Project templates

CREATING ROBUST WORKFLOWS IN PYTHON

Martin Skarzynski

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

Why use templates?

- Avoid repetitive tasks
- Standardize project structure
- Include configuration files:
  - Pytest (`pytest.ini`)
  - Sphinx (`conf.py`)
- Include Makefile to automate further steps:
  - Build Sphinx documentation
  - Create virtual environments
  - Initialize git repositories
  - Deploy packages to the PyPI

- Not just for Python
- Flexible
  - Edit files in template directory
    - Local
    - Remote

Cookiecutter prompts

```
from cookiecutter import main

main.cookiecutter(TEMPLATE_REPO)
```

```
project [PROJECT_NAME]:
>? "My Project"
```

- `cookiecutter()` arguments:
  - `template` : git repository url or path

Cookiecutter prompts

```
from cookiecutter import main

main.cookiecutter(TEMPLATE_REPO)
```

```
project [PROJECT_NAME]: "My Project"
Select license:
1 - MIT
2 - BSD
3 - GPL3
Choose from 1, 2, 3 (1, 2, 3) [1]:
>?
```

- `cookiecutter()` arguments:
  - `template` : git repository url or path

Cookiecutter defaults

```
from cookiecutter import main

main.cookiecutter(
    TEMPLATE_REPO_URL,
    no_input=True
)
```

- `cookiecutter()` arguments:
  - `template` : git repository url or path
  - `no_input`
    - Suppress prompts
    - Use `cookiecutter.json` defaults
      - Key-value pairs

Override defaults

```
from cookiecutter import main

main.cookiecutter(
    TEMPLATE_REPO,
    no_input=True,
    extra_context={'KEY': 'VALUE'}
)
```

```
{
  "project": "Your project's name",
  "license": ["MIT", "BSD", "GPL3"]
}
```

- `cookiecutter()` arguments:
  - `template` : git repository url or path
  - `no_input`
    - Suppress prompts
    - Use `cookiecutter.json` defaults
      - Key-value pairs
  - `extra_context`
    - Override defaults

Access JSON files

```
from json import load
from pathlib import Path

# Local JSON file to dictionary
load(Path(JSON_PATH).open()).values()

# List local cookiecutter.json keys
[*load(Path(JSON_PATH).open())]
```

```
from requests import get

# Remote JSON file to dictionary
get(JSON_URL).json().values()

# List remote cookiecutter.json keys
[*get(JSON_URL).json()]
```

Jinja2 template

```
{"project": "Project Name",
 "author": "Your name (or your organization/company/team)",
 "repo": "{{ cookiecutter.project.lower().replace(' ', '_') }}",
}
```

```
project = "My Project"

project.lower().replace(' ', '_')
```

```
my_project
```

Cookiecutter example

```
from cookiecutter.main import cookiecutter
cookiecutter('https://github.com/marskar/cookiecutter', no_input=True,
             extra_context={'project': 'PROJECT_NAME', 'author': 'AUTHOR_NAME'})
```

```
$ cookiecutter https://github.com/marskar/cookiecutter --no-input \
project="PROJECT_NAME" author="AUTHOR_NAME" \
user=USER_NAME description="DESCRIPTION"
```

Cookiecutter example

```
from cookiecutter.main import cookiecutter
cookiecutter('gh:marskar/cookiecutter', no_input=True,
             extra_context={'project': 'PROJECT_NAME', 'author': 'AUTHOR_NAME',
                            'user': 'USER_NAME', 'description': 'DESCRIPTION'})
```

```
$ cookiecutter gh:marskar/cookiecutter --no-input \
project="PROJECT_NAME" author="AUTHOR_NAME" \
user=USER_NAME description="DESCRIPTION"
```

Project structure

```
...
??? docs
?   ??? Makefile
?   ??? _static
?   ??? authors.rst
?   ??? changelog.rst
?   ??? conf.py
?   ??? index.rst
?   ??? license.rst
??? requirements.txt
??? setup.cfg
??? setup.py
```

```
??? src
?   ??? template
?       ??? __init__.py
?       ??? template.py
??? tests
    ??? conftest.py
    ??? test_template.py
```

```
$ make html
```

PROJECT_NAME

Navigation

Description
License
Authors
Changelog
Module Reference
Test Reference

Quick search

Go

PROJECT_NAME

Welcome to the documentation of PROJECT_NAME!

Note:

This is the main page of your project's Sphinx documentation. It is formatted in reStructuredText. Add additional pages by creating rst-files in `docs` and adding them to the toctree below. Use then references in order to link them from this page, e.g. Contributors and Changelog.

It is also possible to refer to the documentation of other Python packages with the Python domain syntax. By default you can reference the documentation of Sphinx, Python, NumPy, SciPy, matplotlib, Pandas, Scikit-Learn. You can add more by extending the `intersphinx_mapping` in your Sphinx's `conf.py`.

The pretty useful extension autodoc is activated by default and lets you include documentation from docstrings. Docstrings can be written in Google style (recommended!), NumPy style and classical style.

Read *the* Docs

Let's practice using project templates!

