AN UNBIASED EVALUATION OF ENVIRONMENT MANAGEMENT AND PACKAGING TOOLS

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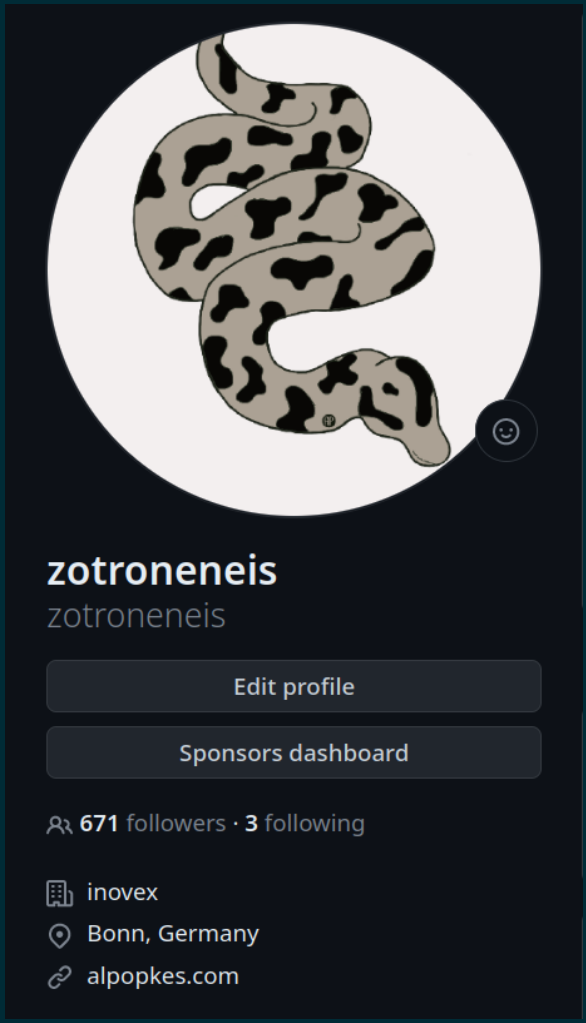
ABOUT ME

Machine Learning Engineer @inovex

inovex

- Github: zotroneneis
- Personal webpage



Github: zotroneneis

machine_learning_basics Public

Plain python implementations of basic machine learning algorithms

Jupyter Notebook 4k 811

magical_universe Public

Awesome Python features explained using the world of magic

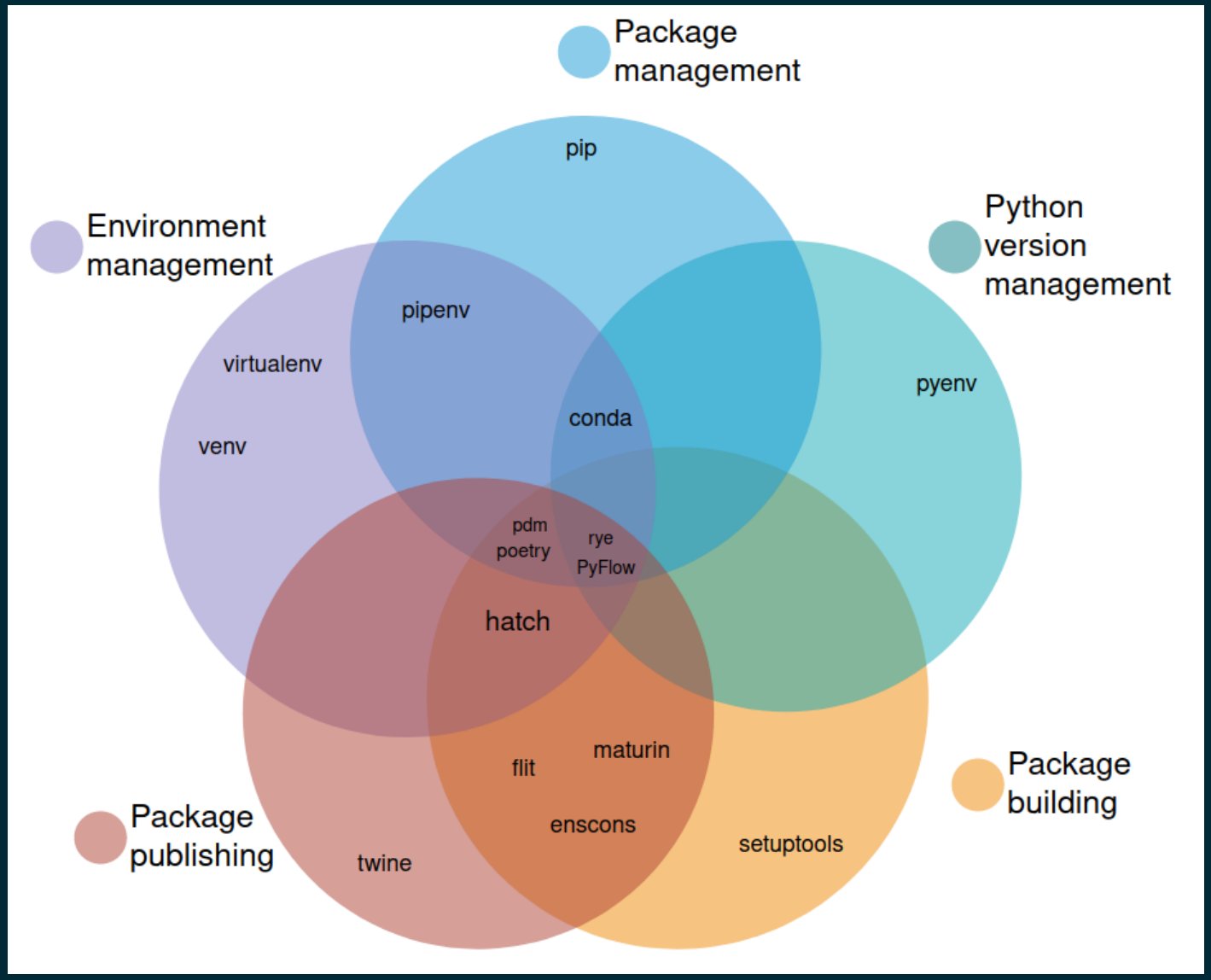
Python 803 59

OVERVIEW

OVERVIEW

1. Goal of the talk
2. Categorization
3. Detailed look at each category
    - Definition
    - Motivation
    - Single purpose tools
4. Multi-purpose tools

