 months ago
Untitled24.ipynb	a month ago
Untitled25.ipynb	a month ago
Untitled26.ipynb	a month ago
Untitled27.ipynb	a month ago

Jupyter lab

- Execute code cell-by-cell and see results instantaneously



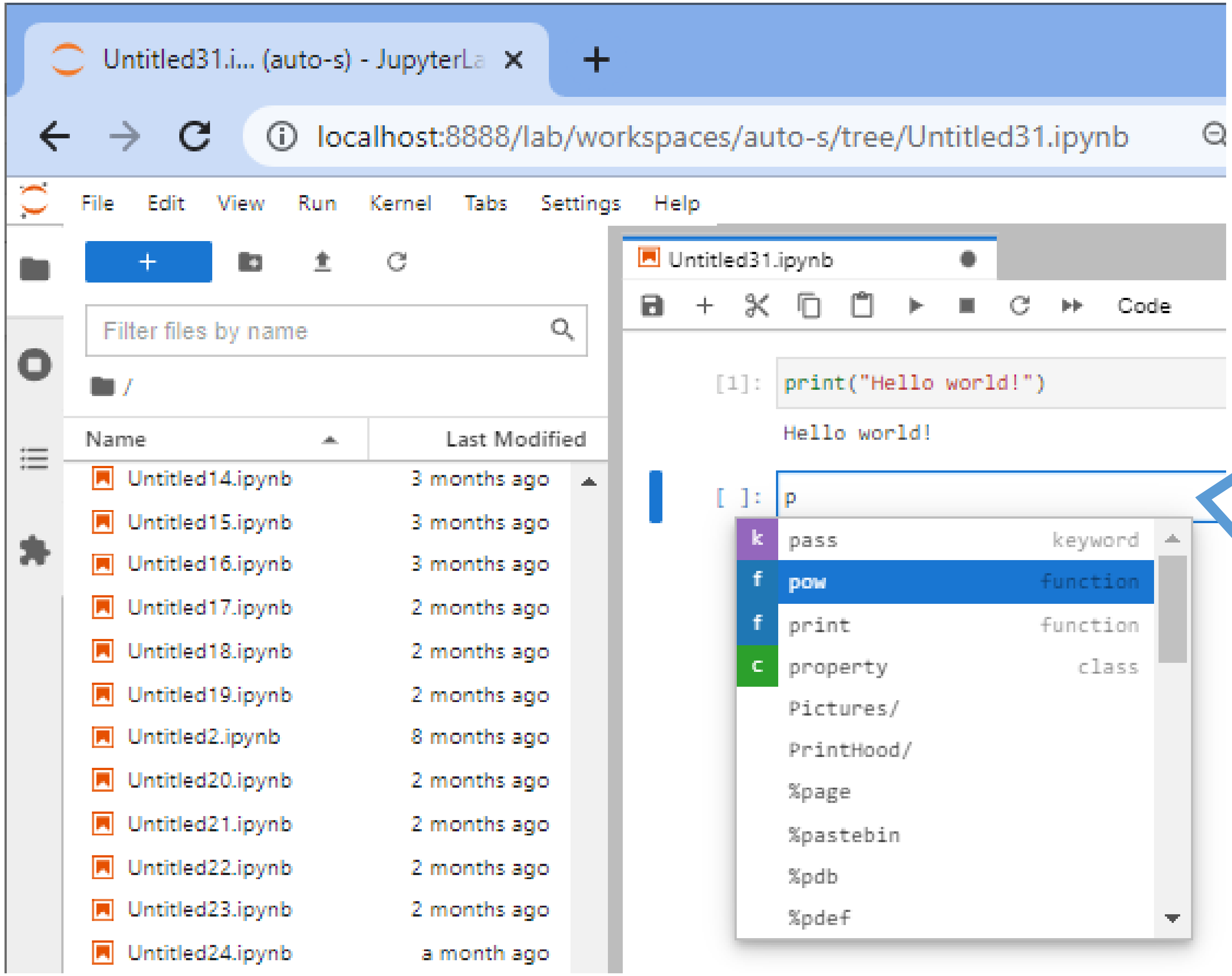
Name	Last Modified
Untitled14.ipynb	3 months ago
Untitled15.ipynb	3 months ago
Untitled16.ipynb	3 months ago
Untitled17.ipynb	2 months ago
Untitled18.ipynb	2 months ago
Untitled19.ipynb	2 months ago

```
[1]: print("Hello world!")

Hello world!

[ ]:
```