CREATING ROBUST WORKFLOWS IN PYTHON

Executable projects

CREATING ROBUST WORKFLOWS IN PYTHON

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Run a module

```
def print_name_and_file():
    print('Name is', __name__,
          'and file is', __file__)
if __name__ == "__main__":
    print_name_and_file()
```

```
prj
??? src
    ??? pkg
        ??? __init__.py
        ??? main.py
```

```
$ python -m prj.src.pkg.main
```

```
Name is __main__ and file is
/Users/USER/prj/src/pkg/main.py
```

Top-level imports

```
# Import module into __main__.py
(from prj.src.pkg.main
 import print_name_and_file)

if __name__ == "__main__":
    print_name_and_file()
```

```
$ python -m prj
```

```
Name is prj.src.pkg.main and file is
/Users/USER/prj/src/pkg/main.py
```

```
prj
??? __main__.py
??? src
    ??? pkg
        ??? __init__.py
        ??? main.py
```

Import error

```
# Import module into __main__.py
(from src.pkg.main
 import print_name_and_file)

if __name__ == "__main__":
    print_name_and_file()
```

```
prj
??? __main__.py
??? src
    ??? pkg
        ??? __init__.py
        ??? main.py
```

```
$ python -m pkg
```

```
...
ModuleNotFoundError:
No module named 'src'
```

Run zipped project

```
import zipapp

zipapp.create_archive('prj')
```

```
$ python -m zipapp prj
$ python prj.pyz
```

```
Name is src.pkg.main and file is
prj.pyz/src/pkg/main.py
```

```
prj
??? __main__.py
??? src
    ??? pkg
        ??? __init__.py
        ??? main.py
```

Pass arguments to projects

```
import sys

if __name__ == "__main__":
    print(sys.argv)
```

```
$ python -m zipapp prj
$ python prj.pyz hello
```

```
['prj.pyz', 'hello']
```

1. Include a command-line interface (CLI) in `__main__.py`
2. Use `zipapp` to create zipped project
3. Pass shell arguments to project

Zipapp main argument

```
import os
import zipapp

os.remove('prj/__main__.py')

zipapp.create_archive('prj', main='src.pkg.main:print_name_and_file')
```

```
$ rm prj/__main__.py
$ python -m zipapp prj --main src.pkg.main:print_name_and_file
```

Zipapp set interpreter

```
import zipapp

zipapp.create_archive('prj', interpreter="/usr/bin/env python")
```

```
$ python -m zipapp prj --python "/usr/bin/env python"
$ ./prj.pyz
```

```
Name is src.pkg.main and file is ./prj.pyz/src/pkg/main.py
```

Self-contained zipped projects

```
import zipapp

zipapp.create_archive('prj', interpreter="/usr/bin/env python")
```

```
$ python -m pip install --requirement prj/requirements.txt --target prj
$ python -m zipapp prj --python "/usr/bin/env python"
$ ./prj.pyz
```

```
Name is src.pkg.main and file is ./prj.pyz/src/pkg/main.py
```

Let's make an executable project!

CREATING ROBUST WORKFLOWS IN PYTHON

Notebook pipelines

CREATING ROBUST WORKFLOWS IN PYTHON

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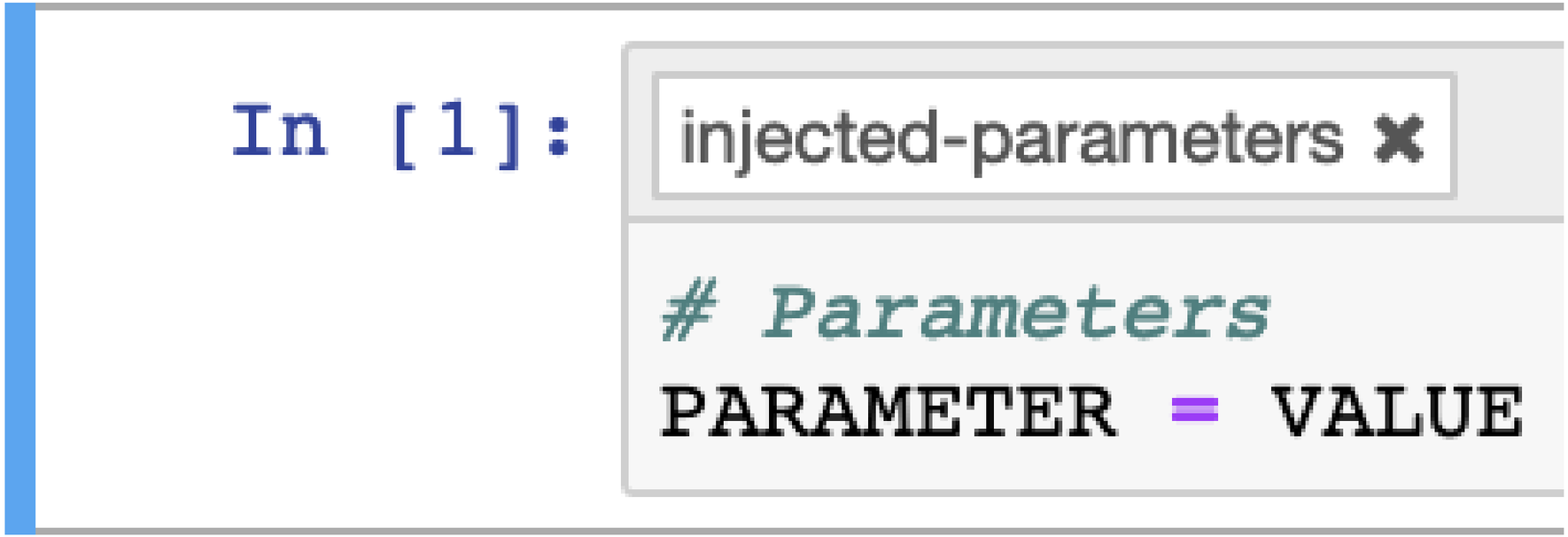
Jupyter nbconvert

