Type hints

CREATING ROBUST WORKFLOWS IN PYTHON

Martin Skarzynski

Co-Chair, Foundation for Advanced Education in the Sciences (FAES)

Dynamic typing

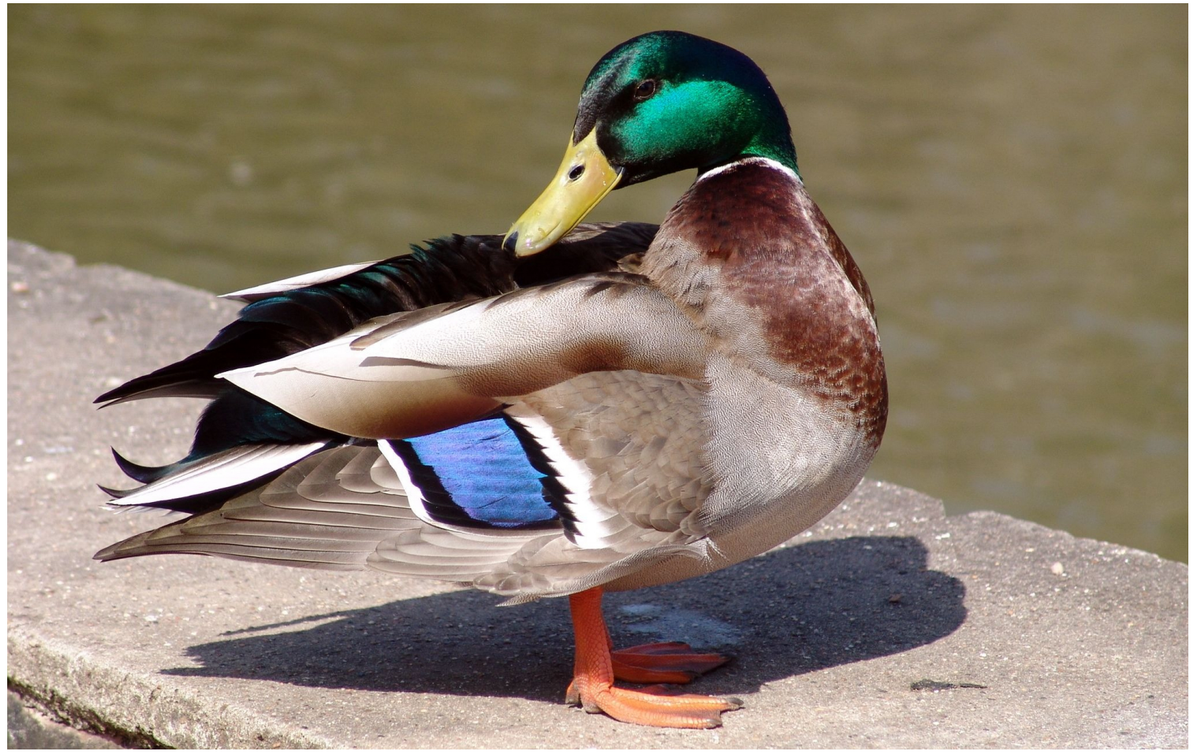
```
def double(n):
    return n * 2
```

```
double(2)

double('2')
```

```
4
'22'
```

- Python
  - Infers types when running code
    - Dynamic (duck) typing



Type hints for arguments

```
def double(n: int):
    return n * 2

double(2)
```

```
4
```

```
def double(n: str):
    return n * 2

double('2')
```

```
'22'
```

Type hints for return values

```
def double(n: int) -> int:
    return n * 2

double(2)
```

```
4
```

```
def double(n: str) -> str:
    return n * 2

double('2')
```

```
'22'
```

Get type hint information

```
from double import double


# The help() function
help(double)
```

```
Help on function double in module double:


double(n:int) -> int
```

Type checker setup

Type checking tool setup:

- `mypy` type checker
- `pytest` testing framework
- `pytest-mypy` pytest plugin

```
$ pip install pytest mypy pytest-mypy
```

