Scientific Software Development with Python

DevOps 1: Testing and packaging Python software

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Agenda

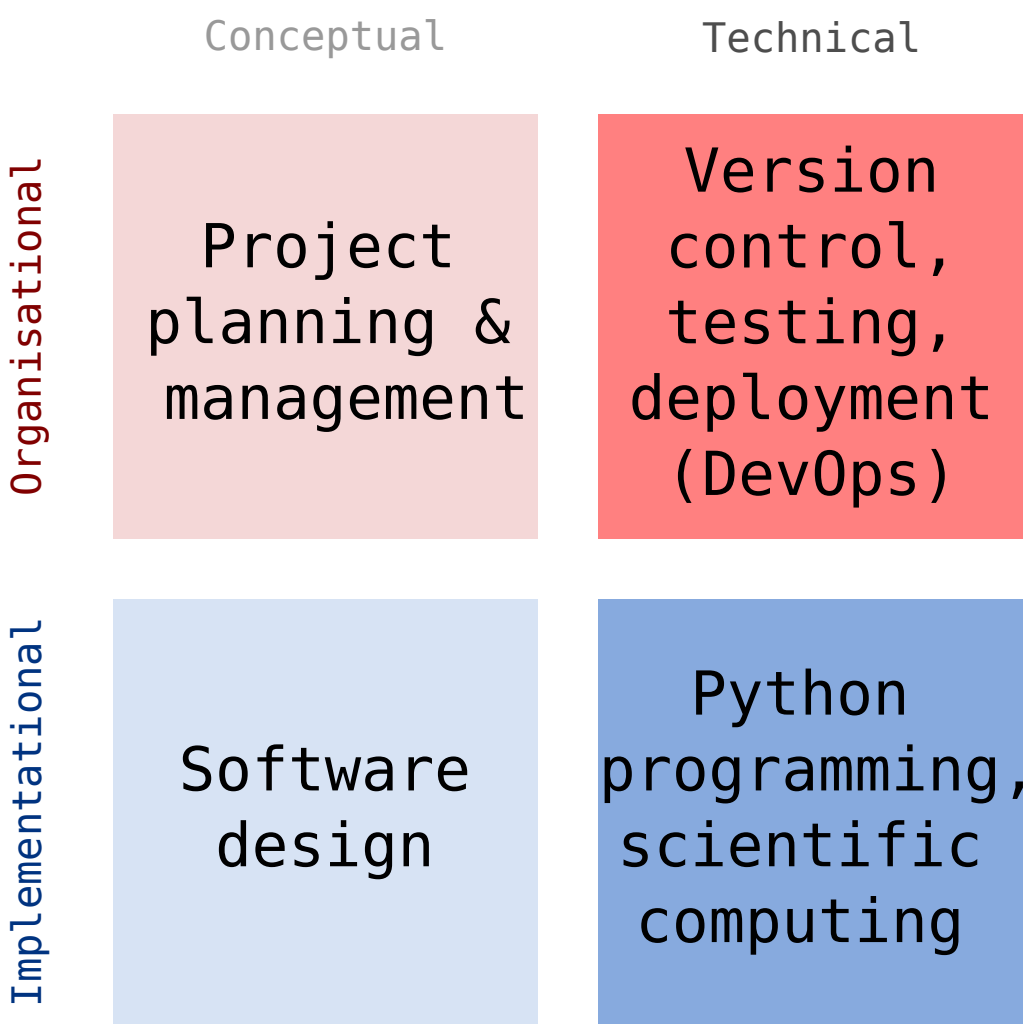
1. Introduction

2. Test driven development

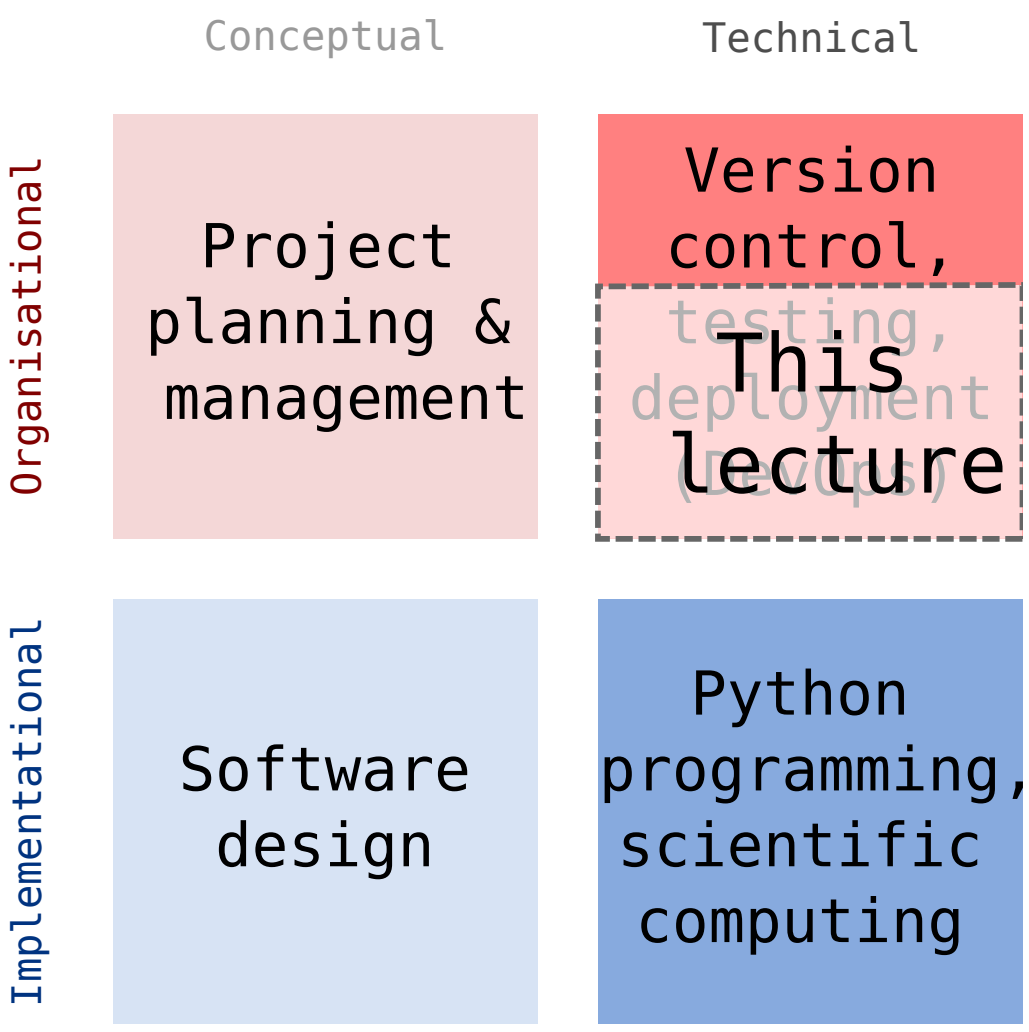
3. Python packaging system

4. Virtual environments

Lecture content



Lecture content



DevOps

- Wikipedia[1]: *set of practices that combines software development (Dev) and IT operations (Ops).*
- Personal definition: The steps that are required to turn code into software, e.g.:
  - Running tests
  - Generating documentation
  - Releasing the package

[1] `https://en.wikipedia.org/wiki/DevOps`

Aims and principles

Aims

- Enable change
- Ensure correctness

Principles

- All code in one place
- Short feedback times: continuous integration (CI)
- Automate everything

Lecture content

This lecture

- Testing
- Packaging

Next lecture

- Documentation
- Automation: Continuous integration with GitHub

Exercise

- Exercise 1 from task sheet
- Time: 10 minutes

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Testing levels

- **Unit tests**: specific section of code (module)
- Integration tests: Interaction between modules
- System testing: Software as a whole
- **Acceptance testing**: Functional requirements (user stories)

Testing and agile development

- Testing enables rapid change and adaptation (flexibility)
- Testing gives you confidence in your code
- Short feedback loops crucial for learning

TDD Workflow:

1. Write test
2. Run test to ensure that it fails
3. Add new code until test passes

Benefits

- All code is verified
- Developer is forced into user role
- Code is more modular
- Code is guaranteed to be testable
- Writing tests first ensures that tests cover only functionality and not implementation details

pytest

- Unit testing framework for python
- There exist others, but general usage is the same.