- Can be used as a Python library, e.g. our `nbconv()` function
- Can execute notebooks

```
$ jupyter nbconvert --execute --to notebook input.ipynb --output output.ipynb
```

  - Cannot pass arguments to code in notebooks

Injected parameters




```
$ papermill input.ipynb output.ipynb --parameters PARAMETER VALUE
```

Default parameters

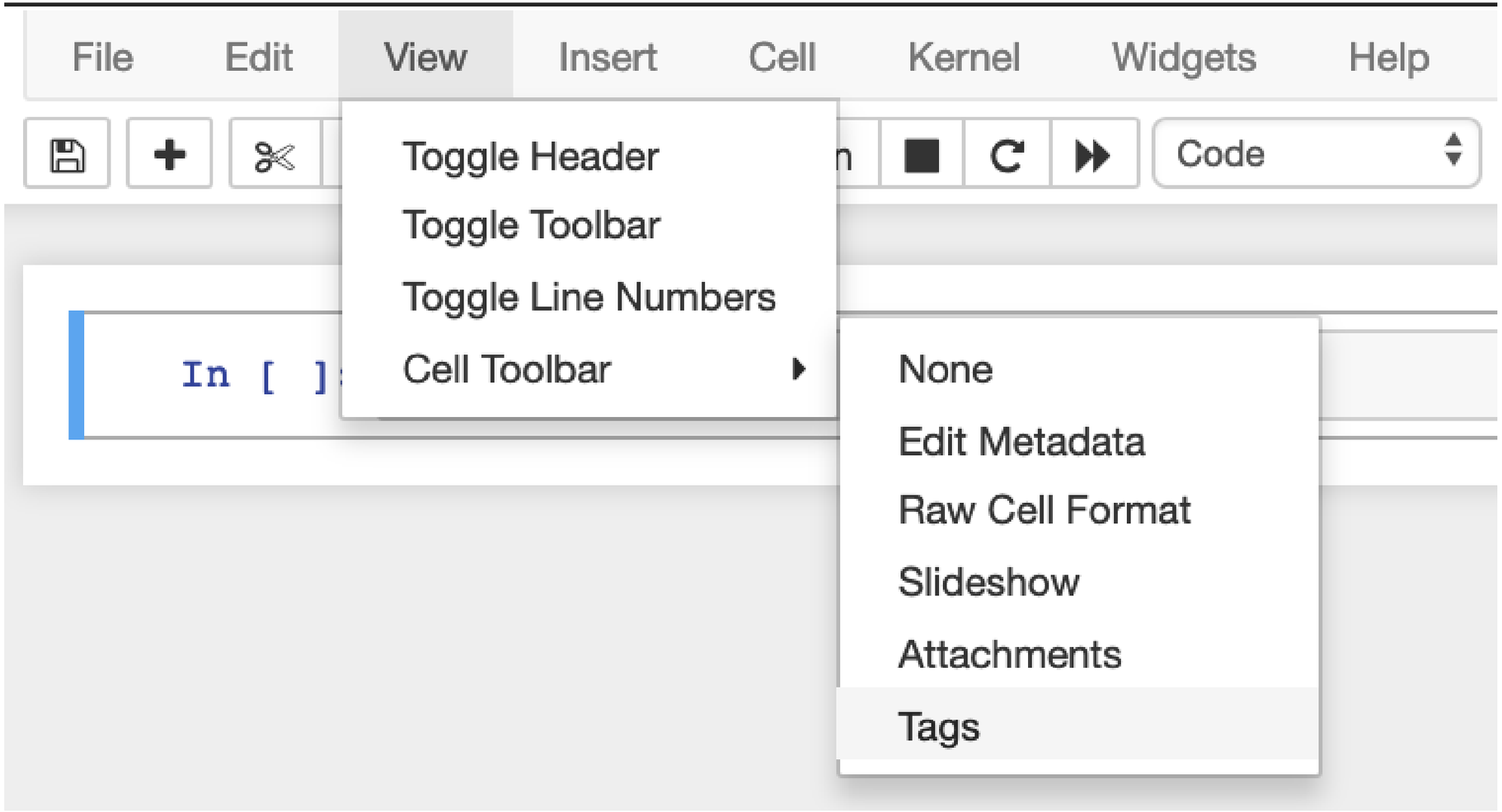
In [1]:

