

Lab Handbook

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Introduction

Lab handbook of the [Machine and Human Intelligence group](#) at the University of Helsinki.

Part I

Python tools

1 How to publish Python packages

We describe here the steps and tips for publishing Python packages on PyPI and conda-forge.

1.1 Publishing on PyPI

Publishing a package on PyPI is generally simpler than publish on conda-forge, and it's easiest to use the PyPI package as the source for a conda-forge recipe anyway, so it's best to start here. More details can be found [here](#).

1. Make sure your package dependencies are all correctly specified, e.g. by creating a new Conda environment and running `pip install -e .` from an up-to-date source and ensuring that all tests pass. Dependencies should be specified with a lower bound, rather than pinned to a specific version, for maximum compatibility.
 - There are a few different ways to specify project dependencies, but the most modern is with a [pyproject.toml](#) file in the root of the project directory. This is what we have used for PyVBMC and GPyReg, this guide may need to be adapted if you are using a different method. From what I understand, it is also good practice to leave a “stub” in setup.py for backwards compatibility, as in [here](#).
2. Make sure `pyproject.toml` contains the appropriate lines. These are taken from PyVBMC, so they may not all be required for your project, but this is a starting point. You may also already have a `pyproject.toml` with other information in it, such as configurations for the [Black formatter](#). That's fine, those sections can remain.

```
# pyproject.toml
#
[project]
name = "PyVBMC" # Naming a project is required
dynamic = ["version"] # use git tags for version, via setuptools_scm
# If you don't want to use setuptools_scm, you can specify the version
# manually:
# version = "v1.0.0"
description = "Variational Bayesian Monte Carlo in Python."
readme = "README.md"
```

```

license = { file = "LICENSE" }
dependencies = [
    "cma >= 3.1.0",
    "corner >= 2.2.1",
    # ...
]
requires-python = ">=3.9"
#
[tool.setuptools]
include-package-data = true
# We want to include some files which are not in the source directory,
# such as the Jupyter Notebooks in /examples.
# See https://setuptools.pypa.io/en/latest/userguide/datafiles.html
# for more info.
packages = ["pyvbm", "pyvbm.examples"]
package-dir = {"pyvbm.examples" = "examples"}
#
[tool.setuptools.package-data]
# Specify the extensions to include as data:
"pyvbm.examples" = ["*.ipynb"]
# Including files which *are* in the source directory but are not
# .py files can also be accomplished with a MANIFEST.in file. See
# e.g. https://github.com/acerbilab/pyvbm/blob/main/MANIFEST.in
#
[project.optional-dependencies]
dev = [
    "myst_nb >= 0.13.1",
    "numpydoc >= 1.2.1",
    # ...
] # These dependencies are for developers. They will only be installed
# with `pip install pyvbm[dev]` (or `pip install .[dev]`, locally).
# You can specify other sets of optional dependencies similarly.
#
[build-system]
# Required for using setuptools.scm, which automatically assigns the
# version number based on Git tags.
requires = [
    "setuptools >= 45",
    "setuptools_scm[toml] >= 6.2",
]
build-backend = "setuptools.build_meta"

```

- `setuptools_scm` is a tool which extracts versioning info from Git tags, so that you don't have to manually specify package versions.

3. Tag the current commit as a release version with

```
git tag vX.Y.Z
```

See [here](#) for some details about semantic versioning.

4. Install Python build tools. It's probably a good idea to create a new environment for the whole build and packaging process.

```
conda create -n build-env # optional, but recommended
conda activate build-env # if you created build-env, otherwise make sure you have activated y
pip install setuptools-scm
pip install build
pip install twine
```

5. Build your package:

```
python -m build
```

(from the project directory)

6. This should create a directory `dist/` with `.whl` and `.tar.gz` files matching your package name and tagged version. Inspect these files and make sure that they contain the contents you expect. By default this should be the source directory corresponding to your project's name, e.g. `/pyvbm`. If you are missing files that should be there, then see the link above (<https://setuptools.pypa.io/en/latest/userguide/datafiles.html>) regarding `package-data` and `MANIFEST.in`.

