Command-line interfaces

CREATING ROBUST WORKFLOWS IN PYTHON

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Synergy with the shell

Photo by Adrianna Calvo from Canva

- Command-line interfaces (CLIs)
  - Pass shell arguments to Python scripts

```
python fit_model.py --alpha 0.2
```

  - Avoid using comments as an on/off switch

```
# To retrain the model,
# Uncomment the line below.
# model.fit(x_train, y_train)
```

Build command-line interfaces

- `argparse`
  - Instantiate the `ArgumentParser` class
  - Call the `add_argument()` method
  - Call the `parse_args()` method
  - Arguments are `Namespace` attributes

```
parser = argparse.ArgumentParser()

parser.add_argument('ARGUMENT_NAME')

namespace = parser.parse_args()

namespace.ARGUMENT_NAME
```

- `docopt`
  - Setup up CLI in file docstring
  - Pass `__doc__` to `docopt()`
  - Arguments are dictionary values

```
"""Pass a single argument to FILENAME.
Usage: FILENAME.py ARGUMENT_NAME"""

argument_dict = docopt.docopt(__doc__)
```

Argparse and methods

```
import datetime
from get_namespace import get_namespace

if __name__ == '__main__':
    namespace = get_namespace()
    print(datetime.datetime.now()
          .strftime(namespace.format))
```

```
import argparse as ap

def get_namespace() -> ap.Namespace:
    parser = ap.ArgumentParser()
    parser.add_argument('format')
    return parser.parse_args()
```

```
$ python now.py %H:%M
```

```
8:30
```

Docopt and docstrings

```
import datetime as dt
from get_arg_dict import get_arg_dict

if __name__ == '__main__':
    arg_dict = get_arg_dict()

    print(dt.datetime.now()
          .strftime(arg_dict['FORMAT']))
```

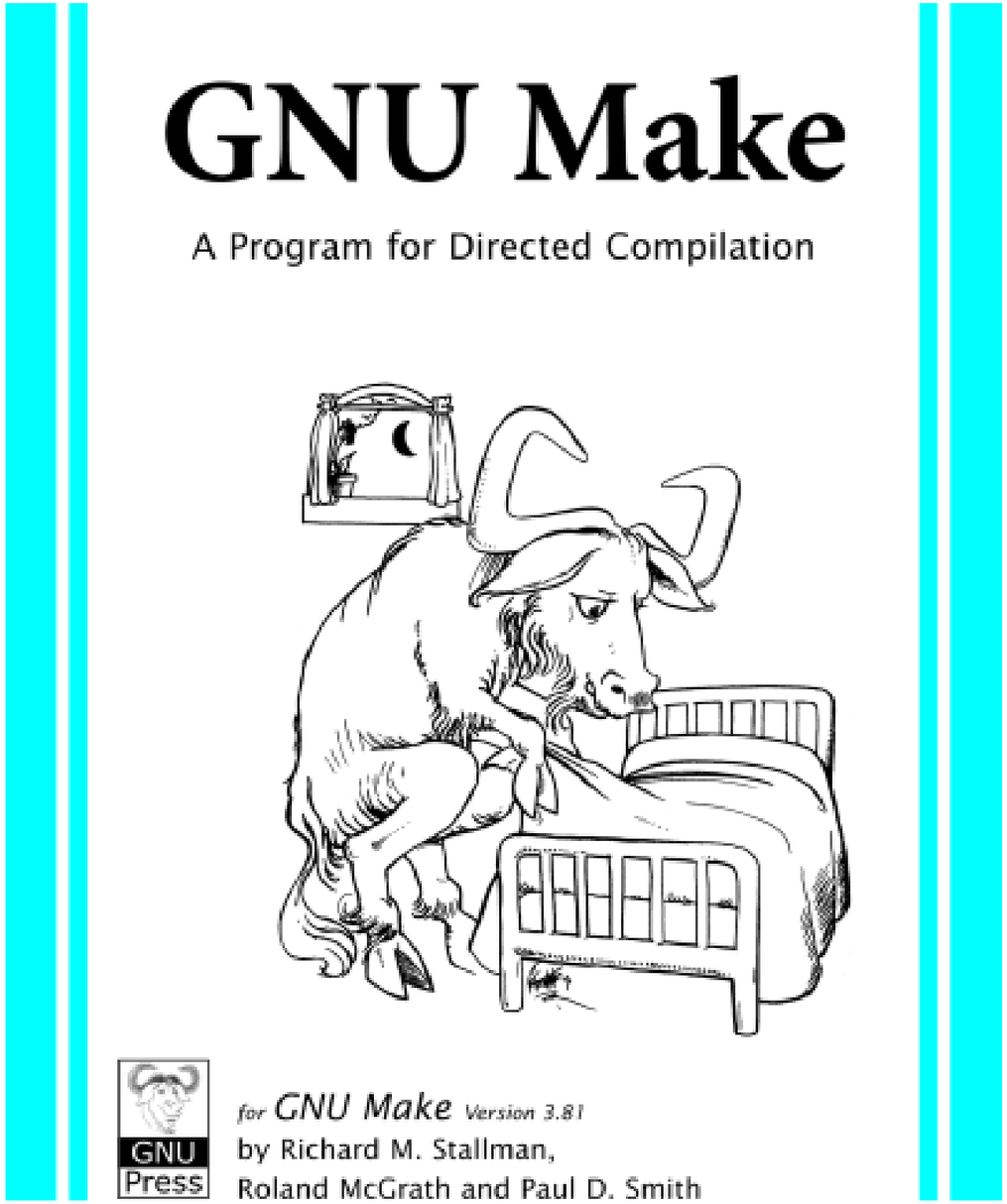
```
"""Get the current date or time.
Usage: now.py FORMAT"""

from typing import Dict
import docopt

def get_arg_dict() -> Dict[str, str]:
    return docopt.docopt(__doc__)
```

```
$ python now.py %B/%d
```

```
March 8
```