Type checker setup

- `pytest.ini` file with the following:

```
[pytest]
addopts = --doctest-modules --mypy --mypy-ignore-missing-imports
```

Mypy to the rescue!

```
$ pytest double.py
```

```
========================== test session starts ==============================
...
================================ FAILURES ===================================
_____________________________ mypy double.py _______________________________
double.py:4: error: Arg. 1 to "double" has incompatible type "str"; expected "int"


======================== 1 failed in 0.36 seconds ===========================
```

List

```
from typing import List

def cook_foods(raw_foods: List[str]) -> List[str]:
    return [food.replace('raw', 'cooked') for food in raw_foods]

cook_foods(['raw asparagus', 'raw beans', 'raw corn'])

cook_foods('raw corn')
```

```
['cooked asparagus', 'cooked beans', 'cooked corn']
['r', 'a', 'w', ' ', 'c', 'o', 'r', 'n']
```

Pytest cook

```
$ pytest cook.py
```

```
============================= test session starts ==============================
...
================================ FAILURES ======================================
_____________________________ mypy cook.py ____________________________________
cook.py:7: error: Arg. 1 to "cook_foods" has ... type "str"; expect. "List[str]"


======================== 1 failed in 0.25 seconds ==============================
```

Optional

```
from typing import Optional

def str_or_none(optional_string: Optional[str] = None) -> Optional[str]:
    return optional_string
```

Let's practice type annotating our code!

CREATING ROBUST WORKFLOWS IN PYTHON

Docstrings

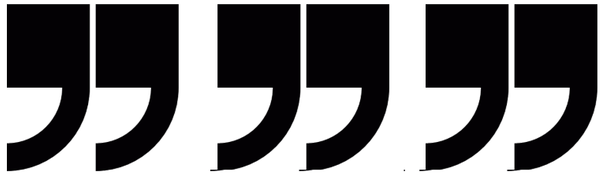
CREATING ROBUST WORKFLOWS IN PYTHON

Martin Skarzynski

Co-Chair, Foundation for Advanced Education in the Sciences (FAES)

Docstrings

- Triple quoted strings
- Include documentation in objects



```
def double(n: float) -> float:
    """Multiply a number by 2."""
    return n * 2
```

Access docstrings

```
help(double)
```

```
Help on function double in module __main__:

double(n: float) -> float
    Multiply a number by 2.
```

Google docstring style

```
"""Google style.

The Google style tends to result in
wider docstrings with fewer lines of code.

Section 1:
    Item 1: Item descriptions don't need line breaks.
"""
```

Numpy docstring style

```
"""Numpy style.

The Numpy style tends to results in
narrower docstrings with more lines of code.

Section 1
---------
Item 1
    Item descriptions are indented on a new line.
"""
```

Docstring types

```
"""MODULE DOCSTRING"""

def double(n: float) -> float:
    """Multiply a number by 2."""
    return n * 2

class DoubleN:
    """CLASS DOCSTRING"""
    def __init__(self, n: float):
        """METHOD DOCSTRING"""
        self.n_doubled = n * 2
```

- Location determines the type:
  - In definitions of
    - Functions
    - Classes
    - Methods
  - At the top of `.py` files
    - Modules
    - Scripts
    - `__init__.py`

Package docstrings

```
import pandas
help(pandas)
```

```
Help on package pandas:

NAME
    pandas

DESCRIPTION
    pandas - a powerful data analysis
    and manipulation library for Python
```

`help()` output highlights:

- NAME
- DESCRIPTION (package docstring)
- FILE (path to `__init__.py`)

Module docstrings

```
import double
help(double)
```

```
Help on module double:

NAME
    double - MODULE DOCSTRING

CLASSES
    builtins.object
        DoubleN
```

```
class DoubleN(builtins.object)
 |  DoubleN(n: float)
 |
 |  CLASS DOCSTRING
 |
 |  Methods defined here:
 |
 |  __init__(self, n: float)
 |      METHOD DOCSTRING
```

