HOW TO PACKAGE AND RELEASE YOUR CODE

Bron Reichardt Chu

Durham University

WHY?

- Reproducibility
- Robustness
- Versatility
- All publicly funded research should be open-source

OPTIONS

Minimal:

release it on your webpage

GADGET-2 released this way

Unclear how to cite

Lack of transparency – no change-log

Can be interpreted as less trustworthy

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Normal:

release on GitHub

Repo + license -> create a release

Get a Zenodo DOI -> permanent link, citeable

Repeat for every new version

Shows more software competence – may be interpreted as more trustworthy

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Maximal:

software paper (e.g. JOSS)

Requires documentation

Add to a package manager (conda and/or PyPI)

Testing

Takes time, which is time not spent on research

CHECKLIST: MINIMAL RELEASE

- ❑ A license
- ❑ A clear readme
- ❑ Documentation
  - o Examples
- ❑ A clear link on your website/in your paper

LICENSES

Grant specific permissions to the user and impose restrictions on how the code can be used, copied and distributed.

A license protects your intellectual property rights.

It also lets other people use your code, which would otherwise be protected by copyright laws.

choosealicense.com

Choose an open source license

An open source license protects contributors and users. Businesses and savvy developers won't touch a project without this protection.

Which of the following best describes your situation?

I need to work in a community.

Use the license preferred by the community you're contributing to or depending on. Your project will fit right in.

If you have a dependency that doesn't have a license, ask its maintainers to add a license.

I want it simple and permissive.

The MIT License is short and to the point. It lets people do almost anything they want with your project, like making and distributing closed source versions.

Babel, .NET, and Rails use the MIT License.

I care about sharing improvements.

The GNU GPLv3 also lets people do almost anything they want with your project, *except* distributing closed source versions.

Ansible, Bash, and GIMP use the GNU GPLv3.

LICENSES

>> For more information:

>> On the legalities of open-source code: https://opensource.guide/legal/

>> On how to choose a license: https://choosealicense.com/

>> On how to add a license to your git repo: https://docs.github.com/en/repositories/managing-your-repositorys-settings-and-features/customizing-your-repository/licensing-a-repository

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README

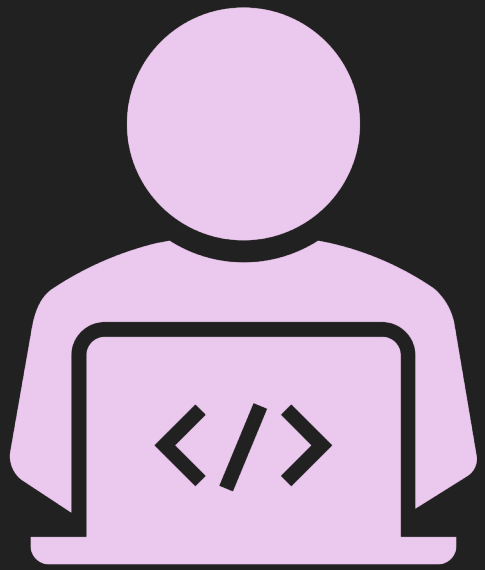
>> Brief description of your code

  >> What does it do?

  >> How does it do that?

>> Installation instructions

>> Brief example of usage



>> Python packaging user guide:
https://packaging.python.org/en/latest/overview/

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CHECKLIST: GITHUB RELEASE

- ☑ A license
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- ☐ Documentation
  - Examples
  - API Documentation
  - Sphinx
- ☐ Tag your release version
- ☐ A persistent identifier: Zenodo

README

>> Brief description of your code

>> What does it do?

>> How does it do that?