SHIFT + ENTER to execute a code cell

Jupyter lab

- Context-specific help, auto-completion


Untitled31.i... (auto-s) - JupyterLa
localhost:8888/lab/workspaces/auto-s/tree/Untitled31.ipynb
File
Edit
View
Run
Kernel
Tabs
Settings
Help
Filter files by name
/
Name
Last Modified
Untitled14.ipynb 3 months ago
Untitled15.ipynb 3 months ago
Untitled16.ipynb 3 months ago
Untitled17.ipynb 2 months ago
Untitled18.ipynb 2 months ago
Untitled19.ipynb 2 months ago
Untitled2.ipynb 8 months ago
Untitled20.ipynb 2 months ago
Untitled21.ipynb 2 months ago
Untitled22.ipynb 2 months ago
Untitled23.ipynb 2 months ago
Untitled24.ipynb a month ago
Untitled31.ipynb
Code

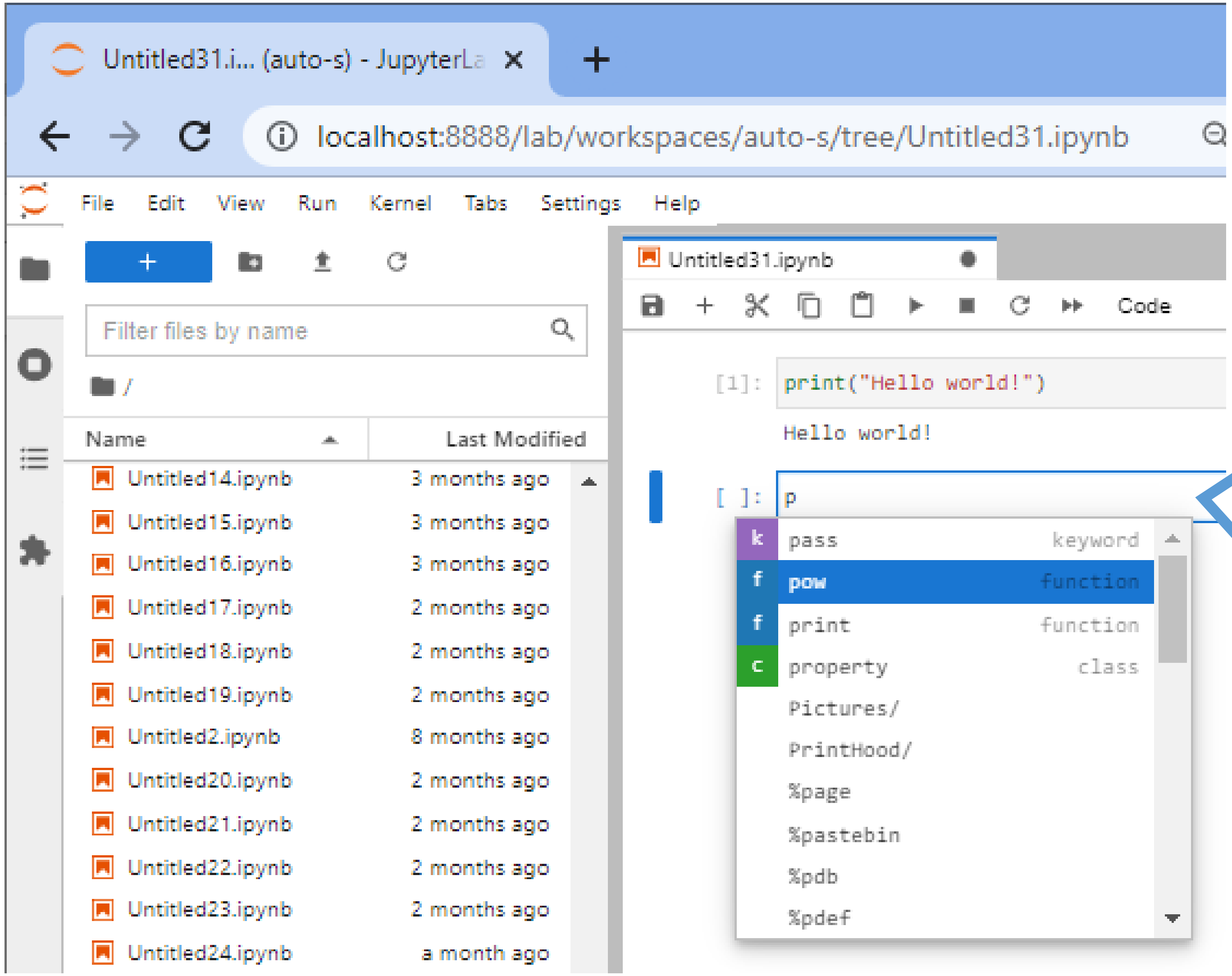
```
[1]: print("Hello world!")

     Hello world!

[ ]: p
```

```
k  pass        keyword
f  pow         function
f  print       function
c  property    class
   Pictures/
   PrintHood/
   %page
   %pastebin
   %pdb
   %pdef
```