Class docstrings

```
class DoubleN:
    """The summary of what the class does.
    Arguments:
        n: A float that will be doubled.
    Attributes:
        n_doubled: A float that is the result of doubling n.
    """

    def __init__(self, n: float) -> None:
        self.n_doubled = n * 2
```

Docstring examples

```
def double(n: float) -> float:
    """Multiply a number by 2.
    Arguments:
        n: The number to be doubled.
    Returns:
        The value of n times 2.
    Examples:
        >>> double(2)
        4.0
    """
    return n * 2
```

Mistake in the docstring example:

```
2 * 2
```

```
4
```

```
2. * 2
```

```
4.0
```

Test docstring examples

```
============== FAILURES ===============
_______ [doctest] double.double _______
005     Returns:
006         The value of n times 2.
007     Examples:
008         >>> double(2)
Expected:
    4.0
Got:
    4
MODULE/square.py:8: DocTestFailure
=== 1 failed, 1 passed in 0.26 sec. ===
```

```
$ pytest double.py
```

- Docstring examples combine
  - Documentation
  - Tests (via `doctest`)

Module docstring examples

```
"""Module docstring
    Examples:
        >>> dn = DoubleN(2)
        >>> dn.n_doubled == double(2)
        True
"""

def double(n: float) -> float:
    return n * 2

class DoubleN:
    def __init__(self, n: float):
        self.n_doubled = n * 2
```

```
$ pytest double.py
```

```
======== test session starts ==========
...

double.py ..                          [100%]

====== 2 passed in 0.36 seconds =======
```

Let's practice writing docstrings!

CREATING ROBUST WORKFLOWS IN PYTHON

Reports

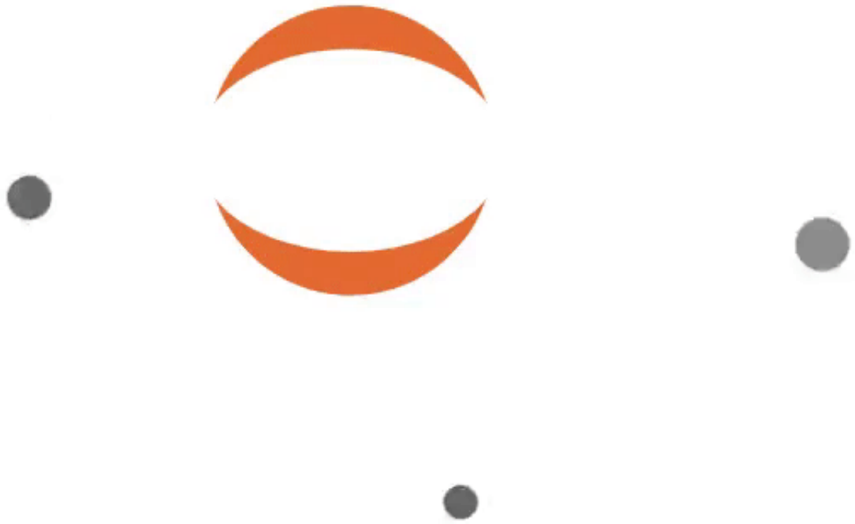
CREATING ROBUST WORKFLOWS IN PYTHON

Martin Skarzynski

Co-Chair, Foundation for Advanced Education in the Sciences (FAES)