Automate execution of

- Shell
  - Commands: `echo hello`
  - Scripts: `bash myscript.sh`
- Python
  - Scripts: `python myscript.py`
  - Modules: `python -m timeit -h`

Make shell command

Makefile:

```
time:
    python now.py %H:%M
```

```
$ make
```

```
python now.py
19:30
```

Makefile structure:

```
TARGET:
    RECIPE
```

Make dependencies

Makefile:

```
time:
    python now.py %H:%M

date:
    python now.py %d/%m

all: date time
```

Makefile structure:

```
TARGET:
    RECIPE

TARGET:
    RECIPE

TARGET: DEPENDENCIES
```

Make all

Makefile:

```
time:
    python now.py %H:%M

date:
    python now.py %m-%d

all: date time
```

```
$ make all
```

```
python now.py %H:%M
19:32
python now.py %d/%m
08/03
```

Command-line interface documentation

Nbless

A Python package for programmatic Jupyter notebook workflows

Star 5

Navigation

Contents:

Quick search

Go

nbuild

Create an unexecuted Jupyter notebook from markdown and code files.

```
nbuild [OPTIONS] IN_FILES...
```

Options

-o, --out_file <out>

Arguments

IN_FILES
Required argument(s)

nbconv

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

```
nbconv [OPTIONS] IN_FILE
```

Options

-e, --exporter <exporter>

-o, --out_file <out>

Arguments

IN_FILE
Required argument

Let's practice building CLIs!

CREATING ROBUST WORKFLOWS IN PYTHON

Git version control

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Git

- Records and manages modifications made to projects
- Prevents lost work or unwanted changes

Basic git workflow

- Make changes in the working directory (`.`)
- Add changes to the index (`./.git/index`)
- Commit changes to version control history (`./.git`)
- A "commit" ~ a milestone