CATEGORIZATION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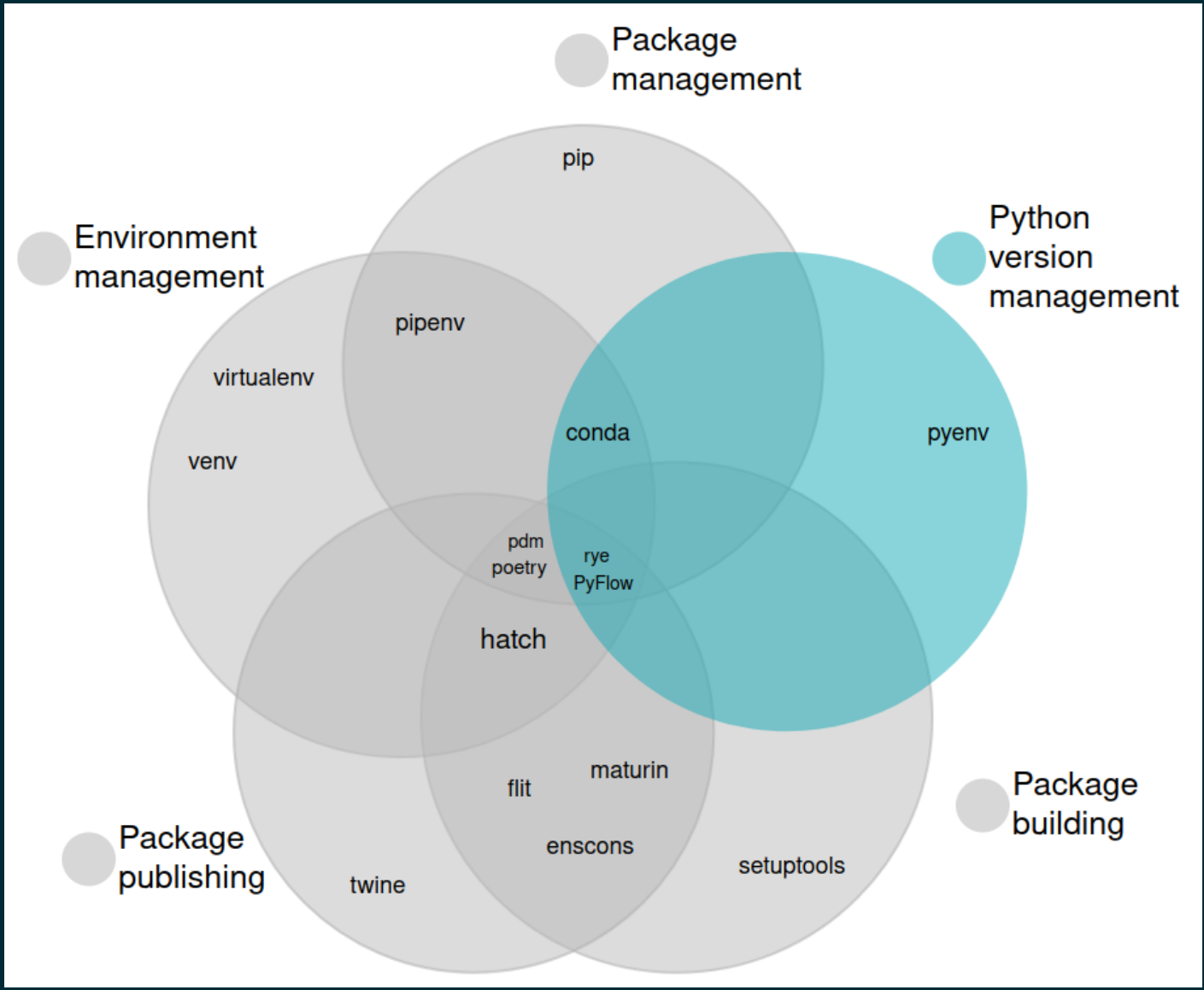
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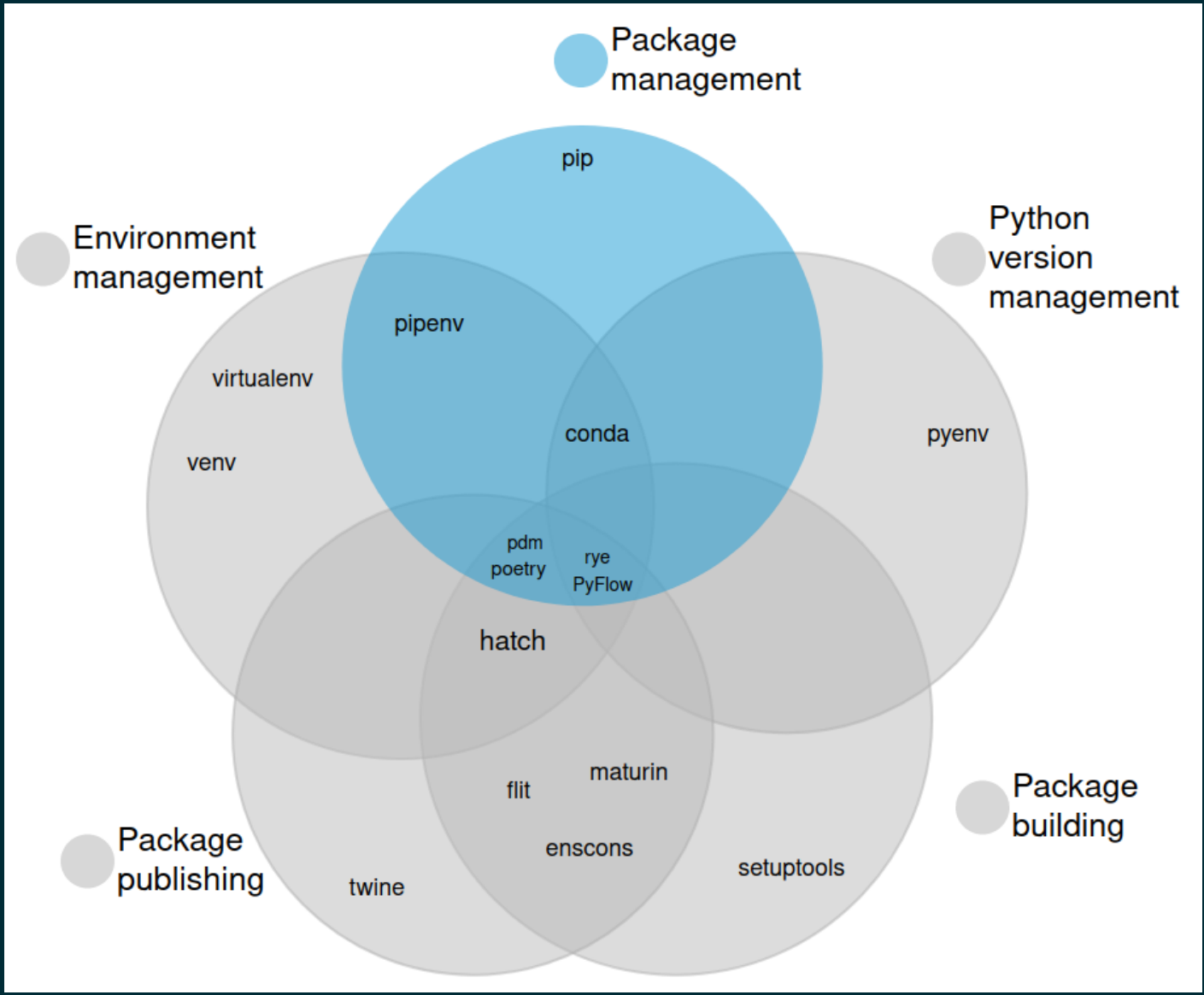