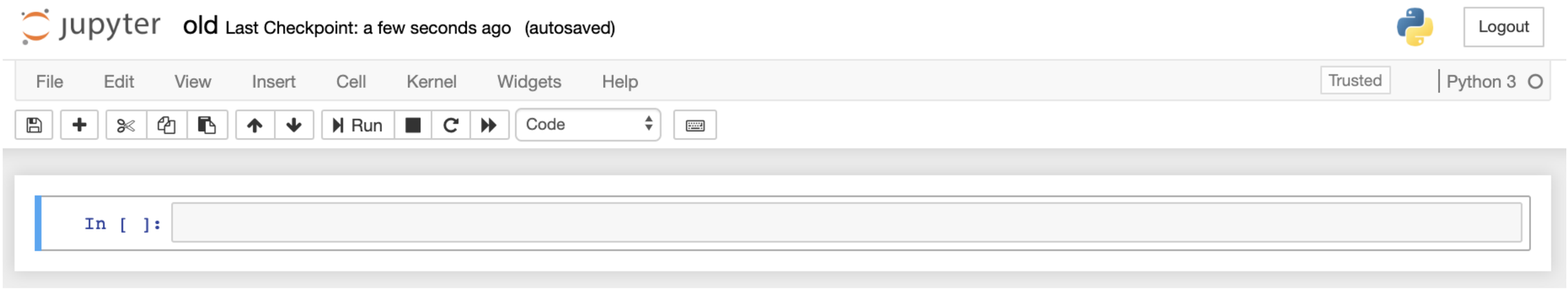
Jupyter notebooks

- Consist of cells
  - Text (Markdown format)
  - Code (Python, R, etc.)
- Have an `.ipynb` extension
- Built on IPython
- Have a structure based on JSON
  - JavaScript Object Notation
  - Similar to a Python dictionary



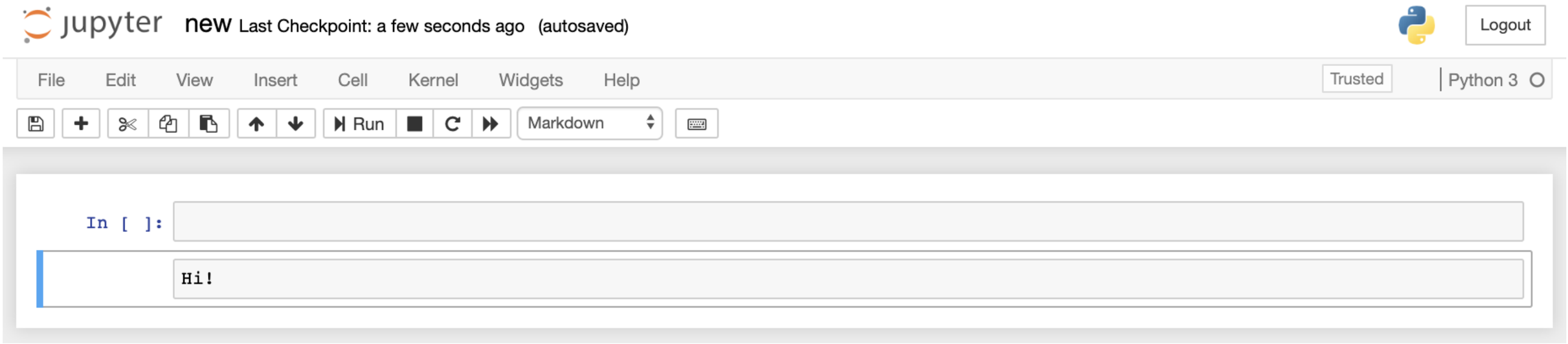
[1] Pérez, F., & Granger, B. E. (2007). IPython: a system for interactive scientific computing. CiSE, 9(3).

Track notebooks changes



- `old.ipynb`
  - Empty code cell

Track notebooks changes



- `new.ipynb`
  - Empty code cell
  - Markdown cell that says `Hi!`

Diff

- View changes made to notebooks
  - With the `diff` shell command

```
$ diff -c old.ipynb new.ipynb
```

```
     "source": []
+    },
+    {
+     "cell_type": "markdown",
+     "metadata": {},
+     "source": [
+      "Hi!"
+     ]
     }
```

Nbdiff

- View changes made to notebooks
  - With the `diff` shell command

```
$ diff -c old.ipynb new.ipynb
```