7. You can also run `twine check dist/*` to ensure that the package name and description will render properly on PyPI.

8. If everything looks correct, test out the build by creating a new environment and running `pip install dist/*.whl` to install the packaged version and test it out. For example, you could run the tests with `pytest --pyargs your-package` (do this from somewhere *outside* the project directory, to ensure that `pytest` is finding the version you just installed, and not the local tests). You could also open a Python REPL and just ensure that your package imports. You may need to open a new shell before the installation can be found on your path.

```
conda create -n test-package-release
conda activate test-package-release
pip install dist/*.whl
cd ~ # Test the build package outside the working directory.
```

```
pytest --pyargs your-package
# Ensure later to come back to the project working directory
```

9. If everything checks out and you are ready to upload, first head to <https://test.pypi.org/> and register an account if you don't already have one. Then you can test uploading your package by running `twine upload --repository testpypi dist/*` from the project directory. Your package should then be visible under your account on the test repository, and you can make sure that the description and other info are correct. You can also attempt to install it with

```
python3 -m pip install --index-url https://test.pypi.org/simple/ --extra-index-url https://p
```

The `--extra-index-url` tells `pip` to also look at the regular PyPI repository, which is important if your package has dependencies which are not on the test repo (this is likely the case).

10. If everything looks good on the test repository, you can run `twine upload dist/*` to upload to the official repository (you will need an account there as well, separate from your test account). Be aware that while a version of a package can be deleted from PyPI (so that it is no longer available), that same version number can never be re-uploaded. So it pays to double-check.

11. Once uploaded, you should be able to run `pip install your-package!`

Other notes

1. You can add another user as an owner or maintainer of a project through your account at <https://pypi.org/>
2. Optionally, you may also want to list the package version on GitHub. You can do this by pushing the version tag(s) to the origin with `git push --tags`, then selecting the tag from <https://github.com/account-name/repo-name/tags> and clicking “Create release”. You can describe the release, and optionally upload the built `.whl` and `.tar.gz` files.

1.2 Uploading to conda-forge

Uploading to `conda-forge` is slightly more involved. Detailed instructions can be found [here](#), but here is a summary of steps:

1. Fork the `conda-forge` [staged-recipes](#) repository from GitHub, and clone the fork locally. Checkout a new branch, e.g. `pyvbmc-recipe`, then `cd` into the `staged-recipes/recipes/` directory.

2. Install `grayskull` with `pip install grayskull` (or `conda install -c conda-forge grayskull`). `Grayskull` is a utility which will help generate the appropriate metadata for your package.
3. If your package is already on PyPI, you can run `grayskull pypi --strict-conda-forge your-package` to generate a `conda-forge` recipe for your package. It should create the file `staged-recipes/recipes/your-package/meta.yaml`.
4. Everything should be filled in automatically (though it's good to double-check), with the exception of

```
|about:
|  home: https://acerbilab.github.io/pyvbmc/
|
|extra:
|  recipe-maintainers:
|    - AddYourGitHubIdHere
```

(ignore the vertical bars, Colab won't let me include leading spaces without them). You can also add other people as recipe maintainers, with their permission. It just means they will receive automated PRs and other updates regarding the project from `conda-forge`, and possibly answer any questions that pop up. 5. Optionally, you can add documentation and development URLs to the `about:` section, e.g.

```
|about:
|  home: https://acerbilab.github.io/pyvbmc/
|  description: |
|    PyVBM is a Python implementation of the Variational Bayesian Monte Carlo (VBM) algorithm
|  doc_url: https://acerbilab.github.io/pyvbmc/
|  dev_url: https://github.com/acerbilab/pyvbmc/
|  ...
```

6. Optionally, you can include commands in the `test` section of the `meta.yaml` recipe, which will be automatically run when `conda-forge` updates the package. The `pyvbmc` test suite is quite expensive to run, so I elected to just include the default basic tests here, which just ensure that the package can be imported.
7. Once you think everything is correct (see a checklist [here](#)), you can commit the changes to your new branch, push them to GitHub, and then open a PR to merge your fork to the original `staged-recipes` repo. Fill out the template checklist which appears when you draft the PR.
8. Once you've opened the PR, the `conda-forge` automation will check your recipe and attempt to install the package. Correct any errors that occur, and comment on GitHub with `@conda-forge-admin, please restart ci` to re-run the automated checks.