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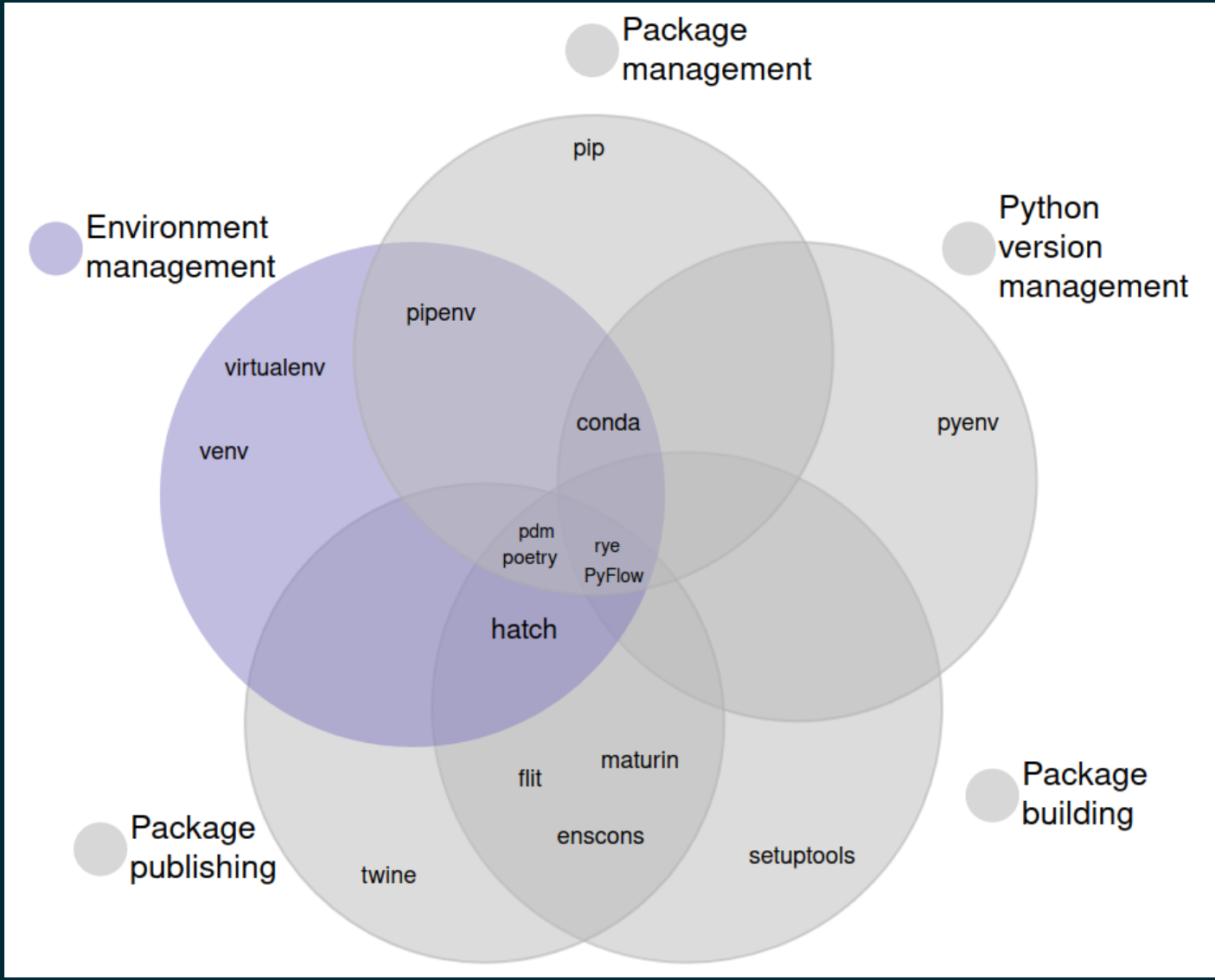
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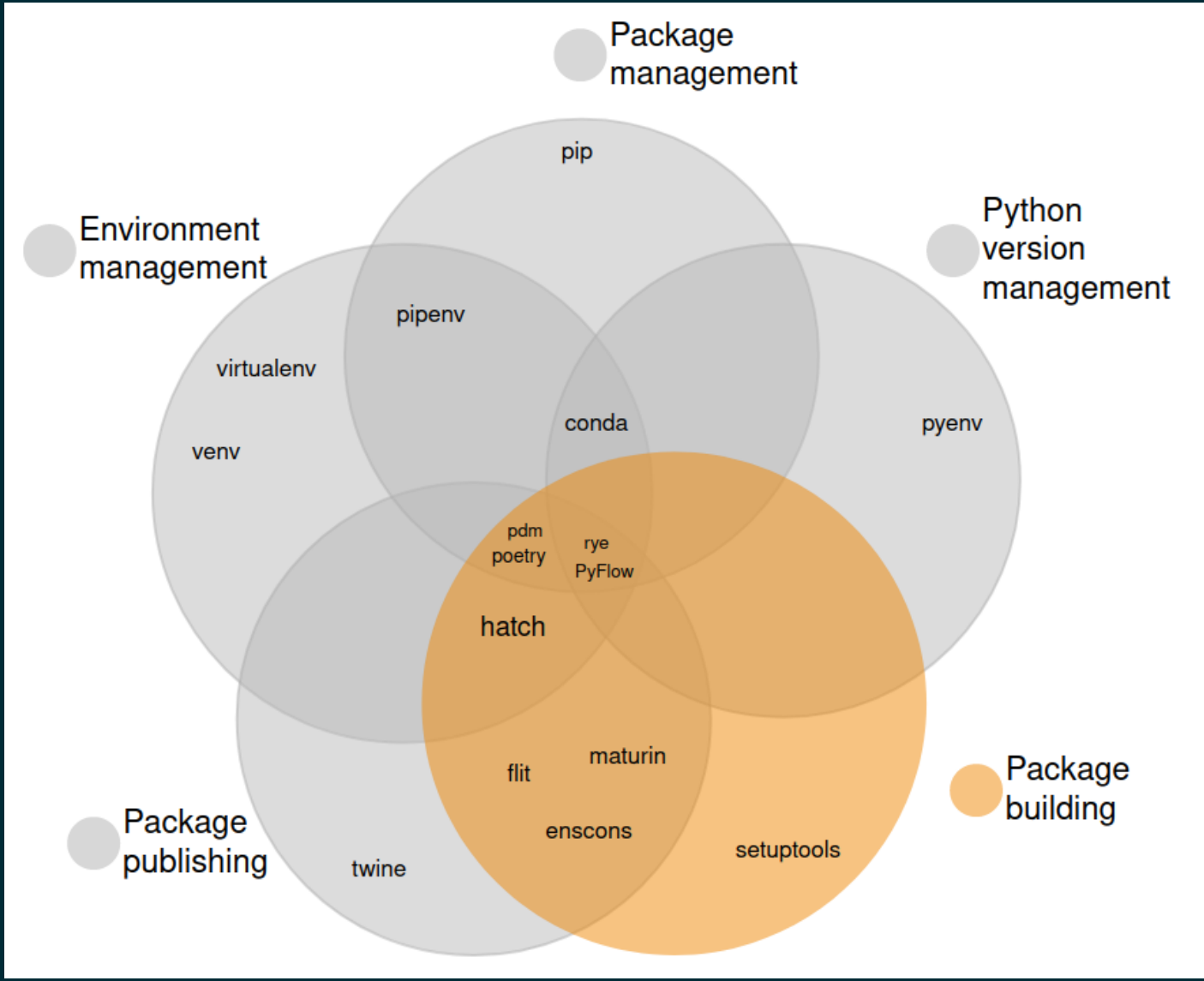
