How to Package and Publish Your Python Codes

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Download Workshop Codes

https://github.com/fjying/PythonPackageWorkshop

1. Open the Repo Link
2. Click the Green Code Button on the Top Right of the Page
3. Click Download Zip to Download the Repo
4. Zip the Download Folder
5. Rename the Folder as PythonPackageWorkshop
6. Put the Folder on the appropriate place

Outline of Workshop

1. Virtual Environment of Packages
2. Build Python Package
3. Create an Automatic Test of Package Codes
4. Documentation Files for Package Publishing
5. Package Versioning
6. Publish Package to TestPyPI or PyPI
7. Create Package Citation

Virtual Environment of Packages

Packages and Virtual Environment

Suppose we just open the terminal and enter

pip install <package>,

the package would be installed on the base environment by default.

What is the main concern with this?

Package Versions Conflict

For instance, when we use pip install torch to install package torch, the latest version of torch would be installed. However, other packages may require the use of older versions of torch as some functions in the older versions are no longer supported by the latest version.

Package Versions Conflict

One Python environment could only support one version of the particular python package. It is not possible to run two different versions of the same package under the same environment. Thus, if we want to use the older version of torch and other packages only compatible with the older version, we need to create another Python environment to install and use them.

Virtual Environment to Manage Different Versions of Packages

Specifically, we could create **different virtual environments** so the **same package of different versions** could be installed **separately inside different environments.**

When we want to use the package of specific version, we could activate the environment related to that package.

Use Python to Create Virtual Environment

```
mkdir ~/packageenvs

cd ~/packageenvs

python -m venv <env_name>

cd <env_name>

source <env_name>/bin/activate

deactivate
```

Use Conda to Create Virtual Environment

This requires the installation of Anaconda.

```
conda create -n <env_name> <python=3.X>

conda activate <env_name>

conda deactivate
```

Set Up Virtual Envrionment of the Workshop

Conda:

```
conda create -n pythonpackageworkshop python=3.9

conda activate pythonpackageworkshop
```

Python:

```
mkdir ~/packageenvs

cd ~/packageenvs

python -m venv pythonpackageworkshop

source pythonpackageworkshop/bin/activate
```

How to Build a Python Package?

The Necessary Directory Structure for a Package

src directory: contain source codes

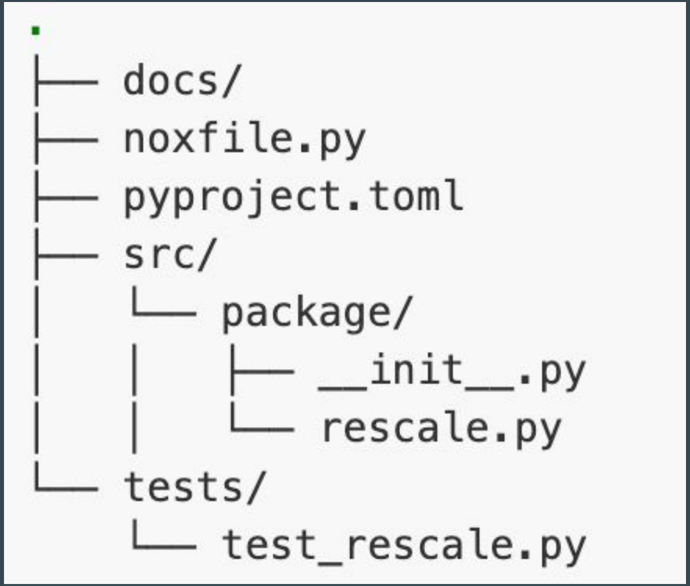
tests directory: tests codes

noxfile.py: main file to run test codes

docs directory: package usage documentation

pyproject.toml: contains the metadata to build and install a package

Need to put __init__.py inside each subdirectory of src to create subpackages.



```
.
├── docs/
├── noxfile.py
├── pyproject.toml
├── src/
│   └── package/
│       ├── __init__.py
│       └── rescale.py
└── tests/
    └── test_rescale.py
```

Pyproject.toml

Contains Package Metadata for Building a Package and Publishing It

Two Categories of Metadata:

Informational (like Package Name, Author)

Functional (like Requirements to install all necessary python packages to run codes)

See toml file for the details

Build the First Python Package

1. Change Directory to the Repo Folder

```
cd <.../PythonPackageWorkshop>
```

2. Build and Install the Package named packageworkshop

```
pip install -e .
```

3. Run Test Codes below to See If The Package Works

```
python

import numpy as np

from packageworkshop.rescale import rescale

rescale(np.linspace(0, 100, 5))
```

Automatic Test of Package Codes

Automatic Test

Test Function: tests/test_rescale.py

Test Session: noxfile.py

Terminal:

cd to the repo folder: <…/PythonPackageWorkshop>

nox

Package Files Documentation

README

A README is a plain text file that sits at the top level of your package and provides general information about your package.