TAB
to open auto-completion

Jupyter lab

- Context-specific help, auto-completion



Untitled31.i... (auto-s) - JupyterLa
localhost:8888/lab/workspaces/auto-s/tree/Untitled31.ipynb
File Edit View Run Kernel Tabs Settings Help
Filter files by name
/
Name
Last Modified
Untitled31.ipynb
Code

Name	Last Modified
Untitled14.ipynb	3 months ago
Untitled15.ipynb	3 months ago
Untitled16.ipynb	3 months ago
Untitled17.ipynb	2 months ago
Untitled18.ipynb	2 months ago
Untitled19.ipynb	2 months ago
Untitled2.ipynb	8 months ago
Untitled20.ipynb	2 months ago
Untitled21.ipynb	2 months ago
Untitled22.ipynb	2 months ago
Untitled23.ipynb	2 months ago
Untitled24.ipynb	a month ago

```
[1]: print("Hello world!")

Hello world!

[ ]: p
```

```
k  pass        keyword
f  pow         function
f  print       function
c  property    class
   Pictures/
   PrintHood/
   %page
   %pastebin
   %pdb
   %pdef
```

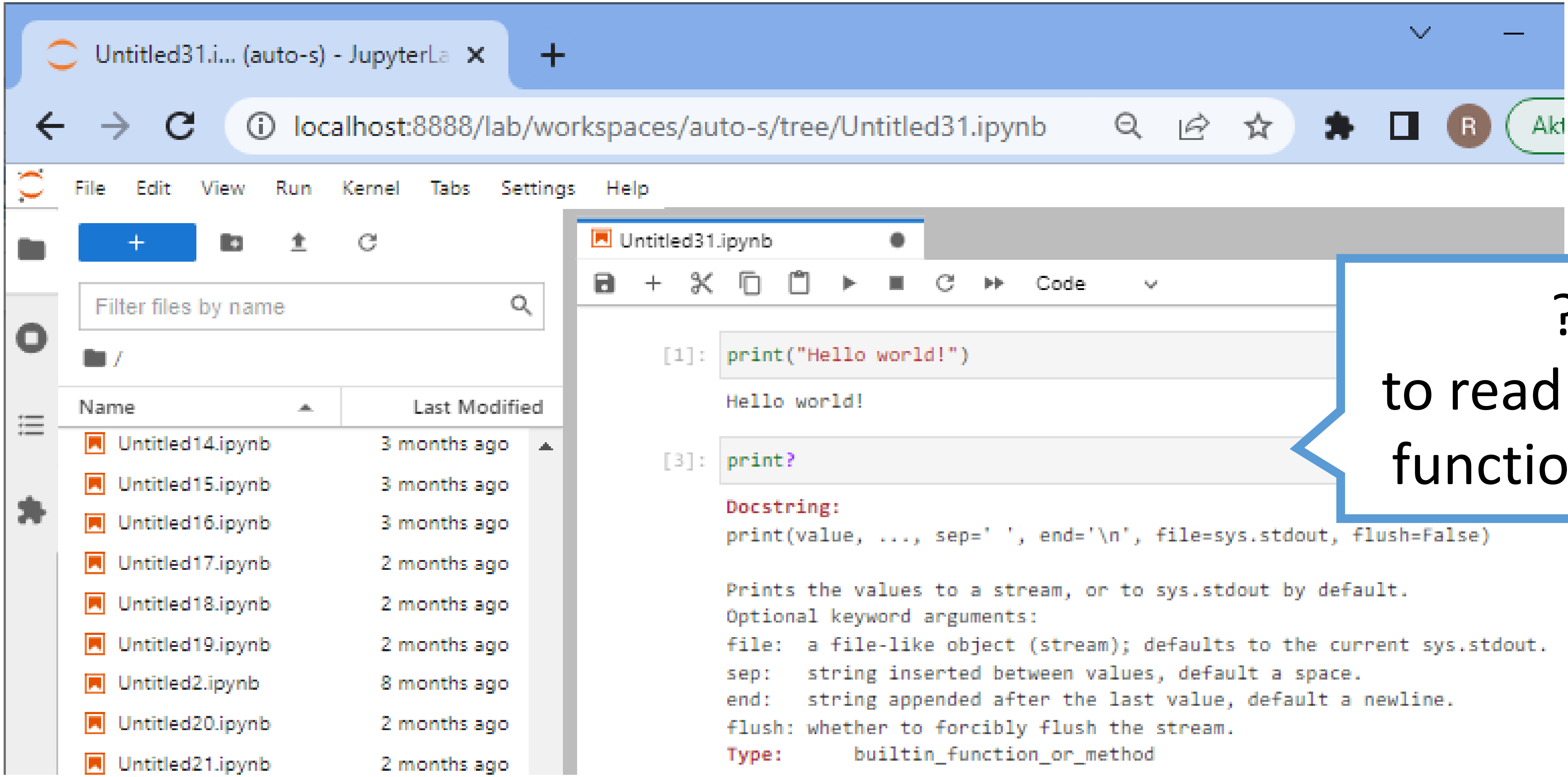
TAB
to open auto-completion

@haesleinhuepf

December 2022

Jupyter lab

- Help / "docstrings"


Untitled31.i... (auto-s) - JupyterLa
localhost:8888/lab/workspaces/auto-s/tree/Untitled31.ipynb
File
Edit
View
Run
Kernel
Tabs
Settings
Help
Filter files by name
Untitled31.ipynb
Code

Name	Last Modified
Untitled14.ipynb	3 months ago
Untitled15.ipynb	3 months ago
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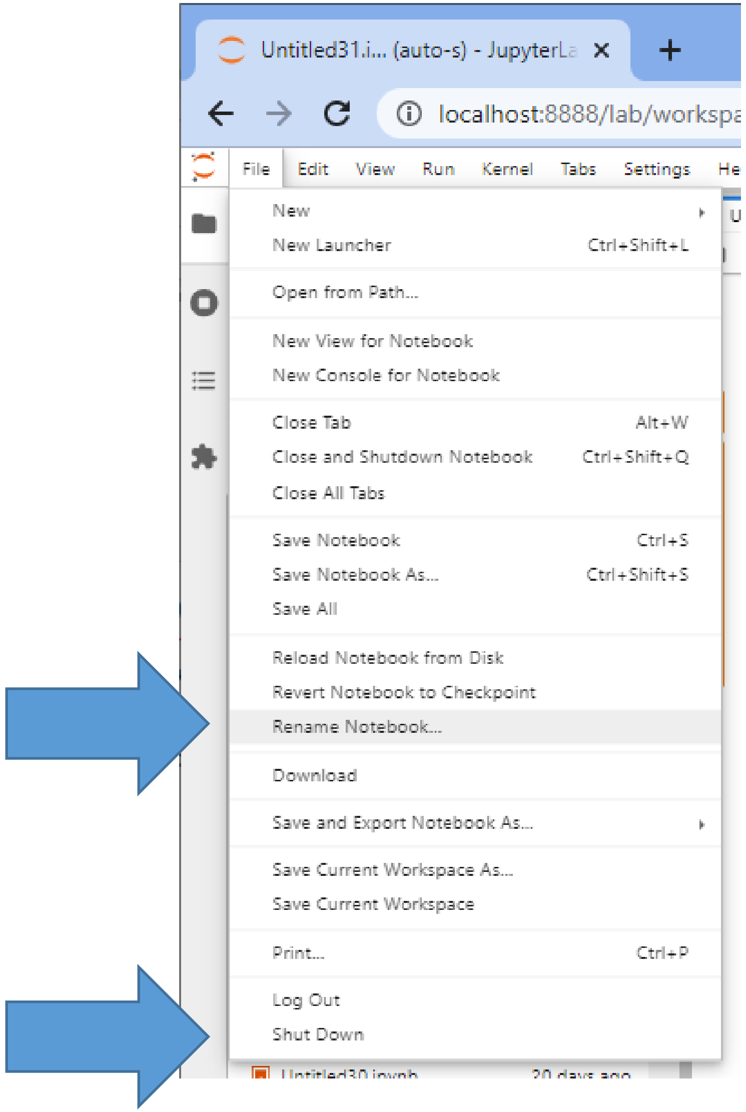
Untitled18.ipynb	2 months ago
Untitled19.ipynb	2 months ago
Untitled2.ipynb	8 months ago
Untitled20.ipynb	2 months ago
Untitled21.ipynb	2 months ago