parameters ✖ ... Add tag

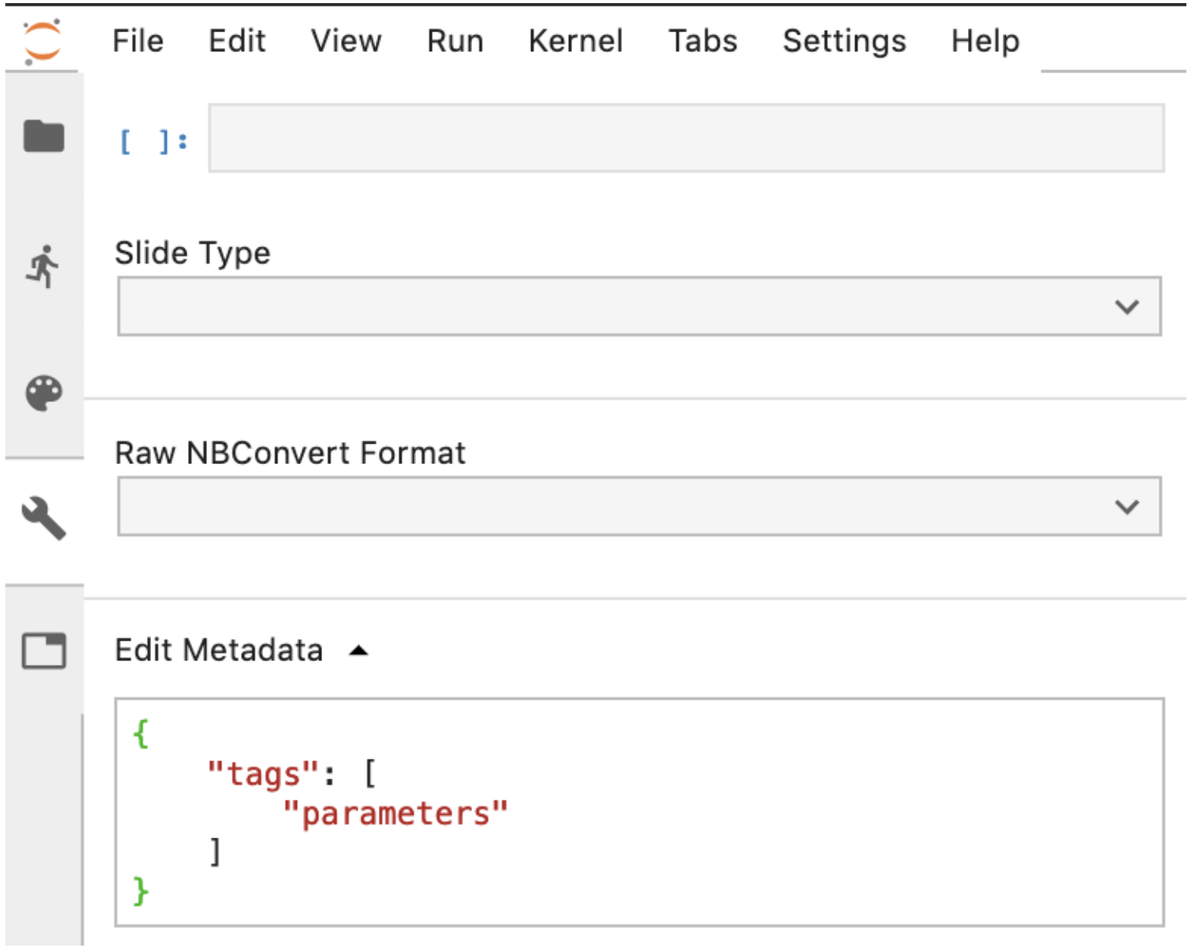
```
1  # This cell is tagged `parameters`
2  alpha = 0.1
3  ratio = 0.1
```

```
$ papermill input.ipynb output.ipynb --parameters alpha 0.2
```

Classic notebook interface



JupyterLab interface



- Edit metadata (JupyterLab)

```
{
  "tags": [
      "parameters"
  ]
}
```

Jupyter nbformat

```
import nbformat

nb = nbformat.read('NOTEBOOK.ipynb',
                   as_version=4)

nb.cells[0].metadata = {'tags':
                        ['parameters']}

nb.cells[0].source = "alpha = 0.4"

nbformat.write(nb, 'NOTEBOOK.ipynb')
```

- `nbformat.read()` : read in a notebook
- Edit the first cell
  - Add a parameters tag to `metadata`
  - Add a default parameter to `source`
- `nbformat.write()` : overwrite the original

Execute notebook

`pm.execute_notebook()`	`$ papermill`
`input_path: str`	NOTEBOOK_PATH
`output_path: str`	OUTPUT_PATH
`cwd: Any = None`	--cwd
`parameters: Any = None`	-p, --parameters
`kernel_name: Any = None`	-k, --kernel
`report_mode: Any = False`	--report-mode / --not-report-mode

Parametrize

```
import papermill as pm

names = ['alpha', 'ratio']
values = [0.6, 0.4]

param_dict = dict(zip(names, values))

pm.execute_notebook(
    'IN.ipynb',
    'OUT.ipynb',
    kernel_name='python3',
    parameters=param_dict
)
```

- Save parameter names and values as lists
- Create a dictionary of custom parameters
- Pass the dictionary
  - To the `execute_notebook()` function
  - As its `parameters` argument

Overwrite defaults

In [1]:
parameters

```
# Parameters
alpha = 0.6
```

In [2]:
injected-parameters

```
# Parameters
alpha = 0.8
```

Notebook parameters

```
# Parameters
dataset_name = "diabetes"
model_type = "ensemble"
model_name = "RandomForestRegressor"
hyperparameters = {"max_depth": 3, "n_estimators": 100, "random_state": 0}
```

Use parameters inside notebooks

```
from importlib import import_module
from typing import Optional, Dict


def get_model(model_type, model_name, hyperparameters=None):
    model = getattr(import_module('sklearn.'+model_type), model_name)
    return model(**hyperparameters) if hyperparameters else model()

keys = ['model_type', 'model_name', 'hyperparameters']
vals = [model_type, model_name, hyperparameters]
model = get_model(**dict(zip(keys, vals)))
```

scrapbook

- `sb.glue('alpha', alpha)` : record a variable
- `sb.read_notebook('NOTEBOOK.ipynb')` : return a `scrapbook.models.Notebook` object
  - `scraps` : a dictionary of recorded values
  - `scrap_dataframe` : a dataframe of recorded values
  - `papermill_metrics` : a dataframe of execution times
  - `parameter_dataframe` : a dataframe of notebook parameters