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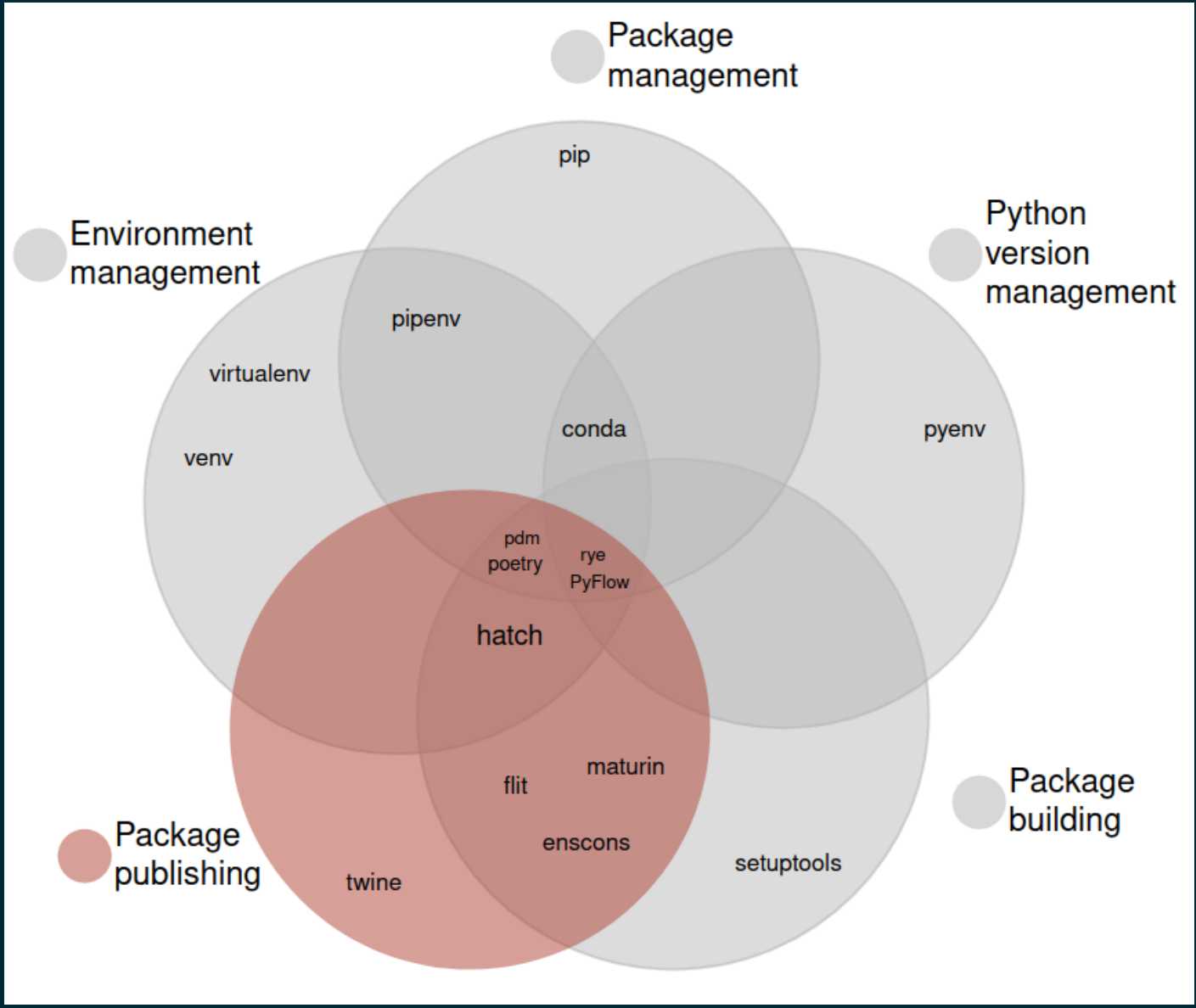
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PYTHON VERSION MANAGEMENT