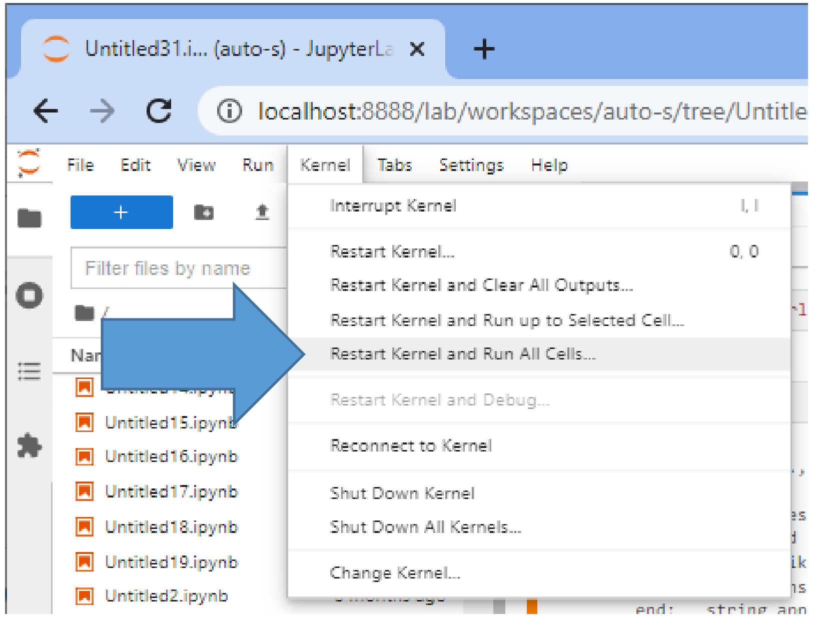
```
[1]: print("Hello world!")

Hello world!

[3]: print?

Docstring:
print(value, ..., sep=' ', end='\n', file=sys.stdout, flush=False)

Prints the values to a stream, or to sys.stdout by default.
Optional keyword arguments:
file:  a file-like object (stream); defaults to the current sys.stdout.
sep:   string inserted between values, default a space.
end:   string appended after the last value, default a newline.
flush: whether to forcibly flush the stream.
Type:      builtin_function_or_method
```

?
to read what a function does

Jupyter lab

- Saving / renaming / closing


Untitled31.i... (auto-s) - JupyterLa
localhost:8888/lab/workspa
File
Edit
View
Run
Kernel
Tabs
Settings
He
New
New Launcher Ctrl+Shift+L
Open from Path...
New View for Notebook
New Console for Notebook
Close Tab Alt+W
Close and Shutdown Notebook Ctrl+Shift+Q
Close All Tabs
Save Notebook Ctrl+S
Save Notebook As... Ctrl+Shift+S
Save All
Reload Notebook from Disk
Revert Notebook to Checkpoint
Rename Notebook...
Download
Save and Export Notebook As...
Save Current Workspace As...
Save Current Workspace
Print... Ctrl+P
Log Out
Shut Down
Untitled30.ipynb 20 days ago



Enforcing a “clean” execution state is important for ensuring reproducibility and repeatability