Basic usage

- Assuming the following project structure:

```
project_dir/
├── module/
│   └── __init__.py
└── test/
    └── test_module.py
```

Basic usage

- module/__init__.py:

```
def multiply(a, b):
    return a * b
```

- test/test_moudle.py:

```
from module import multiply
from random import randint

def test_multiply():
    a = randint(0, 99)
    b = randint(0, 99)
    result = multiply(a, b)
    assert result == a * b
```

Invoking tests:

`pytest` automatically runs all

1. functions prefixed with `test`
2. methods prefixed with `test` inside `Test`-prefixed classes

in files matching `test_*.py` or `*_test.py`.

```
cd project_dir
pytest test/
```

- Example output:

```
=================================== test session starts ===================================
platform linux -- Python 3.7.4, pytest-5.3.5, py-1.8.1, pluggy-0.13.1
rootdir: /home/simon/src/scratch/module
plugins: hypothesis-5.5.4, doctestplus-0.5.0, astropy-header-0.1.2, arraydiff-0.3, ...
collected 1 item

test/test_module.py .                                                              [100%]

==================================== 1 passed in 0.02s ====================================
```

Exercise

- Exercise 2 from task sheet
- Time: 15 minutes

Some comments

- Folder structure is not mandatory
- Source files and test file can also be in same repository

Advanced concepts

- `pytest` provides several ways to handle the setup and teardown of more complex tests (*fixtures*)
- More information can be found in the documentation[2]

[2] `https://docs.pytest.org/en/stable/fixture.html`

Note

Unit tests alone are not sufficient to ensure correctness of your software[3]

Acceptance tests

- Verify that software fulfills requirements
- User stories should be turned into acceptance tests
- Benefits:
  - Ensures that functionality doesn't *decay* over time
  - Can be turned into documentation (examples)
- Example: Your plot script from the first exercise

[3] Although, formally, nothing is:
`https://en.wikipedia.org/wiki/Halting_problem`

Summary

Unit tests

- Force you to write better code
- Basis for iterative improvements
- Ensure correctness on module level

Acceptance tests

- Ensure that your software does what it is expected to.

Although reality may not always allow us to, we should consider test code of equal importance as implementation code.

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Typical usage

```
# Import statments tell Python to load a module
import module
import module as m
from module import function, Class
# Functions and classes defined in the module can
# be accessed through its attributes.
module.function()
m.function()
```

Modules

- Act as namespaces that bundle classes and functions
- Module imports are cached:
  - Once a module is imported, it can't (easily) be changed[4]

[4] To enable autoreload in IPython:
`[get_ipython().magic(m) for m in ["%load_ext autoreload", "%autoreload 2"]]`

What qualifies as a module?

- A python source file: `module.py`
- A directory tree:

```
module/
├── __init__.py
├── submodule_1.py
└── submodule_2/
    └── __init__.py
```

How does Python find them?

- Modules are searched in the folders contained in the `sys.path`[5] path variable
- By default `sys.path` contains:
  1. Working directory from which Python interpreter is executed
  2. Content of `PYTHONPATH` environment variable
  3. Installation-dependent default directory.

[5] To verify: `import sys; print(sys.path)`

Problem

Python only finds our own modules only when we are in the right directory.

Python packaging system

- Python built-in support for:
  - Installing packages (making modules importable)
  - Handling dependencies
  - Distributing packages

Minimal setup

- A project folder containing:
  1. the modules to include in the package
  2. a `setup.py`, which describes the package
  3. a README file
  4. a LICENSE file

```
project_folder/
├── module_name/
│   └── __init__.py
├── setup_.py
├── README.md
└── LICENSE
```

Do choose a license

- No license means exclusive copyright by default
  - This gets messy as soon as you collaborate with others
- MIT license is a popular default and the most permissive
- GNU GPLv3 forbids distributing closed source version of you code