Summarize

```
import papermill as pm

names = ['alpha', 'ratio']
values = [0.6, 0.4]

param_dict = dict(zip(names, values))

pm.execute_notebook(
    'IN.ipynb',
    'OUT.ipynb',
    kernel_name='python3',
    parameters=param_dict
)
```

```
import scrapbook as sb

nb = sb.read_notebook('OUT.ipynb')

nb.parameter_dataframe
```

```
    name  value       type   filename
2  alpha    0.6  parameter  OUT.ipynb
3  ratio    0.4  parameter  OUT.ipynb
```

Let's practice using papermill and scrapbook!

CREATING ROBUST WORKFLOWS IN PYTHON

Parallel computing

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Parallel computing

- Execute multiple jobs at once (in parallel)
- Decrease code execution time

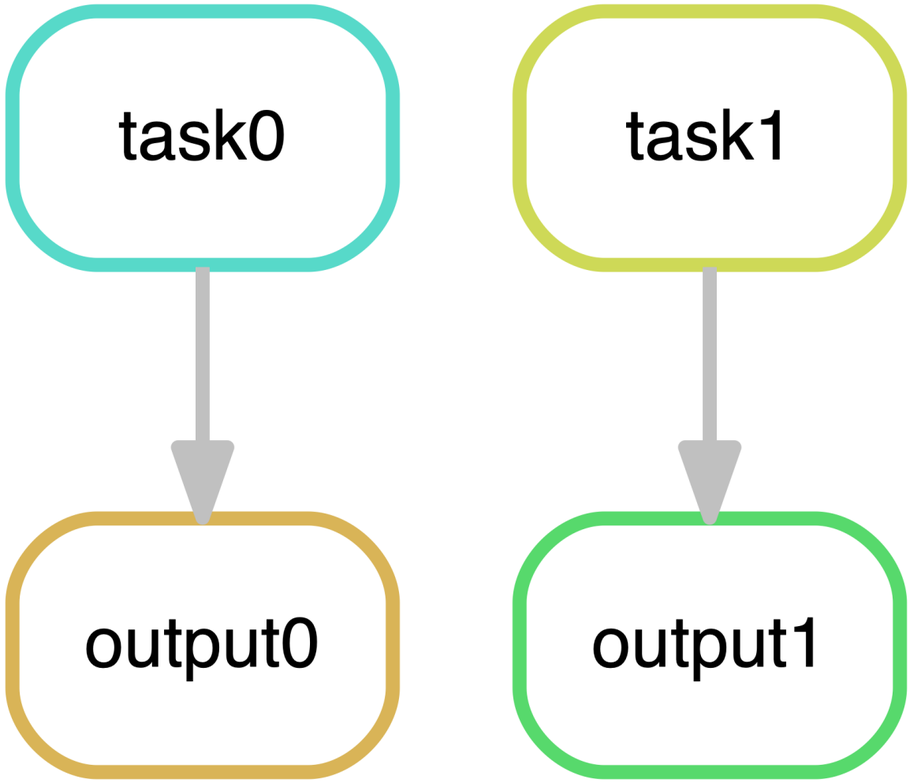
Example:

- Run multiple Make recipes in parallel

```
$ make --jobs 2
```

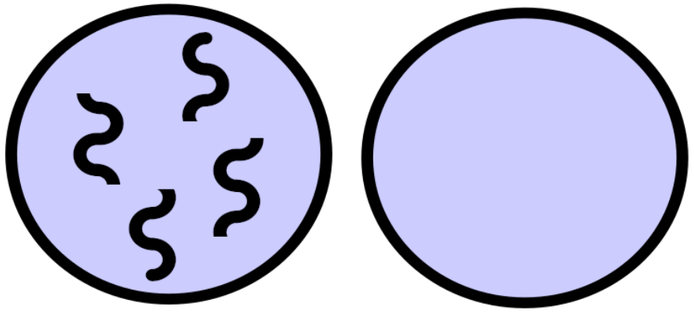
Two parallel computing options:

- Multiprocessing
- Multithreading

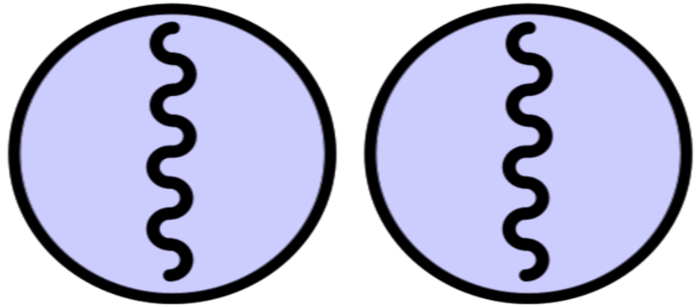


Threads and processes

- Thread ~ task
- Multithreading
  - Like multitasking
    - Assign multiple tasks to one worker

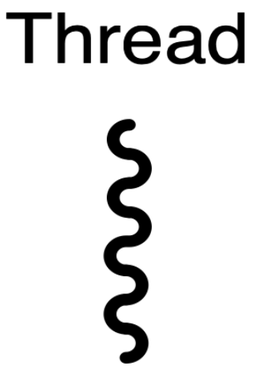


- Process ~ worker
- Multiprocessing
  - Like teamwork
    - Give each worker a task