Python programming basics

Robert Haase

December 2022

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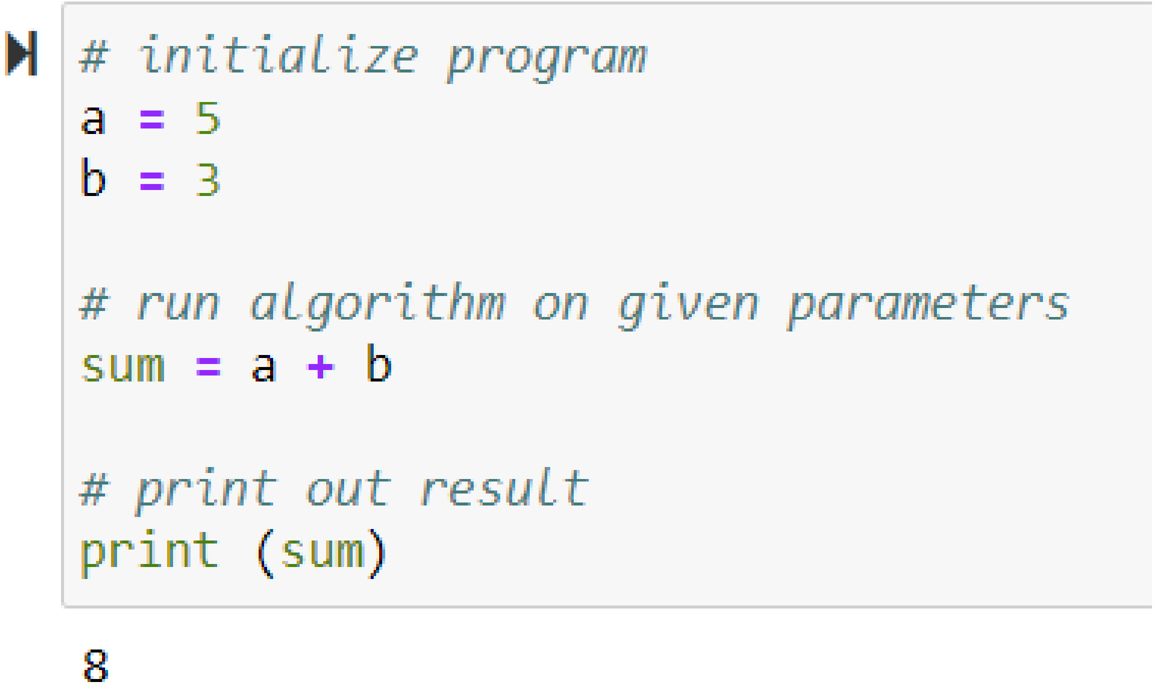
Working with variables

- Variables can hold numeric values and you can do math with them



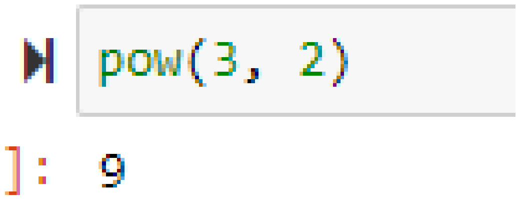
```
# initialize program
a = 5
b = 3

# run algorithm on given parameters
sum = a + b

# print out result
print (sum)
```

```
8
```

Mathematical operations

- Math commands supplement operators to be able to implement any form of calculations

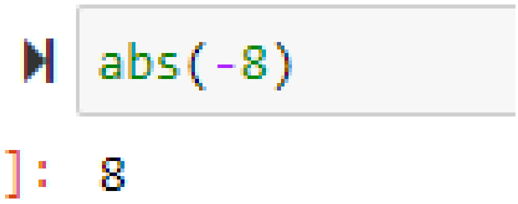
- Power



```
pow(3, 2)
```

```
]:  9
```

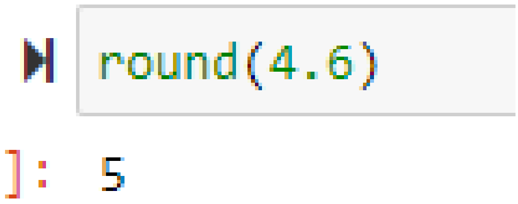
- Absolute



```
abs(-8)
```

```
]:  8
```

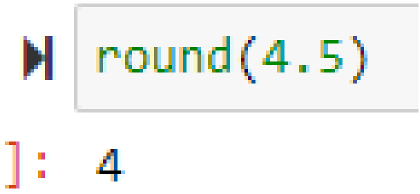
- Rounding



```
round(4.6)
```

```
]:  5
```