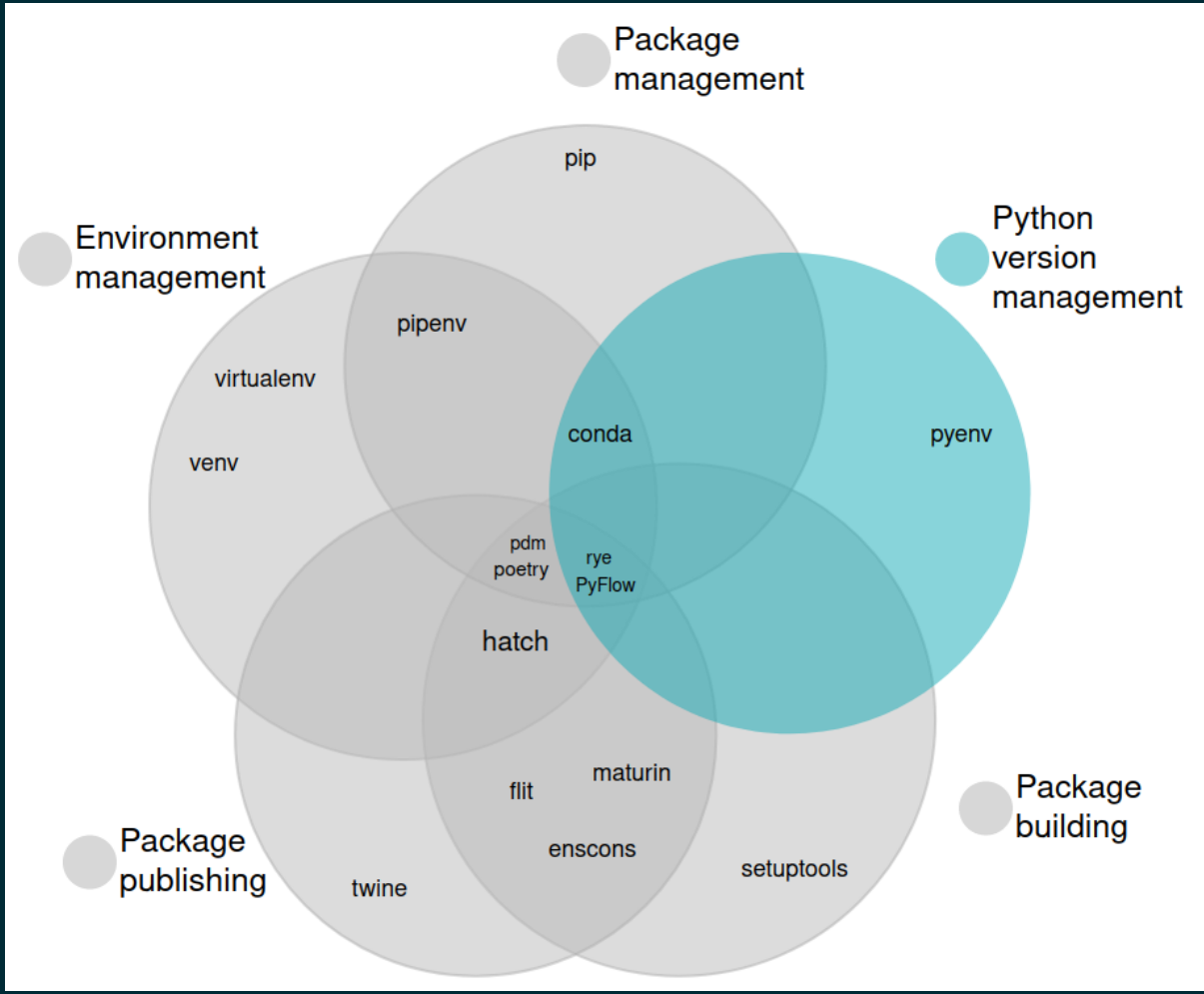
DEFINITION

- Install Python versions
- Switch between Python versions

MOTIVATION

- Projects might require different Python versions
- Projects might support several Python versions
- You might want to test new Python versions

TOOLS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PYENV

- Single-purpose tool to handle multiple Python versions
- Most important commands:

```
# Install specific Python version
pyenv install 3.10.4

# Switch between Python versions
pyenv shell <version>
pyenv local <version>
pyenv global <version>
```

(VIRTUAL) ENVIRONMENT MANAGEMENT

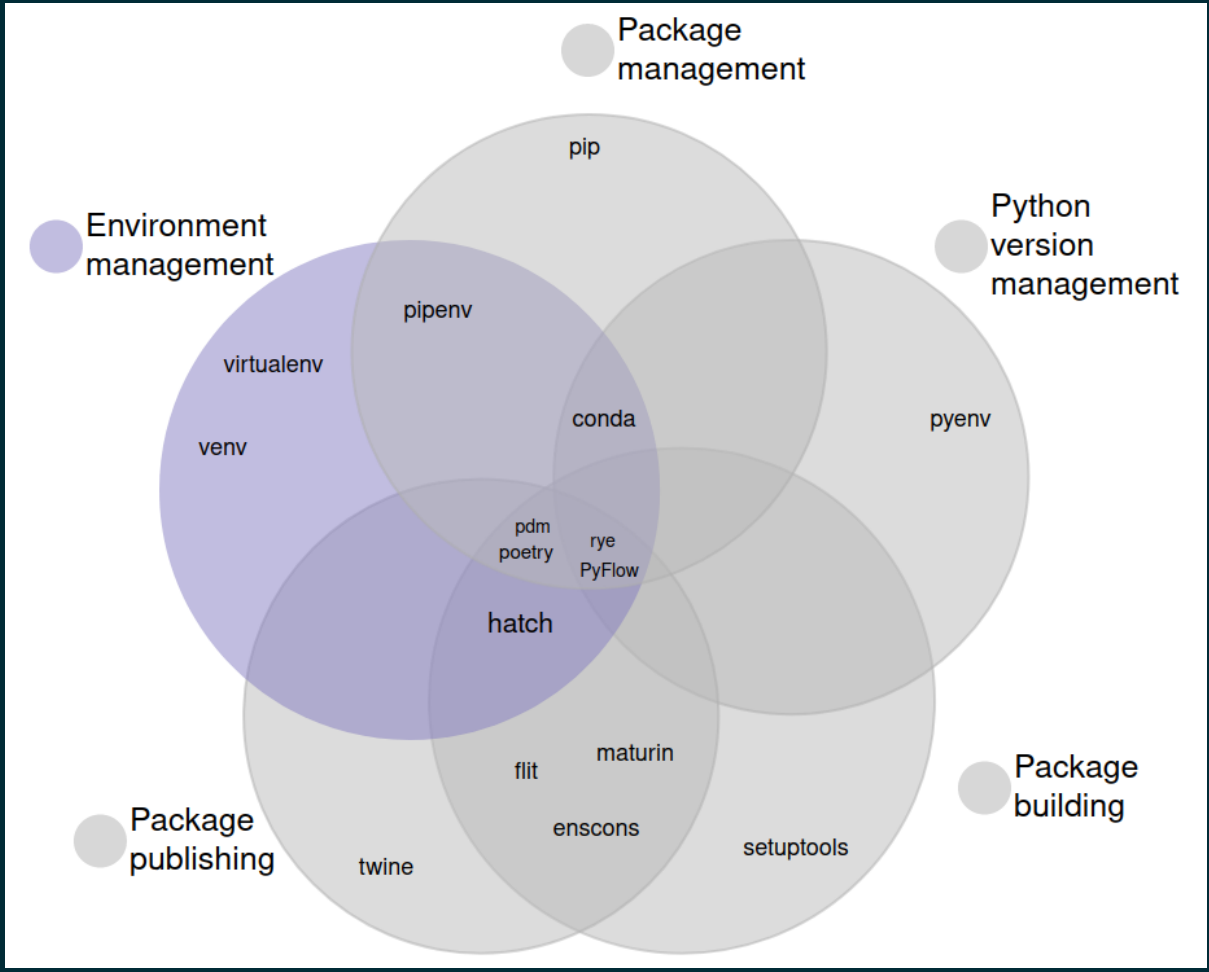
DEFINITION

Creation and management of (virtual) environments

MOTIVATION

- Projects depend on other packages
- Projects might require different versions of the same package
- `pip` installing a package can cause system pollution