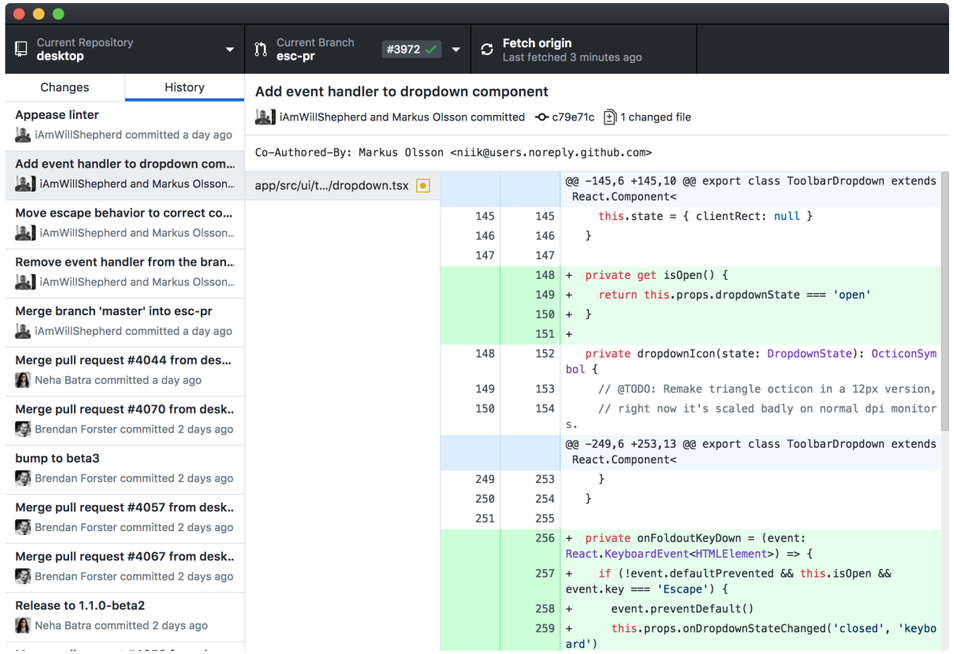
Shell versus API

Use git via

- Graphical User Interface (GUI)
- Command line (shell)
- Application Programming Interface (API)

GitPython (Python interface to git)

- Create a version controlled directory
  - Called a repository
- Add changes to the index
- Commit changes to version control history



Git init

Run `git init` shell command:

```
$ git init
```

```
Initialized empty Git repository in
/Users/USERNAME/REPONAME/.git/
```

Run Python code in a file called `init.py` :

```
import git
print(git.Repo.init())
```

```
$ python init.py
```

```
<git.Repo "/Users/USER/REPO/.git">
```

Make init

Run `git init` using Make:

```
.git/:
    git init
```

```
$ make
```

```
git init
make: '.git/' is up to date.
```

Run `init.py` using Make:

```
.git/:
    python init.py
```

```
$ make
```

```
python init.py
make: '.git/' is up to date.
```

Untracked files

```
import git

repo = git.Repo()
```

```
repo.untracked_files
```

```
['Makefile', 'init.py', 'commit.py']
```

Add untracked files

```
import git

repo = git.Repo()
add_list = repo.untracked_files
if add_list:
    repo.index.add(add_list)
```

```
repo.untracked_files
```

```
[]
```

Commit message

```
import git

repo = git.Repo()
add_list = repo.untracked_files
if add_list:
    repo.index.add(add_list)
    new = f"New files: {', '.join(add_list)}."
```

Commit new files

```
import git

repo = git.Repo()
add_list = repo.untracked_files
if add_list:
    repo.index.add(add_list)
    new = f"New files: {', '.join(add_list)}"
    print(repo.index.commit(new).message)
```

```
$ python commit.py
```

```
New files: Makefile, init.py, commit.py.
```

Diff all files

```
import git

repo = git.Repo()
diff = repo.index.diff(None)
```

Diff modified files

```
import git

repo = git.Repo()
diff = repo.index.diff(None).iter_change_type('M')
edit_list = [file.a_path for file in diff]
```

Commit modified files

```
import git

repo = git.Repo()
diff = repo.index.diff(None).iter_change_type('M')
edit_list = [file.a_path for file in diff]
if edit_list:
    repo.index.add(edit_list)
    modified = f"Modified files: {', '.join(edit_list)}."
    print(repo.index.commit(modified).message)
```