Be careful with some of them!



```
round(4.5)
```

```
]:  4
```

https://en.wikipedia.org/wiki/Rounding#Round_half_to_even

# Comments

Comments should contain additional information such as

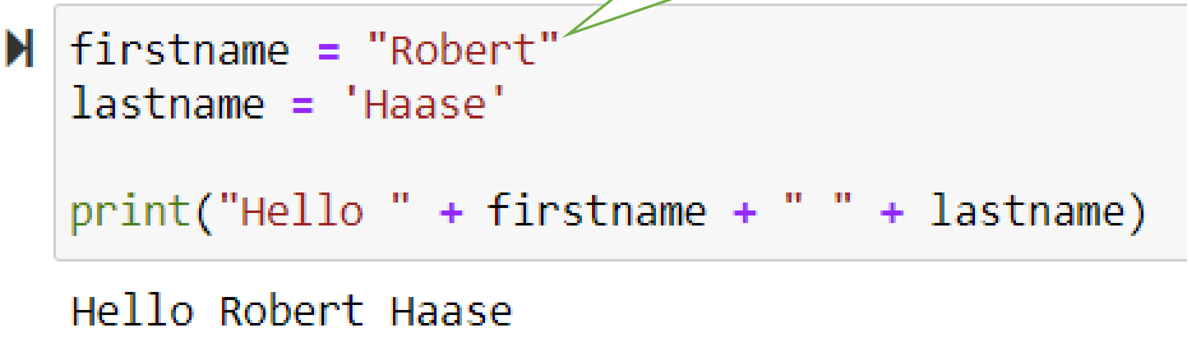
- User documentation
  - What does the program do?
  - How can this program be used?
- Your name / institute in case a reader has a question
- Comment why things are done.
- Do not comment what is written in the code already!

```
#
# This program sums up two numbers.
#
# Usage:
# * Run it in Python 3.8
#
# Author: Robert Haase, PoL TUD
#         Robert.haase@tu-dresden.de
# April 2021

# initialise program
a = 1
b = 2.5

# run complicated algorithm
final_result = a + b

#~~ print the final result~~
print( final_result )
```

Working with variables and string values

- Also strings as values for variables are supported

Single and double quotes allowed

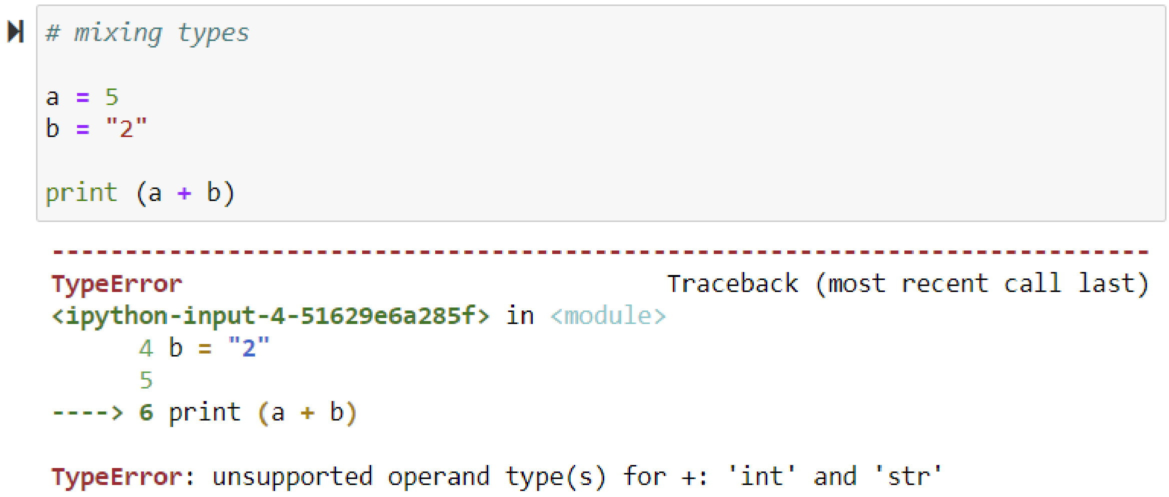


```python
firstname = "Robert"
lastname = 'Haase'

print("Hello " + firstname + " " + lastname)
```

```
Hello Robert Haase
```