TOOLS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VENV

- Built-in Python package for creating virtual environments
- Most important commands:

```
# Create env
python3 -m venv <env_name>

# Activate env
source <env_name>/bin/activate

# Deactivate env
deactivate
```

VIRTUALENV

- Offers more features than venv
- For example, venv is slower and not extendable
- Most important commands:

```
# Create env
virtualenv <env_name>

# Activate env
source <env_name>/bin/activate

# Deactivate env
deactivate
```

RECAP I

PYPROJECT.TOML

- Used to define project settings
- Replaces old `setup.py`
- Example file from `pandas` library:

```toml
[build-system]
# Minimum requirements for the build system to execute.
# See https://github.com/scipy/scipy/pull/12940 for the AIX issue.
requires = [
    "setuptools>=61.0.0",
    "wheel",
    "Cython>=0.29.32,<3",  # Note: sync with setup.py, environment.yml and asv.conf.json
    "oldest-supported-numpy>=2022.8.16",
    "versioneer[toml]"
]
# build-backend = "setuptools.build_meta"

[project]
name = 'pandas'
dynamic = [
  'version'
]
description = 'Powerful data structures for data analysis, time series, and statistics'
readme = 'README.md'
authors = [
  { name = 'The Pandas Development Team', email='pandas-dev@python.org' },
]
license = {file = 'LICENSE'}
requires-python = '>=3.8'
dependencies = [
  "numpy>=1.20.3; python_version<'3.10'",
```

PACKAGE MANAGEMENT

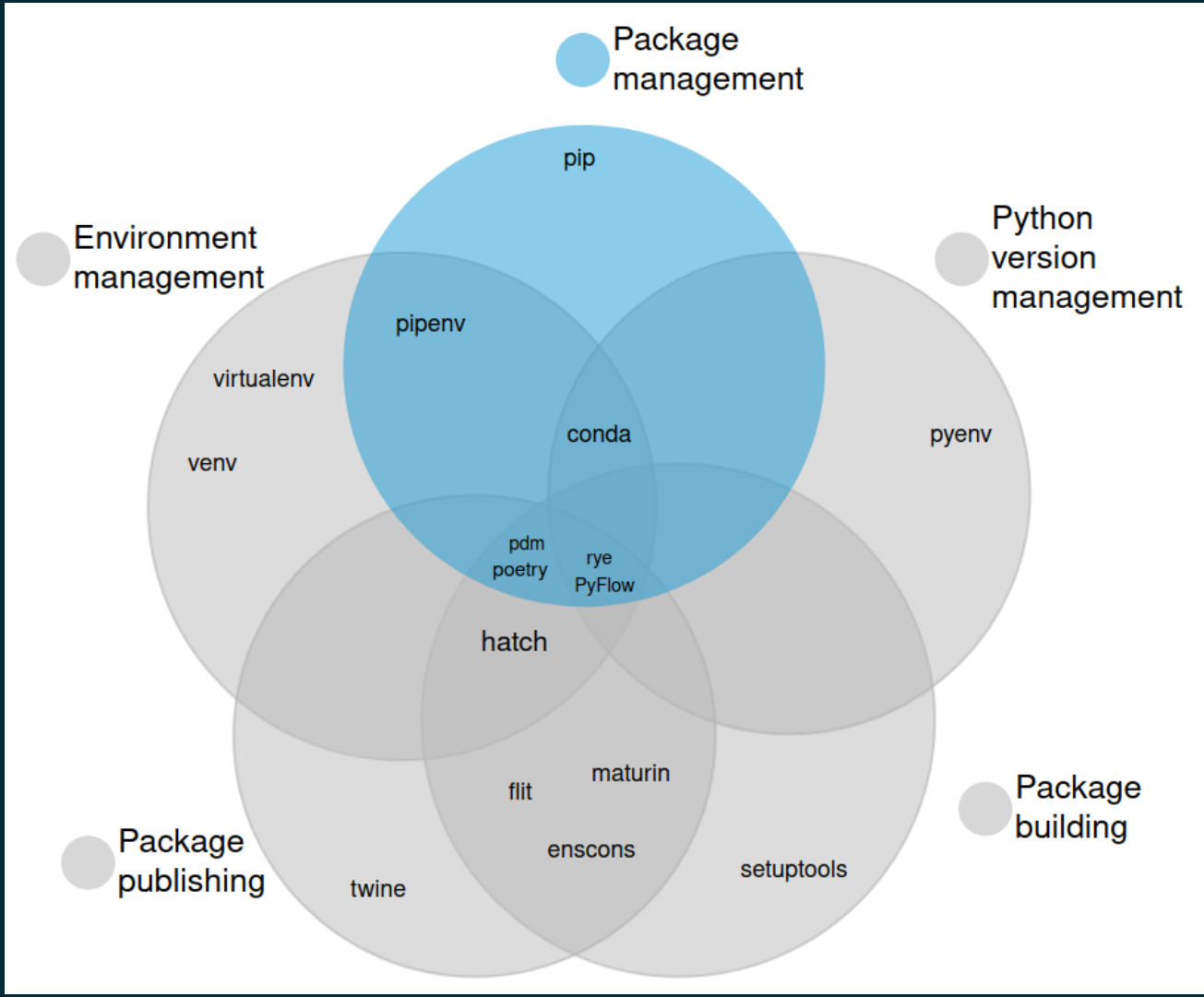
DEFINITION

Download and install libraries and their dependencies

MOTIVATION

- Packages allow us to define a hierarchy of modules
- Modules can be accessed easily using the dot-syntax
- Code can easily be shared with other developers
- Project dependencies are bundled in `pyproject.toml`