9. Once the automated checks all pass, you can ping a member of the `conda-forge` team to review and approve the PR with `@conda-forge-admin`, please ping `conda-forge/help-python`.
10. After the PR is merged, it will take a few hours (and possibly up to 24) for the package to become available on the Conda servers. After that `conda install --channel=conda-forge your-package` should work!
11. A repo will be created at `conda-forge/your-package-feedstock`, and you and any other recipe maintainers will be added to it. This is where automated PRs regarding your package will be issued.

1.3 Updating the package version

Fortunately, this part is simple.

- **Updating the version on PyPI:**

Re-run steps 3-5 from the section [Publishing on PyPI](#) above, and upload the new `.whl` and `.tar.gz` files to PyPI with `twine`.

- **Updating the version on conda-forge:**

After the package becomes available on PyPI, `conda-forge` should automatically find the new version (this will take a few hours). After that, the `conda-forge` process will automatically issue a PR to the feedstock repo, which a recipe maintainer can approve in order to update the `conda-forge` version. After approval, the binary on the `conda-forge` cloud/repo will be automatically updated within 24 hours.

Part II

HPC resources

2 Introduction

Whenever doing research, High Performance Computing (HPC) access and usage is fundamental, you will rarely be running things only on a local machine. The main HPC resources we can use are [CSC](#) and [UH's Turso](#).

2.1 HPC usage tutorial

This is a [tutorial on HPC usage](#) held in June 2021 by Aalto University, very useful. The videos are [here](#).

[HPC user guide for UH](#). They have [support sessions](#) organized every day if you have any questions or need any help with HPC usage.

Slack channel: Join and check out the **#hpc** channel on the lab Slack.

3 Resources for Gaussian processes and Bayesian optimization

Gaussian Processes

- **Gortler et al. (2019)**. A Visual Exploration of Gaussian Processes. [Distill](#)
- **Videos and tutorials** from the Gaussian Process Summer School: [GPSS 2021 Program](#)
 - Start with the first video, “Intro to GPs”, and the sessions on “Kernel Design” and “Representation Learning with GPs” (other videos can be explored later as time permits).
- **Tutorials/workshops (Jupyter notebooks)**: [GPSS 2021 Labs](#)
- **The GP Bible** by Rasmussen and Williams (2006): [Gaussian Processes for Machine Learning](#)

Bayesian Optimization

- **Exploring Bayesian Optimization** (Agnihotri and Batra 2020). [Distill](#)
- **Frazier (2018)**. A Tutorial on Bayesian Optimization. [arXiv](#)
- **Video**: “Introduction to Bayesian Optimization” from the Gaussian Process Summer School, Day 3: [GPSS 2021 Day 3](#)
- **The Bayesian Optimization Book** by Garnett (2023): [BayesOptBook](#)

Slack Channel

- Join and check out the [#gaussian-processes](#) channel on the lab Slack.

4 Seminars

4.1 Ongoing

[Aalto Seminar on Advances in Probabilistic Machine Learning \[APML\]](#)

[Machine Learning Coffee seminars](#)

[Seminar on Gaussian Processes, Spatiotemporal Modeling, and Decision-making Systems](#)

5 Contributing guide

Simply write a (q)markdown file like this one and add the filename (e.g., `contributing.qmd`) to `_quarto.yml` under the field `book: chapters:`. Then make a pull request to merge your changes to the `main` branch.

For other advanced usages, refer to [Quarto documentation](#).

Bibliography

- Agnihotri, Apoorv, and Nipun Batra. 2020. “Exploring Bayesian Optimization.” *Distill*.
<https://doi.org/10.23915/distill.00026>.
- Garnett, Roman. 2023. *Bayesian Optimization*. Cambridge University Press.