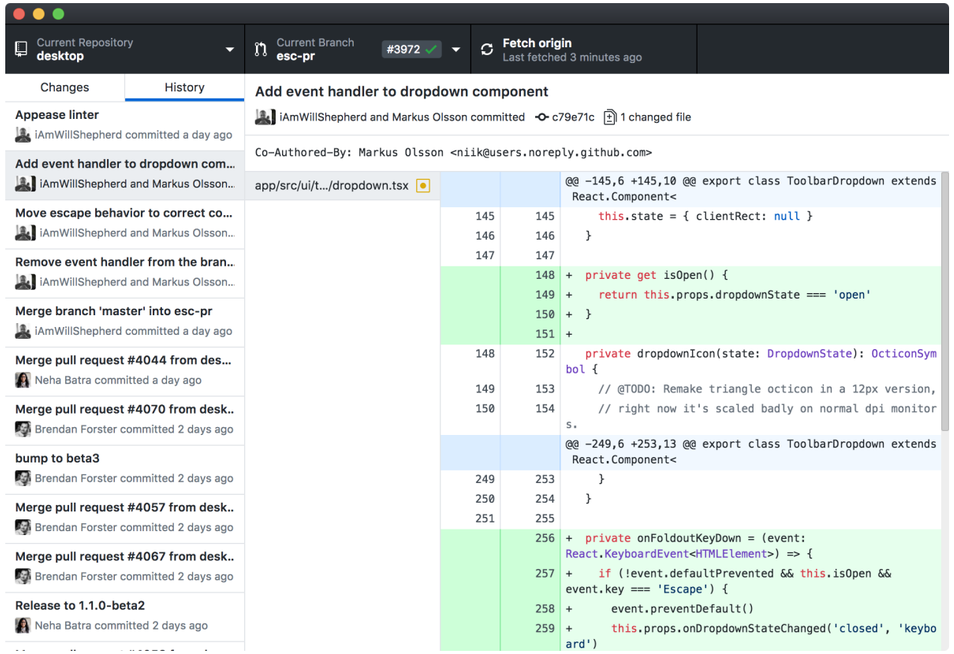
Make commit

```
$ make
```

```
python commit.py
Modified files: Makefile, commit.py.
```

```
$ make
```

```
python commit.py
```



Let's practice automating version control workflows!

CREATING ROBUST WORKFLOWS IN PYTHON

Virtual environments

CREATING ROBUST WORKFLOWS IN PYTHON

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Virtual environments

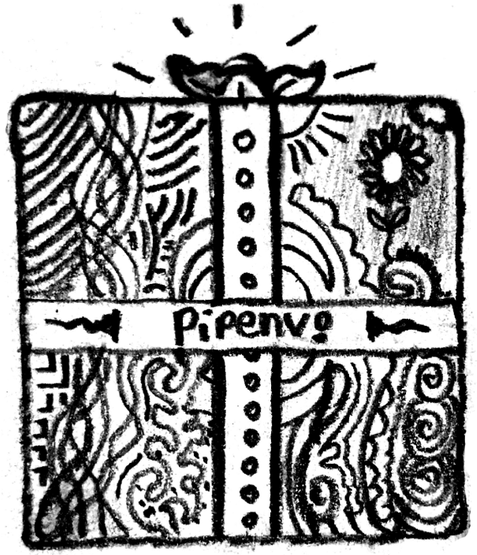
Photo by Katarzyna Modrzejewska from Canva

- Are directories that
  - Contain separate Python installations
  - Facilitate
    - Dependency management
    - Reproducible analysis
    - Python package development

Environment managers

- Tools that create and manage virtual environments

Manager	Superpower
`venv`	Part of the standard library
`virtualenv`	Widely-used
`pipenv`	High-level interface
`conda`	Not only for Python



Dependency managers

Dependency manager
`pip`
`pipenv`
`conda`

- Dependency managers = tools that install and manage dependencies
- `venv` and `virtualenv` use `pip`
- `pipenv` and `conda` manage dependencies and environments

Dependency manager files

Dependency manager	Dependency management file
`pip`	`requirements.txt`
`pipenv`	`Pipfile`
`conda`	`environment.yml`

- Dependency names and versions can be
  - Specified in dependency management files
- All three dependency managers use `requirements.txt`
  - Exact (`jupyter == 4.4.0`)
  - Minimum (`python >= 3.6.0`)

Install dependencies

Create environment

```
$ python -m venv .venv
```

Option 1: Activate environment before `pip install`

```
$ source .venv/bin/activate
$ pip install --requirement requirements.txt
```