TOOLS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PIP

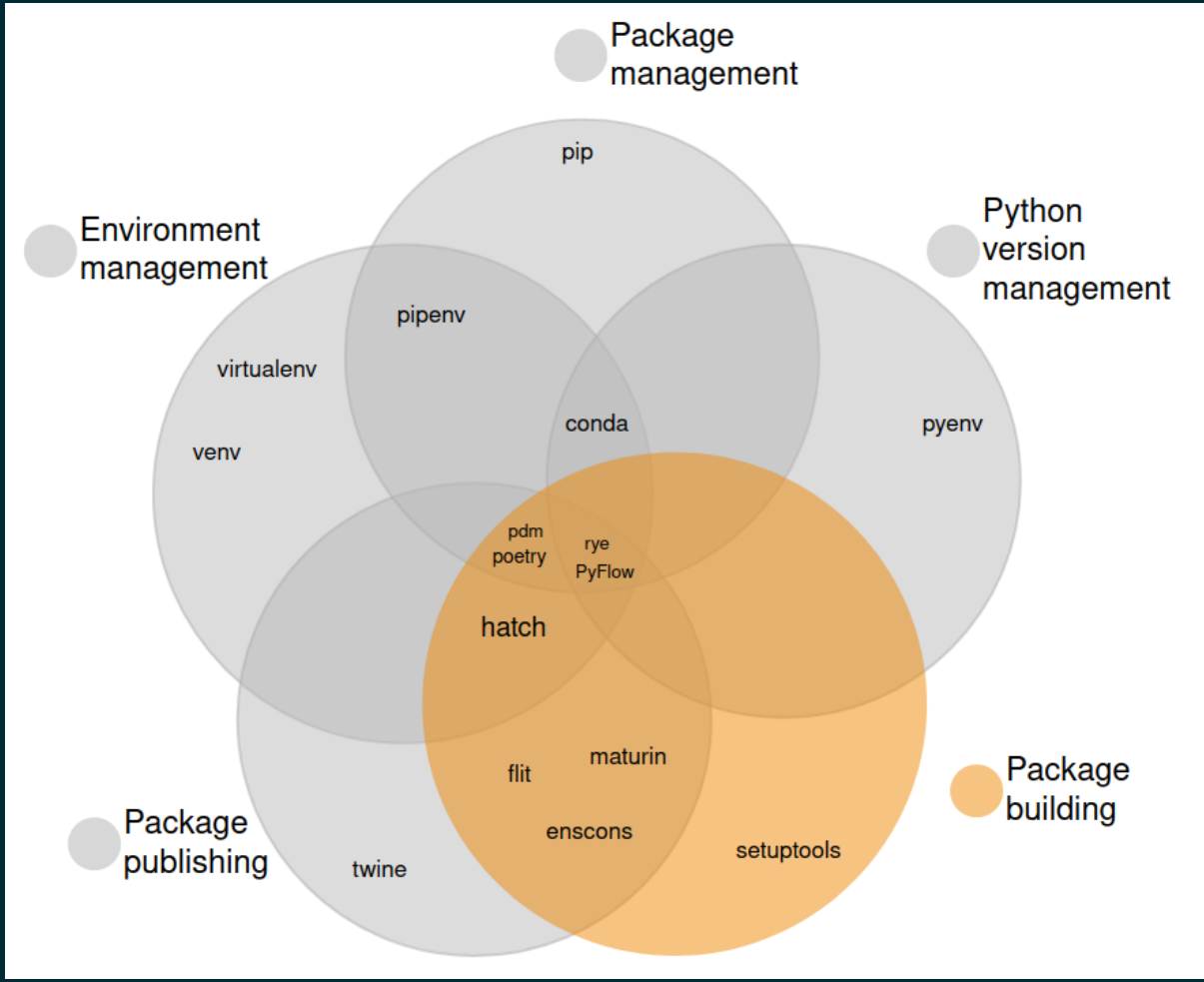
- Standard package manager for Python
- Shipped with Python
- Allows to install packages from PyPI and other indexes
- Main command: `pip install <package_name>`

PACKAGE BUILDING

DEFINITION

Building a package => creating `.whl` and `.tar.gz` files

TOOLS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SETUPTOOLS

- Build backend for Python packages
- Developed as an enhacement for `distutils` in 2004
- Used with a `pyproject.toml` file:

```
[build-system]
requires = ["setuptools"]
build-backend = "setuptools.build_meta"
```

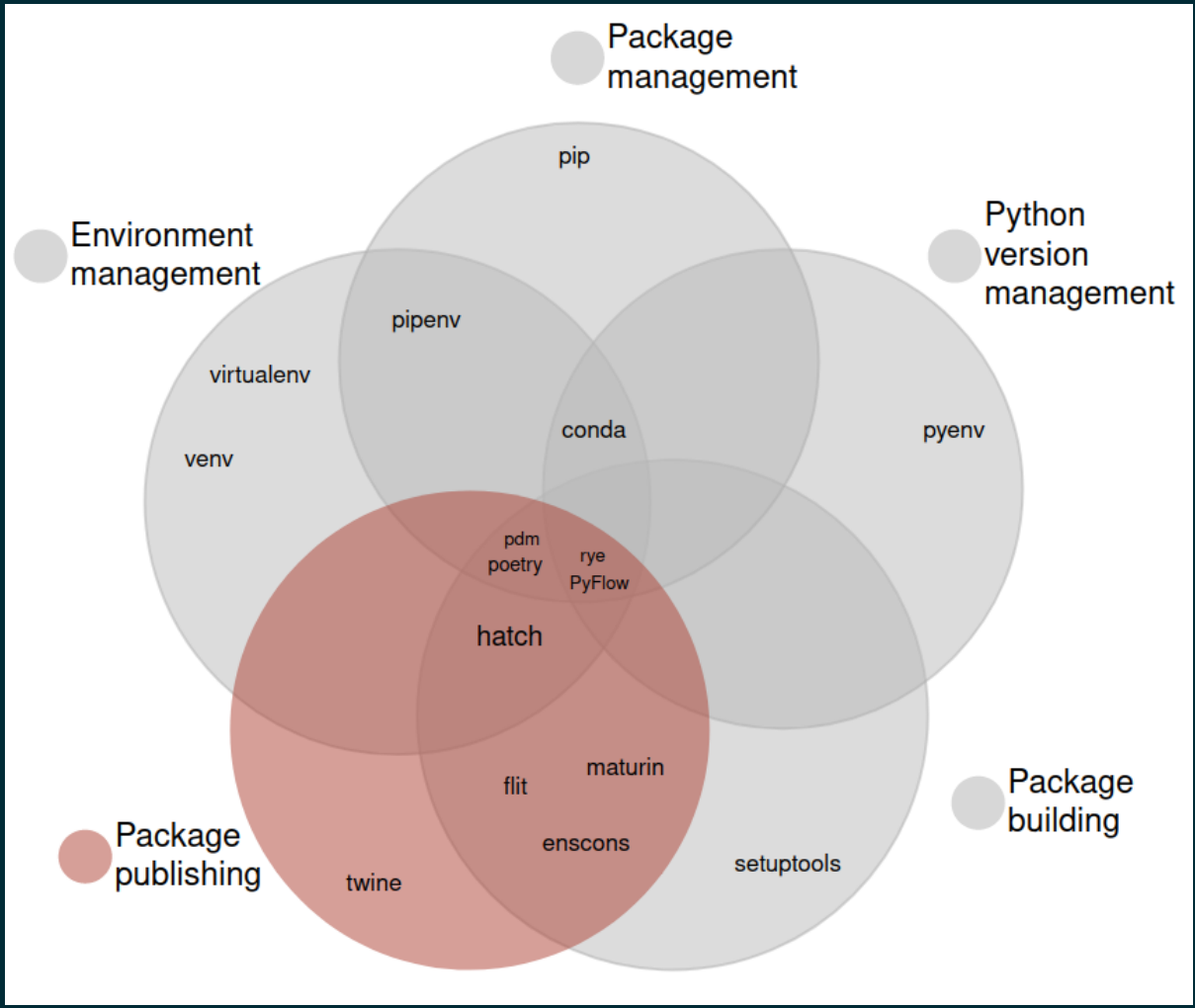
- Build package with build frontend: `python -m build`