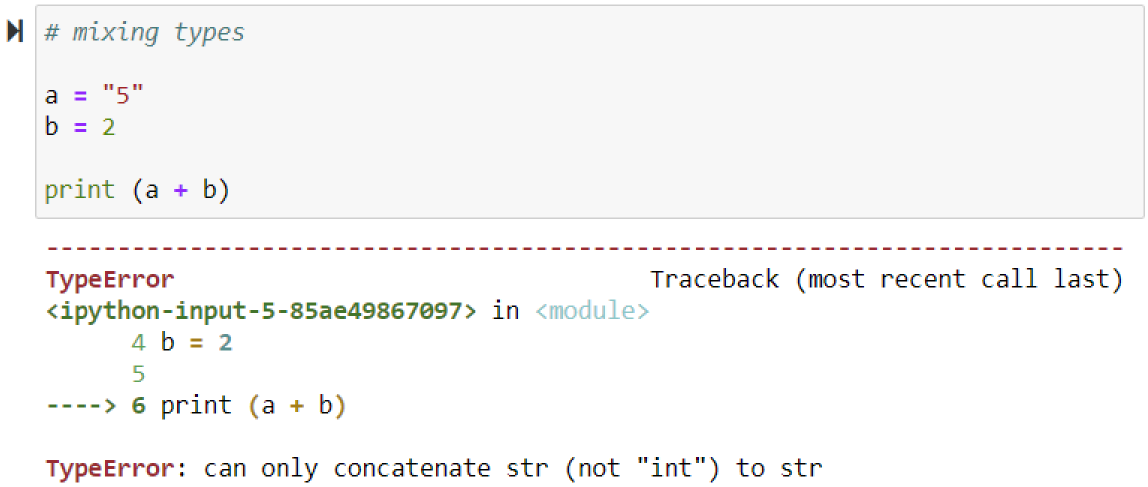
Working with variables and string values

- Also strings as values for variables are supported
- When combining strings and numbers, you need to explicitly define what you want to do.



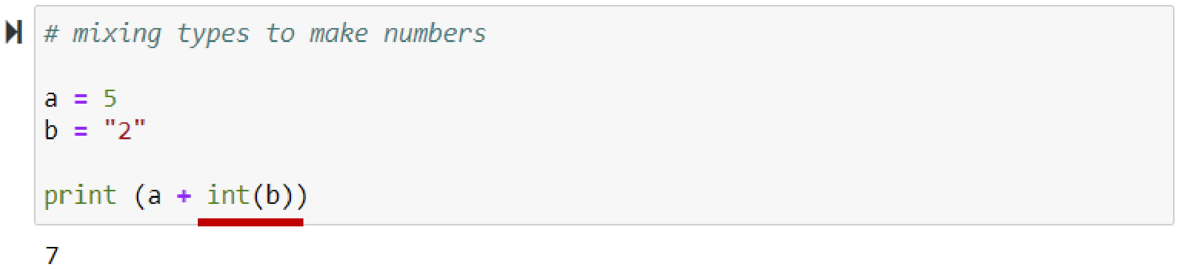
```
# mixing types

a = 5
b = "2"

print (a + b)
```

```
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)
<ipython-input-4-51629e6a285f> in <module>
      4 b = "2"
      5
----> 6 print (a + b)

TypeError: unsupported operand type(s) for +: 'int' and 'str'
```



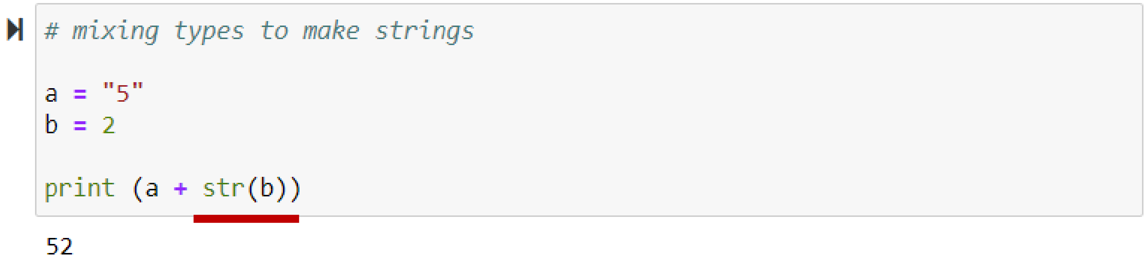
```
# mixing types

a = "5"
b = 2

print (a + b)
```

```
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)
<ipython-input-5-85ae49867097> in <module>
      4 b = 2
      5
----> 6 print (a + b)

TypeError: can only concatenate str (not "int") to str
```



```
# mixing types to make numbers

a = 5
b = "2"

print (a + int(b))
```

```
7
```



```
# mixing types to make strings

a = "5"
b = 2

print (a + str(b))
```

```
52
```

- Conversion to a floating point number: float()