Option 2: Use path to virtual environment Python to `pip install`

```
$ .venv/bin/python -m pip install -r requirements.txt
```

Make venv

1. Create a virtual environment in `.venv`
2. Install the dependencies in the virtual environment
3. Update the "Last Modified" time for the target (.venv/bin/activate)

```
.venv:
    python -m venv .venv

.venv/bin/activate: .venv requirements.txt
    .venv/bin/python -m pip install -r requirements.txt
    touch .venv/bin/activate
```

Make test

- Run all tests in a virtual environment
- Avoid failed tests due to missing or outdated project dependencies

```
.venv:
    python -m venv .venv
.venv/bin/activate: .venv requirements.txt
    .venv/bin/python -m pip install -r requirements.txt
    touch .venv/bin/activate

test: .venv/bin/activate
    .venv/bin/python -m pytest src tests
```

Venv module

```
import venv
venv.create('.venv')
```

1. Create a `venv` environment
    - With `venv` API
        - `create()` function

Subprocess module

```
import subprocess

cp = subprocess.run(
    ['.venv/bin/python', '-m',
     'pip', 'list'], stdout=-1
    )

print(cp.stdout.decode())
```

```
Package                       Version
----------------------------- ----------
PACKAGE_NAME                  0.0.1
...
```

1. Create a `venv` environment
   - With `venv` API
     - `create()` function
2. List packages
   - With `pip` and `subprocess`
     - `subprocess.run()` function
       - Returns `CompletedProcess`
       - `stdout` or `capture_output`
     - `pip list`

Package information

```
cp = subprocess.run(['python', '-m', 'pip', 'show', 'pandas'], stdout=-1)


print(cp.stdout.decode())
```

```
Name: pandas
Version: 0.24.1
Summary: Powerful data structures for data analysis, time series, and statistics
Home-page: http://pandas.pydata.org
...
```

Summary

Environment manager	Dependency manager	Dependency management file	Environment manager Superpower
`venv`	`pip`	`requirements.txt`	Part of the standard library

- `venv` API:
  - `create()`
- Use `subprocess.run()`
  - To run shell commands, such as
    - `pip install`
    - `pip list`
    - `pip show`

Summary

Environment manager	Dependency manager	Dependency management file	Environment manager Superpower
`venv`	`pip`	`requirements.txt`	Part of the standard library
`virtualenv`	`pip`	`requirements.txt`	Widely-used
`pipenv`	`pipenv`	`Pipfile`	High-level interface
`conda`	`conda`	`environment.yml`	Not only for Python

Let's practice using virtual environments!

CREATING ROBUST WORKFLOWS IN PYTHON

Persistence and packaging

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Persistence in a pipeline

- Save files throughout a data analysis pipeline
  - Processed data
  - Plots
  - Trained models

  - Each file should be
    - A target in the project's `Makefile`
    - The sole responsibility of a script (`plot1.py -> plot1.png`)

Save data with pandas

Format	Writer
CSV	`to_csv()`
JSON	`to_json()`
Excel	`to_excel()`
Pickle	`to_pickle()`

```
# Make simple dataframe
df = pd.DataFrame({
    'Evens': range(0, 5, 2),
    'Odds': range(1, 6, 2)
})

# Pickle dataframe
df.to_pickle('numbers.pkl')
```