  - With the `nbdime` `nbdiff` command

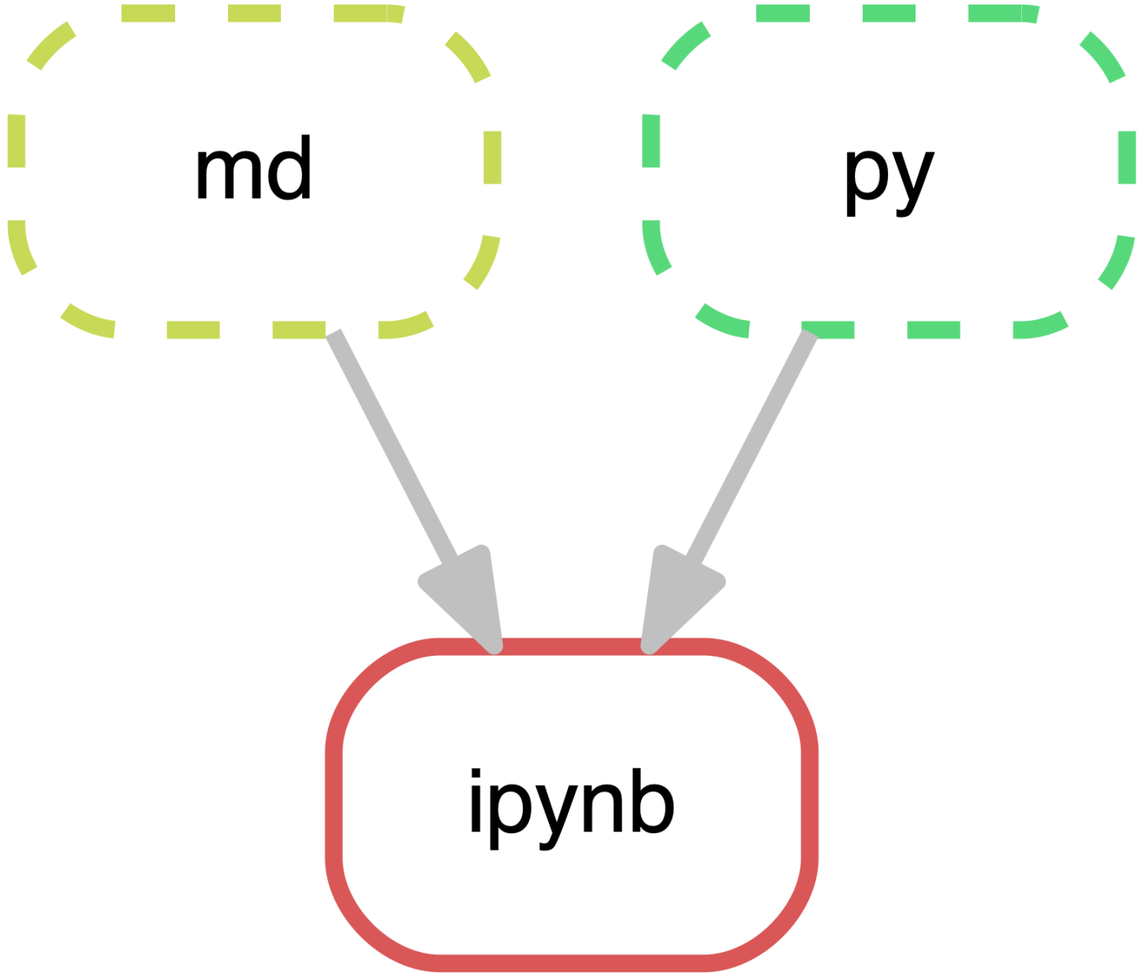
```
$ nbdiff old.ipynb new.ipynb
```

    - https://nbdime.readthedocs.io

```
--- old.ipynb  2020-02-07 20:46:26.4981
+++ new.ipynb  2020-02-07 20:41:18.5494
## inserted before /cells/1:
+  markdown cell:
+    source:
+      Hi!
```