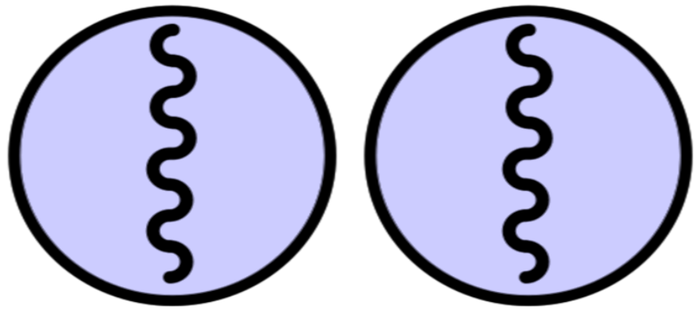


Multiprocessing

```
import time

def task(duration):
    time.sleep(duration)
```



- Process ~ worker
- Multiprocessing
  - Like teamwork
    - Give each worker a task



Multiprocessing

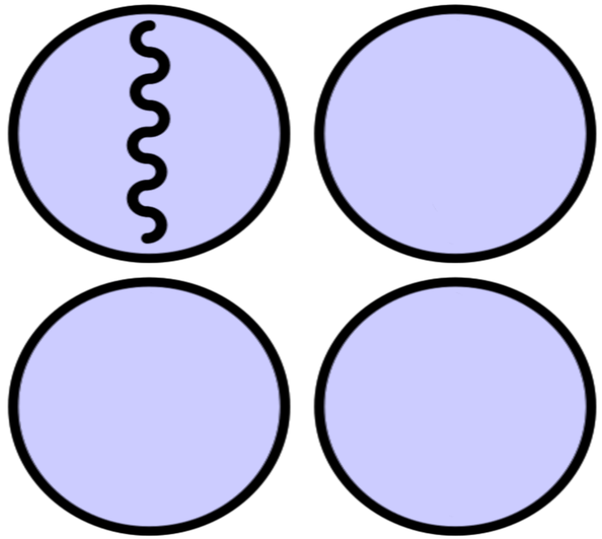
```
import time
from multiprocessing import Pool
from itertools import repeat

def split_tasks(n_workers, n_tasks, task_duration):
    start = time.time()
    Pool(n_workers).map(task, repeat(task_duration, n_tasks))
    end = time.time()
    print("Workers:", n_workers, "Tasks:", n_tasks, "Seconds:", round(end - start))
```

Sequential execution

```
split_tasks(n_workers=1,
            n_tasks=4, task_duration=2)
```

```
Workers: 1 Tasks: 4 Seconds: 8
```

- 1 worker
- 4 tasks
- 1 task at a time



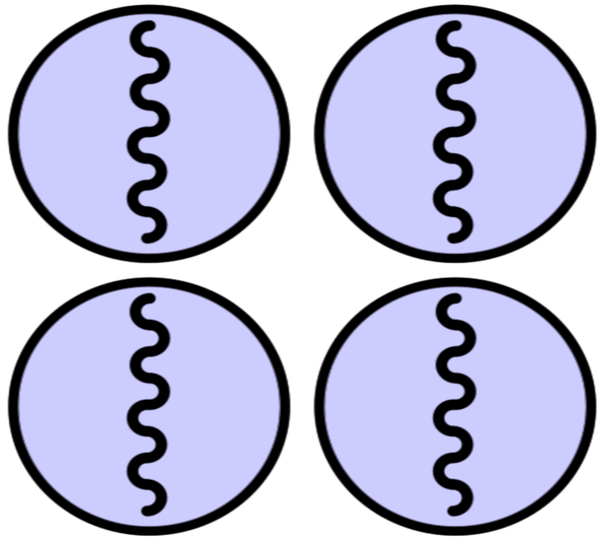
Parallel execution

```
split_tasks(n_workers=4,
            n_tasks=4, task_duration=2)
```

```
Workers: 4 Tasks: 4 Seconds: 2
```

```
from multiprocessing import Pool

Pool(n_workers).map(FUNCTION, ITERABLE)
```

- 4 workers
- 4 tasks
- 4 tasks at a time



Parallelize scitkit-learn

```
from dask.distributed import Client
from sklearn.externals import joblib
```

Parallelize scitkit-learn

```
from dask.distributed import Client
from sklearn.externals import joblib

Client(n_workers=1,
       threads_per_worker=4,
       processes=False)

with joblib.parallel_backend('dask'):
    MODEL.fit(x_train, y_train)
```

1. Instantiate the `Client` class
   - Number of workers (`n_workers`)
   - Set `threads_per_worker` ratio
   - Enable threading (`processes=False`)
2. As part of a `with` statement
   - Pass `'dask'` to `parallel_backend()`
3. Inside the context of the `with` statement
   - Call a model instance's `fit()` method

Dask collections

- Can be used interactively with minimal setup
- Dask bags resemble unordered tuples and are limited to one process per thread
- Numpy and Pandas can handle more than one thread per process
- Replace Numpy arrays and Pandas dataframes with analogous Dask Collections

Dask collection	Similar to	Default scheduler	Advantage
Bag	`tuple` (unordered)	Multiprocessing	1 thread / process
Array	Numpy Array	Threaded	Easy data sharing
DataFrame	Pandas DataFrame	Threaded	Easy data sharing