README.md

- Rendered on GitHub as the frontpage of your repository.
- Uses Markdown markup language.
- Also used for package description on PyPI.

```
# Header 1

Normal text, *Italic text*, **Bold text**, ...

## Header 2

1. A numerated ...
2. ... list

- A bulletted ...
- ... list

[A text link](https://link.target).
```

setup.py

- Python source file defining package metadata
- Good template can be found on `https://packaging.python.org/tutorials/packaging-projects/`
- It is good practice to use the same name for the package and the included modules

```
import setuptools

with open("README.md", "r") as fh:
    long_description = fh.read()

setuptools.setup(
    name="package_name",
    version="0.0.1",
    author="Your name",
    author_email="your@address.com",
    description="My first package.",
    long_description=long_description,
    long_description_content_type="text/markdown",
    url="https://github.com/you_username/your_project",
    packages=setuptools.find_packages(), # Searches modules in current directory.
    python_requires='>=3.6',
)
```

Installing your package locally

Install using pip:

```
$ cd project_folder
$ pip install .
```

- Alternatively, you could use `python setup.py install`
- Advantages of using pip:
  - `pip` automatically downloads dependencies
  - `pip` can be used to uninstall the package again

Installing your package locally

Issue with normal install

- Installing copies the module code into an installation-dependent directory
- Changes made to the the code in the `project_folder` therefore do not affect the installed module
- This is impractical when a package is in development

Solution

```
$ pip install -e . # or pip install --editable
```

Install requires

- Required packages are specified as argument to the `setuptools.setup` call.
- Packages listed here are installed automatically before the package is installed.

```
setuptools.setup(
    ...
    install_requires([
        package_name,
        another_name>=1.0,
    ])
    ...
)
```

Exercise

- Exercise 3 from task sheet
- Time: 10 minutes

Distributing packages

Python provides two built-in ways of distributing packages:

Source distributions

- A source distribution (sdist) is simply the source code as a `tar.gz` archive.

Wheel

- Built distribution already containing files and metadata required to install a package
- Advantages over sdist:
  - Smaller in size
  - Faster to install
  - More secure (no `setup.py` execution)

Tools

- The `wheels` package is required to build Python wheels:

```
$ pip install wheels
```

- We will use the `twine` package to upload your package distributions to PyPI:

```
$ pip install twine
```

Generating wheels

```
$ python setup.py sdist bdist_wheel
```

Package indices

- Python packages can be published via package indices
- The Python Package Index (PyPI) is the most popular one

Uploading your package

- For testing, uploading to the test index[6] of PyPI is recommended. This avoids polluting the standard PyPI name space.
- To upload to `test.pypi.org`:

```
$ python -m twine upload --repository testpypi dist/*
```

[6] Requires account at `https://test.pypi.org`

Uploading your package

- To upload to the real PyPI[7]:

```
$ python -m twine upload --repository testpypi dist/*
```

[7] Requires account at `https://pypi.org`

Installing your package from PyPI

- Since the package has been upload to `test.pypi.org`, we need to specify the URL of the index:

```
python3 -m pip install --index-url https://test.pypi.org your_package
```

Exercise

- Exercise 4 on exercise sheet
- Time: 10 minutes

What you have learned

- How to declare a package (`setup.py`)
- How to package it into wheels
- How to upload it to a package index

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Dependency hell

- The problem with the presented workflow:
  - By default `pip` will install packages system- or user-wide
  - This can lead to clashes if packages depend on different versions of a given package
- It possible to end up in a configuration where not all requirements for all packages can be resolved simultaneously (dependency hell)

The solution

- Virtual environment
- A virtual environment is project-specific Python environment

`venv`

- `venv` is a tool to create virtual environments
- part of Python standard library
- usage:

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

Creating a virtual environment

- To create a virtual environment in the folder `.venv`: `project_folder`:

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

Activating the environment

- To activate the environment: `project_folder`:

```
$ source .venv/bin/activate
```

- Note that you will need to reinstall any non-standard-library packages in the new environment

Listing installed packages

- To extract names of currently installed packages:

```
$ pip freeze > requirements.txt
```

- The `requirements.txt` file can be shared with others who can install file from it:

  `$ pip install -r requirements.txt`

Listing installed packages

- To extract names of currently installed packages:

```
$ pip freeze > requirements.txt
```

- The `requirements.txt` file can be shared with others who can install file from it:

  `$ pip install -r requirements.txt`

Exercise

- Exercise 5 on exercise sheet
- Time: 10 minutes

What we have learned

- How to avoid dependency hell (`venv`)
- How to share specific environments with others (`requirements.txt`)