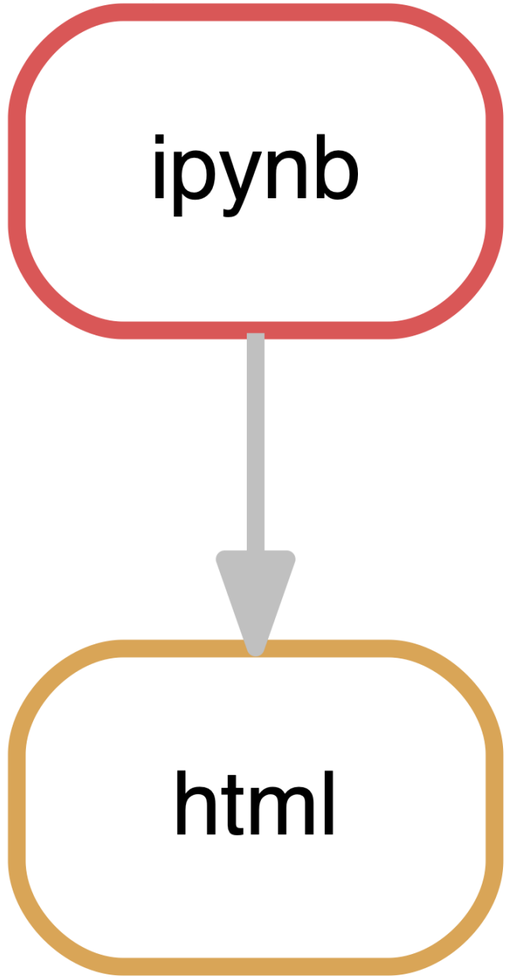
Notebook workflow package

1. Use `nbformat` to create notebooks from:
   - Markdown files (`.md`)
   - Code files (`.py`)



Convert notebooks

1. Use `nbformat` to create notebooks from:
   - Markdown files (`.md`)
   - Code files (`.py`)
2. Use `nbconvert` to convert notebooks



Code cells

```
from nbformat.v4 import (new_notebook,
                         new_code_cell)

nb = new_notebook()

nb.cells.append(new_code_cell('1+1'))

nb.cells
```

```
[{'cell_type': 'code', 'metadata': {},
  'execution_count': None,
  'source': '1+1', 'outputs': []}]
```

- Use `nbformat` 's `v4` module to create:
- Notebook objects
  - `new_notebook()`
- Code cell objects
  - `new_code_cell()`
- Code cell keys
  - `execution_count`
  - `source`
  - `outputs`

Unexecuted code cells

From Altair's Example Gallery:

```
[ ]: import altair as alt
     from vega_datasets import data
     alt.Chart(data.cars()).mark_circle(size=60).encode(
         x='Horsepower', y='Miles_per_Gallon', color='Origin',
         tooltip=['Name', 'Origin', 'Horsepower', 'Miles_per_Gallon']
     ).interactive()
```

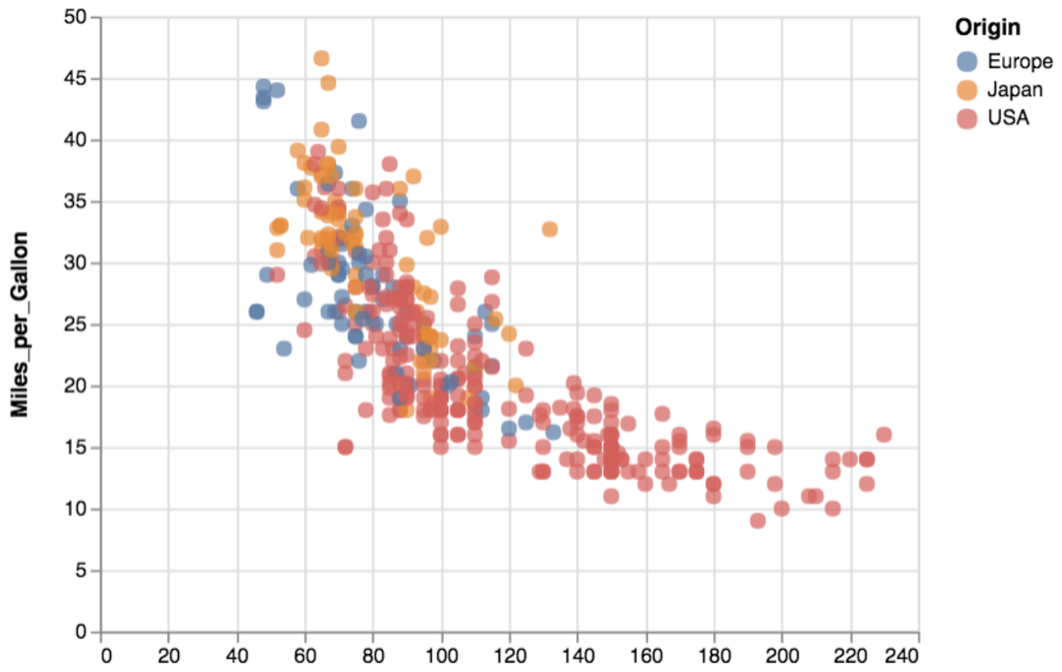
- Square brackets (`[ ]:`) on the left
  - Correspond to `execution_count` key-value pair