Read data with pandas

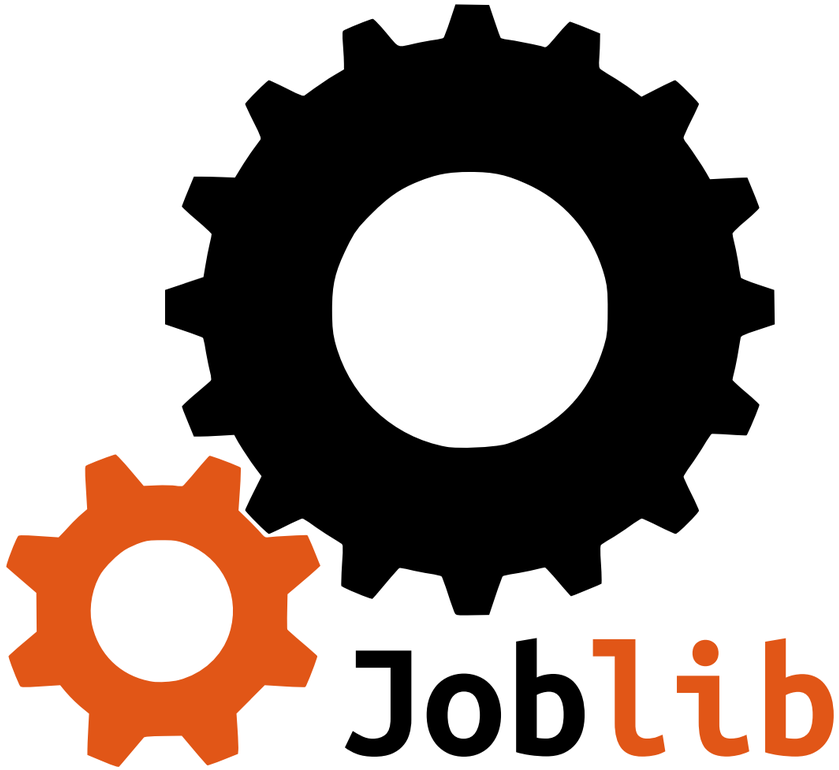
Format	Writer	Reader
CSV	`to_csv()`	`read_csv()`
JSON	`to_json()`	`read_json()`
Excel	`to_excel()`	`read_excel()`
Pickle	`to_pickle()`	`read_pickle()`

```
# Unpickle dataframe
pd.read_pickle('numbers.pkl')
```

```
   Evens  Odds
0      0     1
1      2     3
2      4     5
```

Why pickle?

- Built into `pandas`
  - `df.to_pickle('df.pkl')`
- Standard library includes `pickle` module
- `joblib` is optimized for `scikit-learn`
- Fast and memory efficient
- Works for many types of Python objects
- Supports on-the-fly (de)compression
  - `df.to_pickle('df.pkl.xz')`



Pickle models

```
import joblib
from sklearn import datasets, model_selection, neighbors

diabetes = datasets.load_diabetes()

x_train, x_test, y_train, y_test = model_selection.train_test_split(
    diabetes.data, diabetes.target, test_size=0.33, random_state=42)

knn = neighbors.KNeighborsRegressor().fit(x_train, y_train)

# Pickle the k-nearest neighbors model with joblib
joblib.dump(knn, 'knn.pkl')
```

Why package code?