Pandas dataframes

```
import pandas as pd

df = pd.read_csv('FILENAME.csv')

(df
 .groupby('COLUMN_NAME')
 .mean()
)
```

1. Import `pandas`
2. Read in csv file as `df`
3. Chain methods
    - `groupby()`
    - `mean()`

Dask dataframes

```
import dask.dataframe as dd

df = dd.read_csv('FILENAME*.csv')

(df
 .groupby('GROUP')
 .mean()
 .compute()
)
```

1. Import `dask.dataframe`
2. Read in csv file(s) as `df`
3. Chain methods
   - `groupby()`
   - `mean()`
   - `compute()`

Persist dask dataframe

```
import dask.dataframe as dd

df = dd.read_csv('FILENAME*.csv')

df = df.persist()

(df
 .groupby('GROUP')
 .mean()
 .compute()
)
```

1. Import `dask.dataframe`
2. Read in csv file(s) as `df`
3. Store `df` on disk with `persist()`
4. Chain methods
   - `groupby()`
   - `mean()`
   - `compute()`

Let's practice using Dask!

CREATING ROBUST WORKFLOWS IN PYTHON

Wrap-up

CREATING ROBUST WORKFLOWS IN PYTHON

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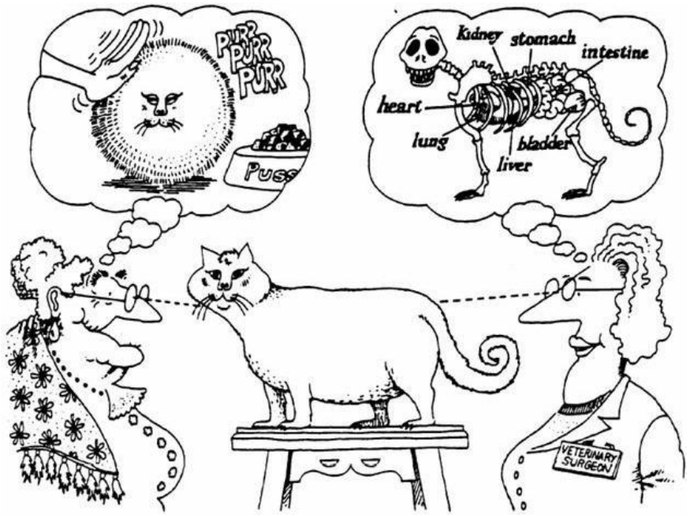
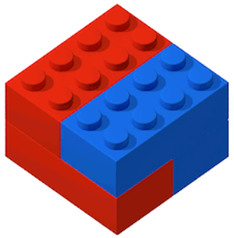
Principles

- DRY (Don't repeat yourself)
- Modularity
- Abstraction



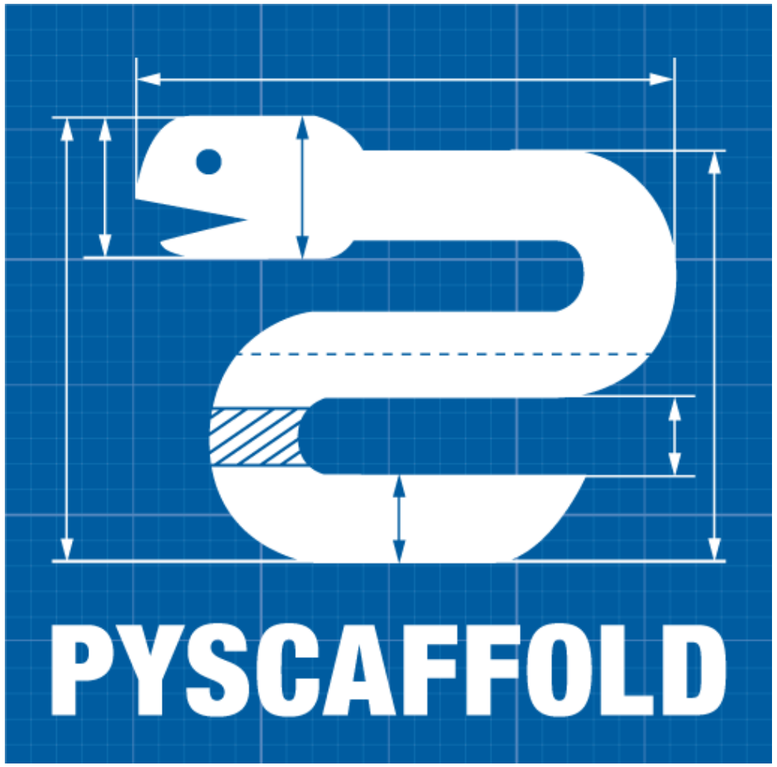
Booch, G. et al. *Object-Oriented Analysis and Design with Applications*. Addison-Wesley, 2007, p. 45.