Executed code cells

From Altair's Example Gallery:

[1]:
```
import altair as alt
from vega_datasets import data
alt.Chart(data.cars()).mark_circle(size=60).encode(
    x='Horsepower', y='Miles_per_Gallon', color='Origin',
    tooltip=['Name', 'Origin', 'Horsepower', 'Miles_per_Gallon']
).interactive()
```

[1]:



Running notebook code cells

- Increments the
  - Number in `[ ]:` (rendered)
  - `execution_count` value
- Produces output (e.g. a plot)
  - Below the code cell
  - In the `outputs` list

Markdown cells

```
from nbformat.v4 import (
    new_markdown_cell
)

nb.cells.append(new_markdown_cell('Hi'))

len(nb.cells)

nb.cells[1]
```

```
2
[{'cell_type': 'markdown',
  'source': 'Hi', 'metadata': {}}]
```

- Use `nbformat` 's `v4` module to create:
- Markdown cell objects
  - `new_markdown_cell()`

```
import nbformat


nbformat.write(nb, "mynotebook.ipynb")
```

Nbconvert exporters

- Convert notebooks
  - Import and instantiate exporter

```
from nbconvert.exporters import HTMLExporter
html_exporter = HTMLExporter()
```

  - Obtain via by `get_exporter()`

```
from nbconvert.exporters import get_exporter
html_exporter = get_exporter('html')()
```

Export files

- Create an HTML report from a Jupyter notebook:
  - Pass a notebook filename to the exporter's `from_filename()` method

```
contents = html_exporter.from_filename('mynotebook.ipynb')[0]
```

  - Save the `contents` of the converted file

```
from pathlib import Path

Path('myreport.html').write_text(contents)
```

Let's write a package for Jupyter notebook workflows!

CREATING ROBUST WORKFLOWS IN PYTHON

Pytest

CREATING ROBUST WORKFLOWS IN PYTHON

Martin Skarzynski

Co-Chair, Foundation for Advanced Education in the Sciences (FAES)

Pytest tests

```
import pytest

def test_addition():
    assert 1 + 2 == 3

@pytest.mark.parametrize('n', [0, 2, 4])
def test_even(n):
    assert n % 2 == 0

def test_assert():
    with pytest.raises(AssertionError):
        assert 1 + 2 == 4
```

- Are functions
- Typically use `assert` statements
- Can test
  - Multiple values (`@parametrize`)
  - For expected errors (`raises()`)

Test-driven development

```
def double(n: float) -> float:
    """Multiply a number by 2."""
```

```
from double import double

def test_double():
    assert double(2) == 4
```

- Define a function
  - With a docstring, but no code block
- Write a test
- Run the failing test

```
$ pytest test_double.py
```

Run failing tests

```
============== FAILURES ===============
_____________ test_double _____________
    def test_double():
>       assert double(2) == 4
E       assert None == 4
E        +  where None = double(2)

test_double:4: AssertionError
====== 1 failed in 0.10 seconds =======
```