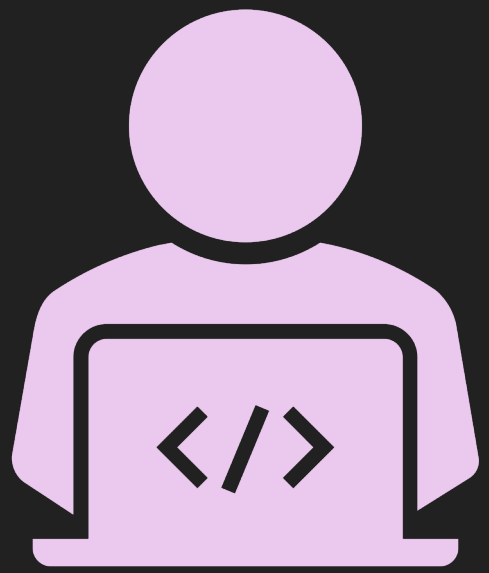
>> Installation instructions

>> Brief example of usage

>> Requirements (what do you need in your environment?)

>> How to contribute

>> How to cite your code



README

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   >> What does it do?
   >> How does it do that?
>> Installation instructions
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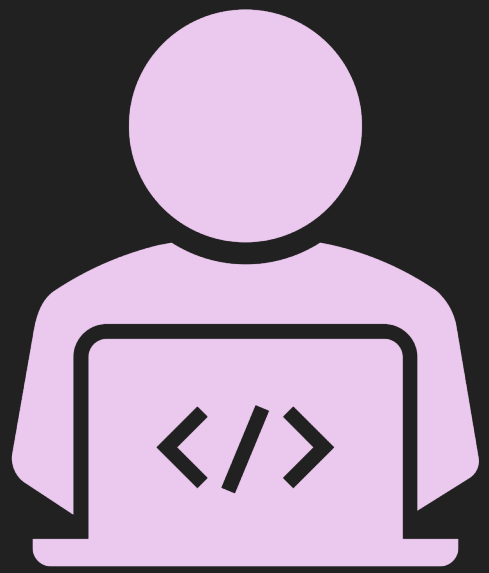
>> Requirements (what do you need in your environment?)
>> How to contribute
>> How to cite your code