Documentation

- Includes:
  - Docstrings """
  - Type hints `x: int`

Project templates



- Includes:
  - Docstrings """
  - Type hints `x: int`

Tests

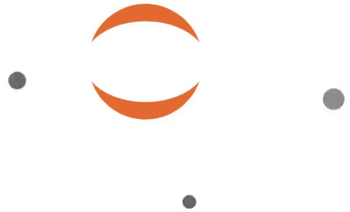
- `pytest` testing framework
  - `pytest.ini` configuration file
    - `doctest` : run docstring examples
    - `mypy` : check types

pytest

: my[py]

Jupyter notebooks

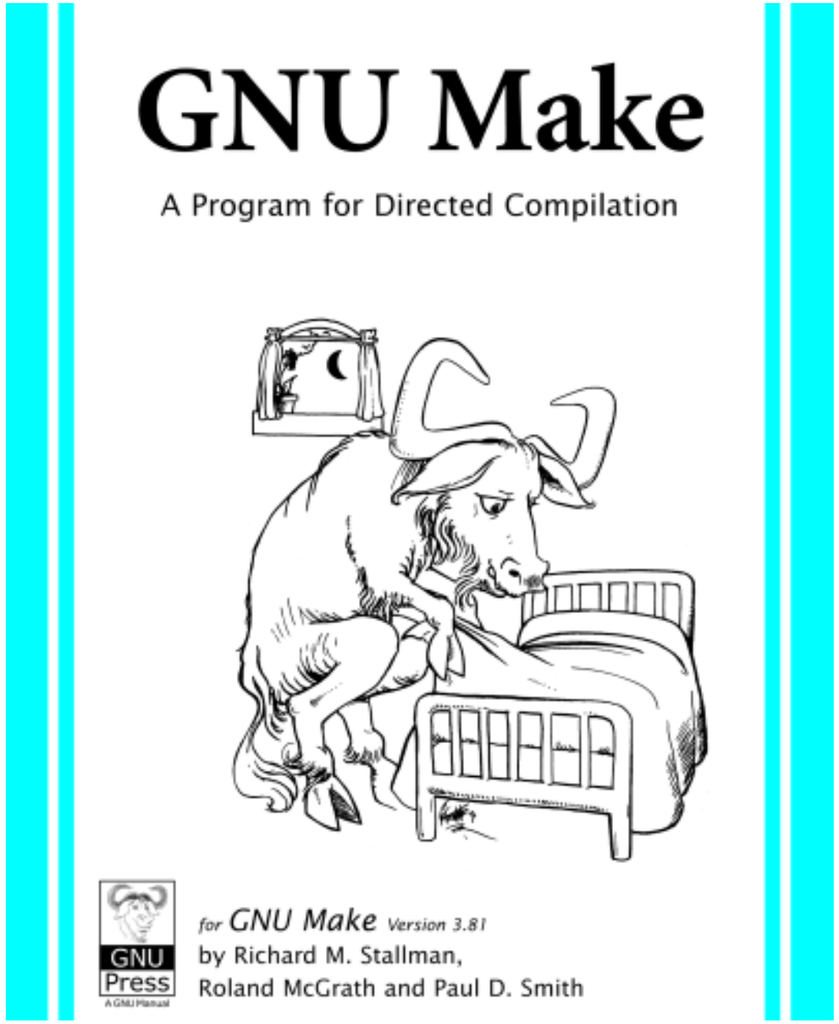
- Create and edit notebooks
  - `nbformat`
- Convert notebooks to other formats
  - `nbconvert`
- Execute notebooks with parameters
  - `papermill`
- Access notebook data
  - `scrapbook`
- Check out `rmarkdown` !



papermill

scrapbook

Pipelines

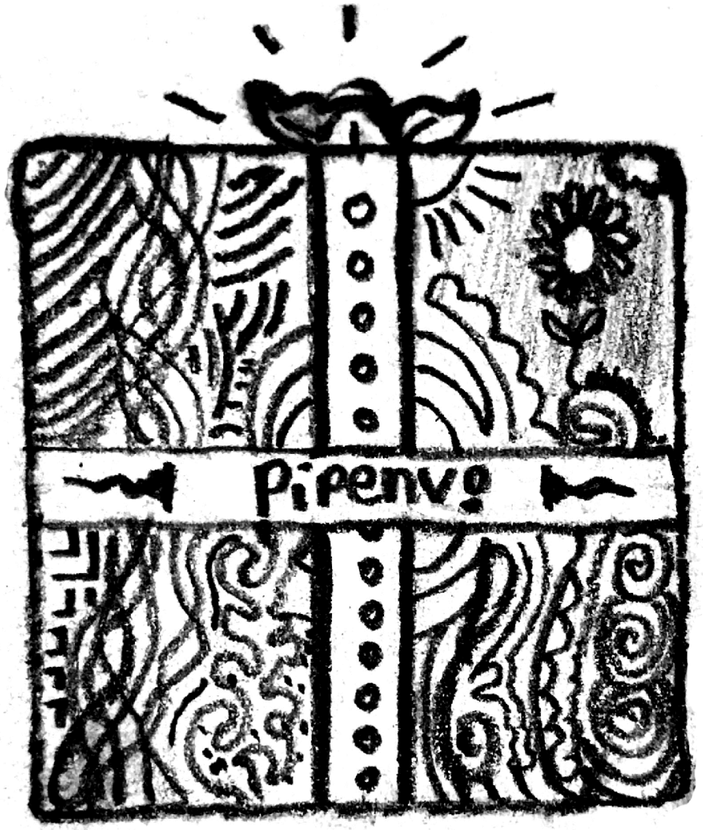


Snakemake

Apache Airflow

DASK

Virtual environments



- Create virtual Python environments
  - `venv` , `virtualenv` , or `pipenv`
- Install Python packages
  - `pip` or `pipenv`
- Not limited to Python

CONDA

Packaging

python™ Package Index

- Package Python code
  - `setuptools`
- Deploy packages to PyPI
  - `twine`

Poetry

Keep learning!

CREATING ROBUST WORKFLOWS IN PYTHON