- Write a function
  - With a docstring, but no code block
- Write a test
- Run the failing test

```
$ pytest test_double.py
```

- Work on the module until it passes

```
def double(n: float) -> float:
  """Multiply a number by 2."""
  return n * 2
```

Run passing tests

```
========= test session starts =========
platform linux -- Python 3.7.2, ...
rootdir: PROJECT_PATH, inifile: ...
plugins: mypy-0.3.2
collected 1 item

test_double .                        [100%]

====== 1 passed in 0.03 seconds =======
```

- Write a function
  - With a docstring, but no code block
- Write a test
- Run the failing test

```
$ pytest test_double.py
```

- Work on the module until it passes

```
def double(n: float) -> float:
  """Multiply a number by 2."""
  return n * 2
```

Test change

```
============== FAILURES ==============
_____________ test_raises _____________

    def test_raises():
        with pytest.raises(TypeError):
>           double('2')
E           Failed: DID NOT RAISE
            <class 'TypeError'>

test_raises.py:6: Failed
== 1 failed, 1 passed in 1.6 seconds ==
```

```
import pytest
from double import double

def test_raises():
    with pytest.raises(TypeError):
        double('2')
```

```
$ pytest test_raises.py
```

Make change

```
========== test session starts ==========
platform linux -- Python 3.7.2, ...
rootdir: PROJECT_PATH, inifile: ...
plugins: mypy-0.3.2
collected 1 item

test_raises .                      [100%]

====== 2 passed in 0.32 seconds =======
```

```
def double(n: float) -> float:
    """Multiply a number by 2."""
    if type(n) == float:
        return n * 2
    else:
        raise TypeError
```

```
$ pytest test_raises()
```

Make change

```
========= test session starts =========
platform linux -- Python 3.7.2, ...
rootdir: PROJECT_PATH, inifile: ...
plugins: mypy-0.3.2
collected 1 item

test_raises .                      [100%]

====== 2 passed in 0.32 seconds =======
```

```
def double(n: float) -> float:
    """Multiply a number by 2."""
    return n * 2.
```

```
$ pytest test_raises()
```

Project organization

```
myproject
?
??? tests
?   ??? test_mymodule.py
?   ??? test_raises.py
?
??? src
    ??? mypackage
        ??? __init__.py
        ??? double.py
```

- Test files (e.g. `test_mymodule.py`)
  - Kept in `tests/` directory
- Modules (e.g. `double.py`)
  - Kept in packages
  - Along with `__init__.py`

Nbless

A Python package for programmatic Jupyter notebook workflows

Star 5

Navigation

Contents:

Quick search

Go

Welcome to Nbless's documentation!

Fork me on GitHub

Contents:

Indices and tables

Nbless

A Python package for programmatic Jupyter notebook workflows

Star 5

Navigation

Contents:

Quick search

Go

Module contents

`nbless.nbuild`(*filenames: List[str]*) → nbformat.notebooknode.NotebookNode [source]

Create an unexecuted Jupyter notebook from markdown and code files.

Parameters: **filenames** – A list of source file names.

`nbless.nbexec`(*nb_name: str*, *kernel: str = 'python3'*) → Tuple[str, nbformat.notebooknode.NotebookNode] [source]

Create an executed notebook without modifying the input notebook.

Parameters:
- **nb_name** – The `NotebookNode` object to be executed.
- **kernel** – The programming language used to execute the notebook.

`nbless.nbconv`(*nb_name: str*, *exporter: str = 'python'*) → Tuple[str, str] [source]

Convert a notebook into various formats using `nbformat` exporters.

Parameters:
- **input_name** – The name of the input notebook.
- **exporter** – The exporter that determines the output file type.

Note: The exporter type must be ‘asciidoc’, ‘pdf’, ‘html’, ‘latex’, ‘markdown’, ‘python’, ‘rst’, ‘script’, or ‘slides’. pdf requires latex, ‘notebook’ does nothing, slides need to served (not self-contained).

Let's practice writing tests!

CREATING ROBUST WORKFLOWS IN PYTHON