A README should at least contain information below:

The name of the software package

A brief description of what the software does

Installation instructions

A brief usage example

The type of software license (with more information in a separate LICENSE file, described next)

(See README.md on the codes repo and README on Github Page)

LICENSE

Common Licenses Used by Research Software:

MIT License, BSD 3-Clause License, Apache License 2.0

Please do not write your own license!

Could create a license from Github Repo:

https://docs.github.com/en/communities/setting-up-your-project-for-healthy-contributions/adding-a-license-to-a-repository

CHANGELOG

In the CHANGELOG file, you should record major changes to the package made since the last released version. Then, when you decide to release a new version, you add a new section to the file above this list of changes.

There are 6 types of changes:

Added for new features,

Changed for changes in existing functionality,

Deprecated for soon-to-be removed features,

Removed for now-removed features,

Fixed for any bug fixes, and

Security in case of vulnerabilities.

Package Versioning

Three Types of Package Versioning

SemVer: Semantic Versioning

ZeroVer: Modified Semantic Versioning Starting with 0

CalVer: Calendar Based Versioning

SemVer: Semantic Versioning

SemVer: Three numbers in a Semantic Versioning; <major>.<minor>.<patch>

If the package changes in a breaking way, the major number must be incremented.

If the package has more features but the existing one still works fine, the minor number must be incremented.

If only bugs are fixed, the patch number must be incremented.

For instance:

Package version upgrades from 1.0.0 to 2.0.0: Users definitely need to check the latest version.

Package version upgrades from 1.0.0 to 1.0.1: Users doesn't need to check the latest version. If something is broken on current use case, users may check the latest version to see if the use case could be fixed.

ZeroVer: Modified Semantic Versioning

Exactly the same as Semantic Versioning

Except that the lowest package version starts with 0.X.X.

The zero version (0.X.X) means that users could use this zero version stably, but there are huge parts of codes which would be rewritten and huge features would be added. This means that this package is still in a development phase.

CalVer: Calendar based versioning

This sets the version number based on the release date. There are several variations. Some projects literally place the date (two or four digit year followed by month then day) as a version number, and some project blend a little bit of semantic versioning by making the second or third digit SemVer-like.

For instance:

22.04 version indicates that the package was released on April, 2022.

23.1.0 version indicates that the package was released on January, 2023. 0 indicates that this package version is a major version without any patches.

Semver versus Calver: Which one should we use?

For most packages especially research software packages, we should use Semver or ZeroVer.

If a package needs to talk to many external services regarding its version released date automatically, we should use Calver. For instance, several core Python packaging projects (like pip, packaging, and virtualenv) use CalVer.

Publish Package on TestPyPI or PyPI

Do you need to publish a package to PyPI？

Not every package needs to go on PyPI. Users can pip install the package directly from Git by following the same commands we have done before. Also, if apackage is used for the front-end development such as building a web application, such package does not need to be on PyPI.

Publish Package to TestPyPI

Before publishing any package officially to PyPI, we should always do a test drive by publishing it to TestPyPI. The steps of publishing packages are exactly the same between TestPyPI and PyPI.

Two Ways to Do It:

(1) Manual

(2) Github Action

Usually, the manual way is preferred because we want to manually check if package codes work as expected before publishing it instead of letting Github automatically publish the package.

Set Up TestPyPI Account and Make an API Token

1. Register account at https://test.pypi.org/

2. Verify your email address (check your account settings)

3. Make an API Token:

Under your user name, click account settings, go to the API tokens section and select "Add API token"

3. Add API Token to Local Computer so we don't need to enter username and password whenever we want to publish a package to TestPyPI

Create the file .pypirc inside the home directory

Open the file using vim or any text editor

```
vim ~/.pypirc
```

Inside the file:

```
[testpypi]

username = __token__

password =
<api_token_generated_in_the_previous_step>
```

Manually Publish Package to TestPyPI

Note that the package name needs to be unique across TestPyPI

Need to change packagename in the pyproject.toml first if you want to publish a package on your own