This can be as simple as **git clone** instructions



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SPHINX

```
MyProject/
   |--src/
      |-- __init__.py
      |-- module1.py
   |--tests/
      |--__init__.py
      |--test_module1.py
   |--docs/
   |--examples/
      |--tutorial.ipynb
   |--.gitignore
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>> To install:

- `$ pip install -U sphinx`
- `$ conda install sphinx`

- `$ pip install myst-parser`
- `$ conda install -c conda-forge myst-parser`

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```

>> To setup, from within your docs folder:

- `$ sphinx-quickstart`

>> Separate source and build directories (y/n) [n]: <hit enter>

>> Project name: <your project name>

>> Author name(s): <your name>

>> Project release []: 0.1

>> Project language [en]: <hit enter>

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>> To enable markdown, in conf.py:

- extensions = ["myst_parser"]

https://myst-parser.readthedocs.io/en/v0.16.1/sphinx/intro.html

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>> Build from within source/:

- `$ sphinx-build . _build`

>> Tip: Creates _build folder, which you should add to your .gitignore so that it is not added to your Git repo

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```

>> To see your website locally:

Linux:

- `$ xdg-open _build/index.html`

macOS:

- `$ open _build/index.html`

Windows:

- `$ start _build/index.html`

SPHINX

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```

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   |--examples/
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```

>> Auto-generate documentation – in the conf.py file:

- `extensions = ["myst_parser", "autodoc2"]`
- `autodoc2_packages = ["multiply.py"]`

>> In the index.rst file:

- `.. toctree::`
- `  :maxdepth: 2`
- `  :caption: Contents:`
- `  apidocs/index`

https://sphinx-autodoc2.readthedocs.io/en/latest/quickstart.html

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SPHINX

>> Host your docs on a GitHub pages website:

https://coderefinery.github.io/documentation/gh_workflow/

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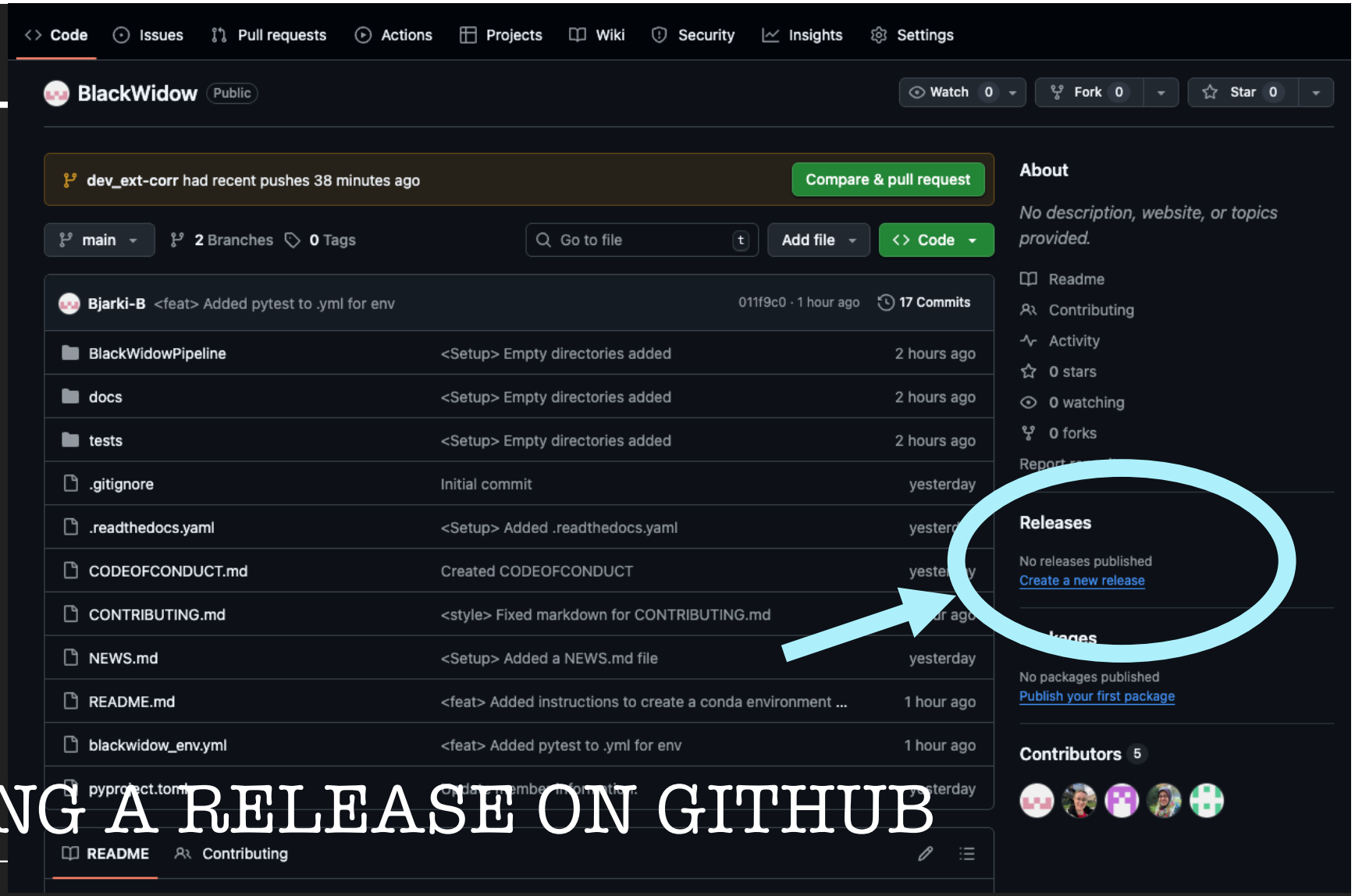
- ☐ Tag your release version
- ☐ A persistent identifier: Zenodo

TAGGING A RELEASE ON GITHUB



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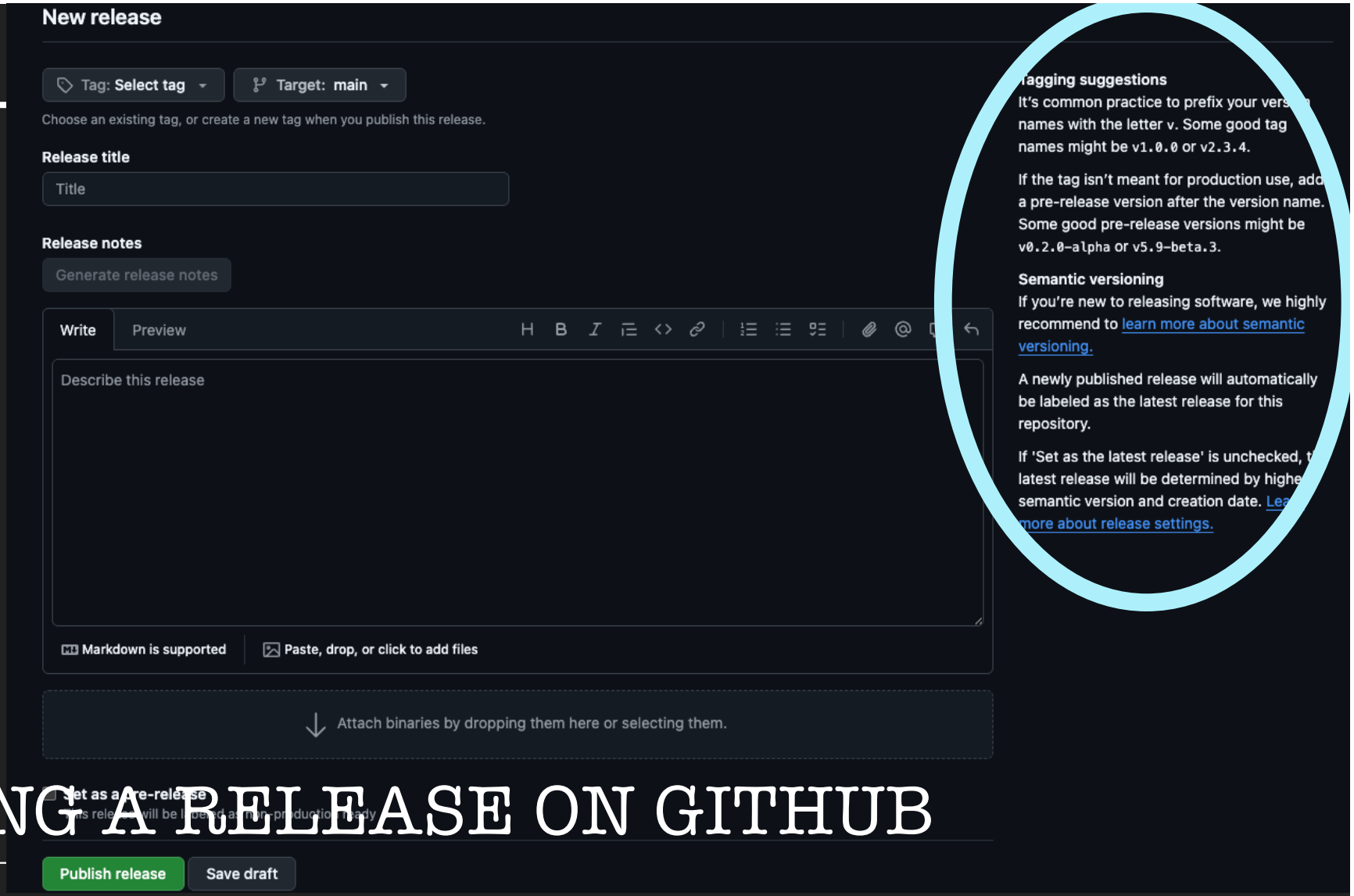

TAGGING A RELEASE ON GITHUB

MAJOR.MINOR.PATCH

>> MAJOR version when you make incompatible API changes
>> MINOR version when you add functionality in a backward compatible manner
>> PATCH version when you make backward compatible bug fixes

For more on semantic versioning: https://semver.org/

For more on how to create a release: https://docs.github.com/en/repositories/releasing-projects-on-github/managing-releases-in-a-repository