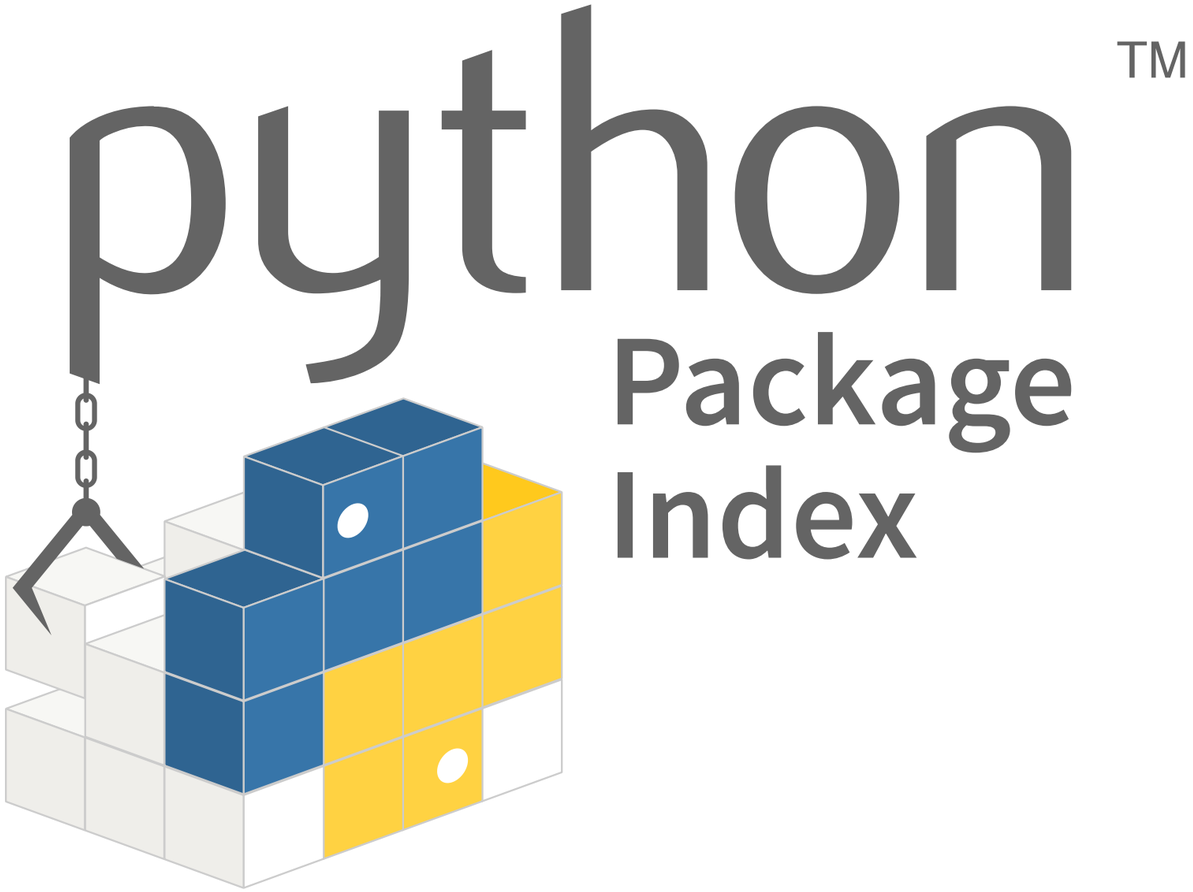
- Everything in one place
  - code
  - documentation
  - data files
- Easy to share
  - Install from Python Package Index (PyPI):

    ```
    pip install mypkg
    ```

  - Install from git repository:

    ```
    pip install git+REPO_URL
    ```

  - Install local package: `pip install .`



Package pickled objects

```
setuptools.setup(
    name="PACKAGE_NAME",
    version="MAJOR.MINOR.PATCH",
    description="A minimal example of packaging pickled data and models.",
    packages=setuptools.find_packages("src"),
    package_dir={"": "src"},
    # Include files in the data and models directories
    package_data={"": ["data/*", "models/*"]},
)
```

Install local package

```
.venv:
    python -m venv .venv

.venv/bin/activate: requirements.txt
    .venv/bin/python3 -m pip install --requirement requirements.txt
    touch .venv/bin/activate
```

`requirements.txt` :

```
--editable .
```

Automated release

- Create a Python Package Index (PyPI) account:

https://pypi.org/account/register/

```
clean:
    rm -rf dist/
dist: clean
    python setup.py sdist bdist_wheel
release: dist
    twine upload dist/*
```

```
$ make release
```

```
...
Uploading distributions to https://...
Uploading ...-0.0.8-py3-none-any.whl
100%|???????????| 22.7k/22.7k...
Uploading ...-0.0.8.tar.gz
100%|???????????| 32.3k/32.3k...
```

Access package data

```
import pkgutil
from pickle import loads

loads(pkgutil.get_data(
    'PACKAGE_NAME',
    'data/numbers.pkl'
    ))
```

```
   Evens  Odds
0      0     1
1      2     3
2      4     5
```

```
??? setup.py
??? src
    ??? PACKAGE_NAME
        ??? __init__.py
        ??? data
        ?   ??? data.pkl
        ??? MODULE.py
```

Access package model

```
import pkg_resources
from joblib import load

load(pkg_resources.resource_filename(
    'PACKAGE_NAME',
    'models/knn.pkl'
    ))
```

```
KNeighborsRegressor(algorithm='auto',
leaf_size=30, metric='minkowski',
metric_params=None, n_jobs=None,
n_neighbors=5, p=2, weights='uniform')
```

```
??? setup.py
??? src
    ??? PACKAGE_NAME
        ??? __init__.py
        ??? models
        ?   ??? knn.pkl
        ??? MODULE.py
```

Let's practice pickling!

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