1. Install All Necessary Packages for Publishing

```
python -m pip install build twine
```

2. Build Your Own Package

```
python -m build
```

3. Publish Package to Testpypi

```
twine upload -r testpypi dist/*
```

See Published Package and Install It from TestPyPI

See Package on TestPyPI Package

https://test.pypi.org/project/packageworkshop/

Install Package from TestPyPI

```
pip install -i https://test.pypi.org/simple/packageworkshop
```

Manually Publish a Package to PyPI

Exactly the same as publishing it to TestPyPI

Need to make sure your package is finalized before publishing it to PyPI

```
python -m build
twine upload dist/*
```

(instead of twine upload -r testpypi dist/*)

Publish A New Version of Package to TestPyPI/PyPI

- Remove Previously Built Files on dist Folder
  - rm -r dist
- Change Version
  - Change version in the pyproject.toml if it is fixed
  - Change version in the version global variable if it is not fixed
- Rebuild Package
  - python -m build
- Upload Package to TestPyPI/PyPI
  - twine upload -r testpypi dist/*
  - twine upload -r dist/*
  - twine upload packageworkshop-2.0.0-py3-none-any.whl
  - Options: --verbose
- View Release History on TestPyPI/PyPI
  - https://test.pypi.org/project/packageworkshop/#history

Advanced: Use Github CI to Automatically Publish Python Packages

Use Github Action to Automate the Process of Publishing package:

Whenever we make a new release on Github, the corresponding release would be published to TestPyPI or PyPI automatically.

1. Need to fill out the form on the following link:

https://test.pypi.org/manage/account/publishing/

2. Create PythonPackageWorkshop/.github/workflows/publishtopypi.yml

(In general, not applicable for daily use case)

Make Package Citable

Zenodo for a Software Citation

1. Log into Zenodo by using **Sign In with Github** :

https://zenodo.org/

2. Under Username on the top right, Click Github Section

3. Follow the instructions: Zenodo would automatically update the citation page when the new version is released on Github

4. Add a DOI badge to README

On Zenodo, click on the badge which opens up the markdown of badge.

Put the markdown of the badge at the top of README on Github

Could go to the citation page by clicking on the Badge

ZENODO Citation Page of Software

https://zenodo.org/records/10516336

Citation of the software with the unique DOI number in different styles is on the page.

Create CITATION.cff

CITATION.cff file on the Github Repo helps people to know how to cite your package.

Should not create CITATION.cff file manually

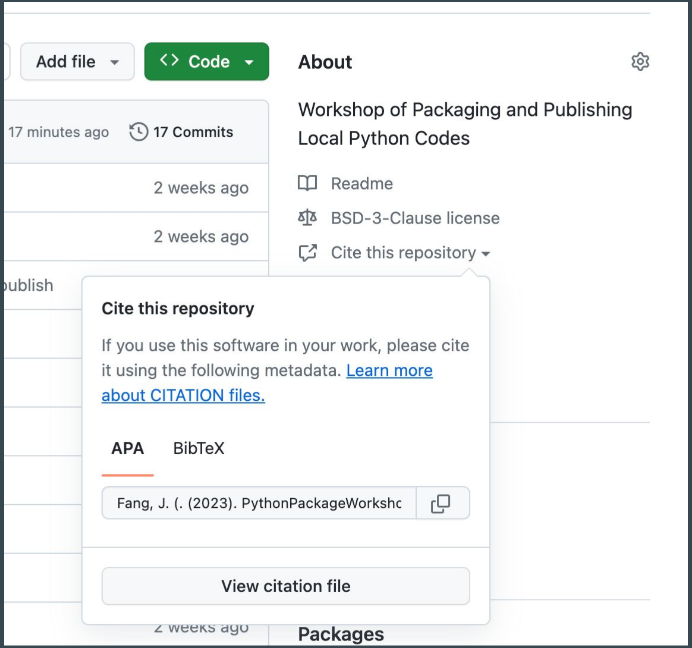
Generate CITATION.cff file using the below link:

https://citation-file-format.github.io/cff-initializer-javascript/#/

See CITATION.cff file on the repo for details

Push CITATION.cff file to Github

After pushing the CITATION.cff file to Github, people could easily cite the package by visiting the github repo:



Workshop of Packaging and Publishing Local Python Codes

Readme

BSD-3-Clause license

Cite this repository

Cite this repository

If you use this software in your work, please cite it using the following metadata. Learn more about CITATION files.

APA | BibTeX

Fang, J. (. (2023). PythonPackageWorkshc

View citation file