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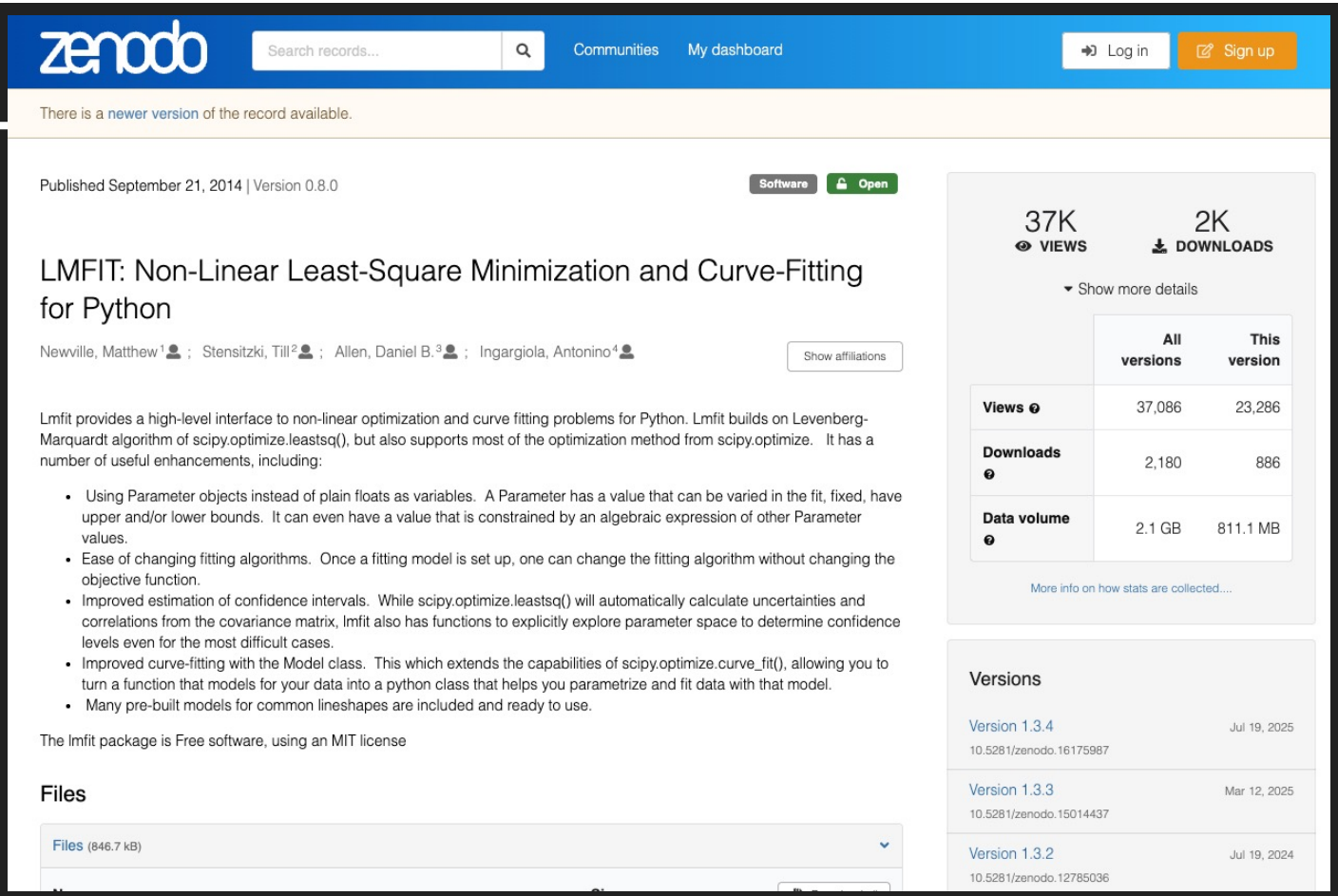
ZENODO

DOI: Digital Object Identifier

Log in with GitHub



https://docs.github.com/en/repositories/archiving-a-github-repository/referencing-and-citing-content

CHECKLIST: JOSS RELEASE

- ☑ A license
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- ☑ Documentation
  - o API Documentation
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  - o Sphinx
- ☐ Ability to pip install your code
- ☐ Software paper

CHECKLIST: JOSS RELEASE

>> How to make your package pip installable: https://packaging.python.org/en/latest/tutorials/packaging-projects/

- ☑ A license
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  - o Sphinx
- ☐ Ability to pip install your code
- ☐ Software paper

JOSS REQUIREMENTS

Functionality

- **Installation:** Does installation proceed as outlined in the documentation?
- **Functionality:** Have the functional claims of the software been confirmed?
- **Performance:** If there are any performance claims of the software, have they been confirmed? (If there are no claims, please check off this item.)

Documentation

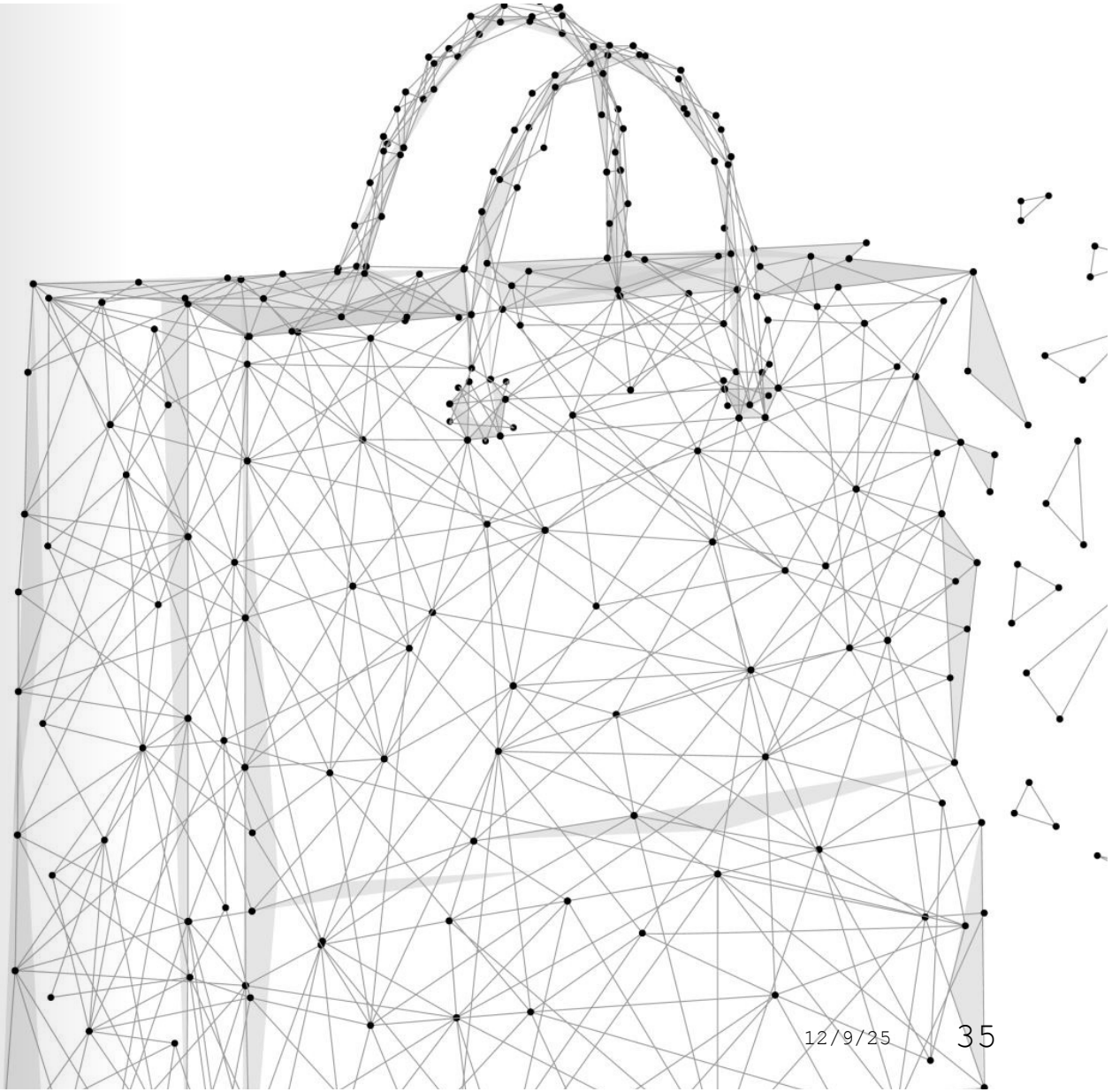
- **A statement of need:** Do the authors clearly state what problems the software is designed to solve and who the target audience is?
- **Installation instructions:** Is there a clearly-stated list of dependencies? Ideally these should be handled with an automated package management solution.
- **Example usage:** Do the authors include examples of how to use the software (ideally to solve real-world analysis problems).
- **Functionality documentation:** Is the core functionality of the software documented to a satisfactory level (e.g., API method documentation)?
- **Automated tests:** Are there automated tests or manual steps described so that the functionality of the software can be verified?
- **Community guidelines:** Are there clear guidelines for third parties wishing to 1) Contribute to the software 2) Report issues or problems with the software 3) Seek support

Software paper

- **Summary:** Has a clear description of the high-level functionality and purpose of the software for a diverse, non-specialist audience been provided?
- **A statement of need:** Does the paper have a section titled 'Statement of need' that clearly states what problems the software is designed to solve, who the target audience is, and its relation to other work?
- **State of the field:** Do the authors describe how this software compares to other commonly-used packages?
- **Quality of writing:** Is the paper well written (i.e., it does not require editing for structure, language, or writing quality)?
- **References:** Is the list of references complete, and is everything cited appropriately that should be cited (e.g., papers, datasets, software)? Do references in the text use the proper citation syntax?

SUMMARY

- Easily accessible
- Clear installation and usage instructions
- Clear how to cite it



MORE RESOURCES

>> Making good README files:

https://www.makeareadme.com/

>> Convert from markdown to rst:

https://pandoc.org/

>> How to document your research software:

https://coderefinery.github.io/documentation/wishlist/

>> Python packaging user guide:

https://packaging.python.org/en/latest/overview/

>> Sphinx documentation:

https://www.sphinx-doc.org/en/master/usage/quickstart.html

>> Connecting Sphinx documentation to a GitHub Pages website:

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>> Connect Zenodo DOI to GitHub release:

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>> Make your package conda installable:

https://docs.conda.io/projects/conda-build/en/stable/user-guide/tutorials/building-conda-packages.html

>> GitHub's instructions for building and testing Python packages:

https://docs.github.com/en/actions/tutorials/build-and-test-code/python

>> Run your tests automatically every time you push changes to the repo:

https://coderefinery.github.io/testing/continuous-integration/

>> Submitting a paper to JOSS:

https://joss.readthedocs.io/en/latest/submitting.html