PACKAGE PUBLISHING

DEFINITION

Publish package to PyPI or other index

TOOLS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TWINE

- Official PyPI tool to upload packages
- Also works with other indexes
- Single-purpose tool
- Main command: `twine upload dist/*`

RECAP II

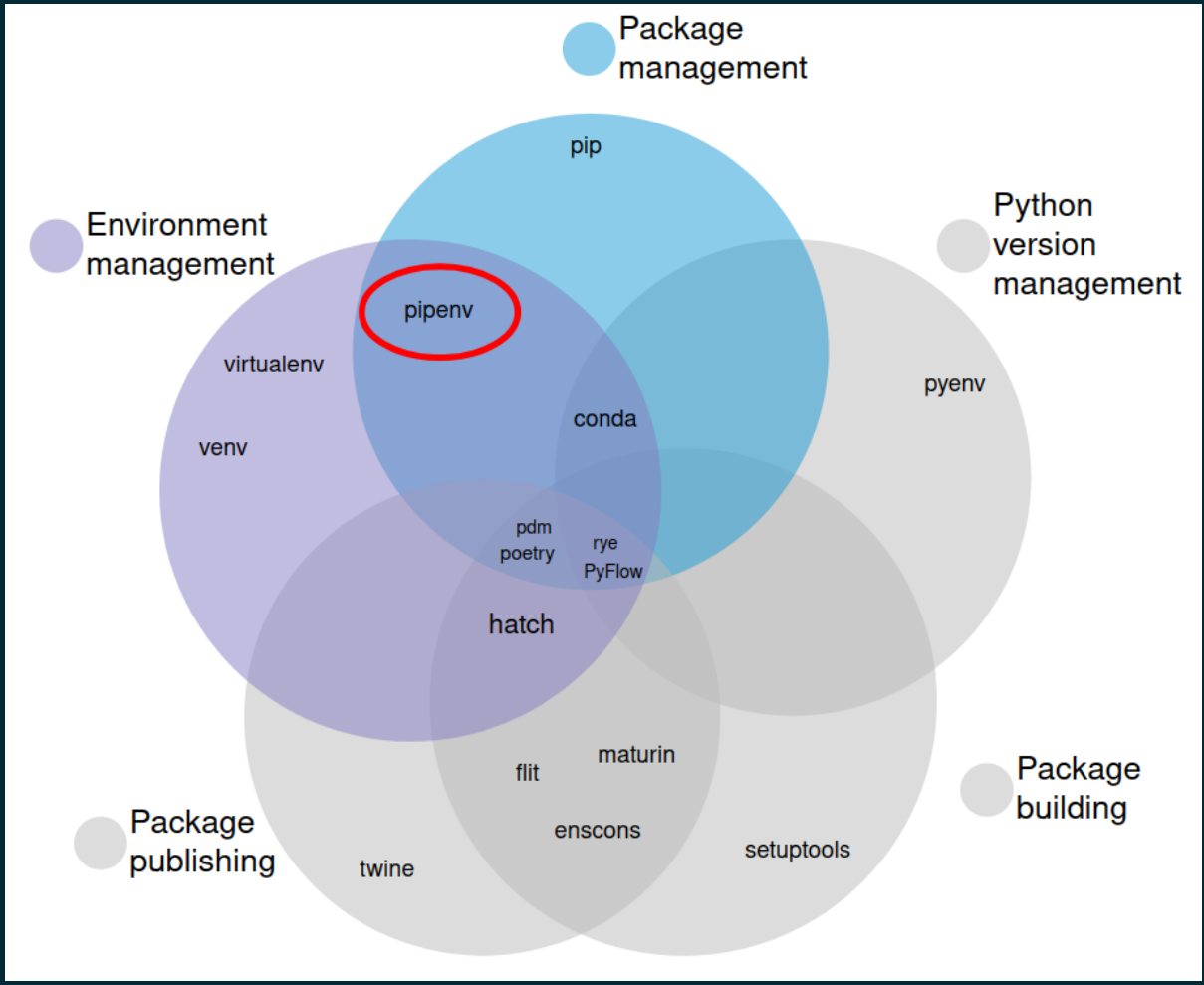
LOCK FILE

- Records exact versions of all dependencies installed for a project
- This enables reproducability of projects across multiple platforms
- Example file from `poetry`:

```
# This file is automatically @generated by Poetry and should not be changed by hand.

[[package]]
name = "attrs"
version = "22.1.0"
description = "Classes Without Boilerplate"
category = "main"
optional = false
python-versions = ">=3.5"
files = [
    {file = "attrs-22.1.0-py2.py3-none-any.whl", hash = "sha256:86efa402f67bf2df34f51a335487cf46b1ec130d02b8d39fd248abfd30da551c"},
    {file = "attrs-22.1.0.tar.gz", hash = "sha256:29adc2665447e5191d0e7c568fde78b21f9672d344281d0c6e1ab085429b22b6"},
]

[package.extras]
dev = ["cloudpickle", "coverage[toml] (>=5.0.2)", "furo", "hypothesis", "mypy (>=0.900,!=0.940)", "pre-commit", "pympler", "pytest (>=4.3.0)", "pytest-mypy-plug
docs = ["furo", "sphinx", "sphinx-notfound-page", "zope.interface"]
tests = ["cloudpickle", "coverage[toml] (>=5.0.2)", "hypothesis", "mypy (>=0.900,!=0.940)", "pympler", "pytest (>=4.3.0)", "pytest-mypy-plugins", "zope.interfac
tests-no-zope = ["cloudpickle", "coverage[toml] (>=5.0.2)", "hypothesis", "mypy (>=0.900,!=0.940)", "pympler", "pytest (>=4.3.0)", "pytest-mypy-plugins"]

[[package]]
name = "backports-cached-property"
version = "1.0.2"
description = "cached_property() - computed once per instance, cached as attribute"
category = "main"
optional = false
python-versions = ">=3.6.0"
files = [
    {file = "backports.cached-property-1.0.2.tar.gz", hash = "sha256:9306f9eed6ec55fd156ace6bc1094e2c86fae5fb2bf07b6a9c00745c656e75dd"},
    {file = "backports.cached_property-1.0.2-py3-none-any.whl", hash = "sha256:baeb28e1cd619a3c9ab8941431fe34e8490861fb998c6c4590693d50171db0cc"},
]
```

MULTI-PURPOSE TOOLS

PIPENV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PIPENV

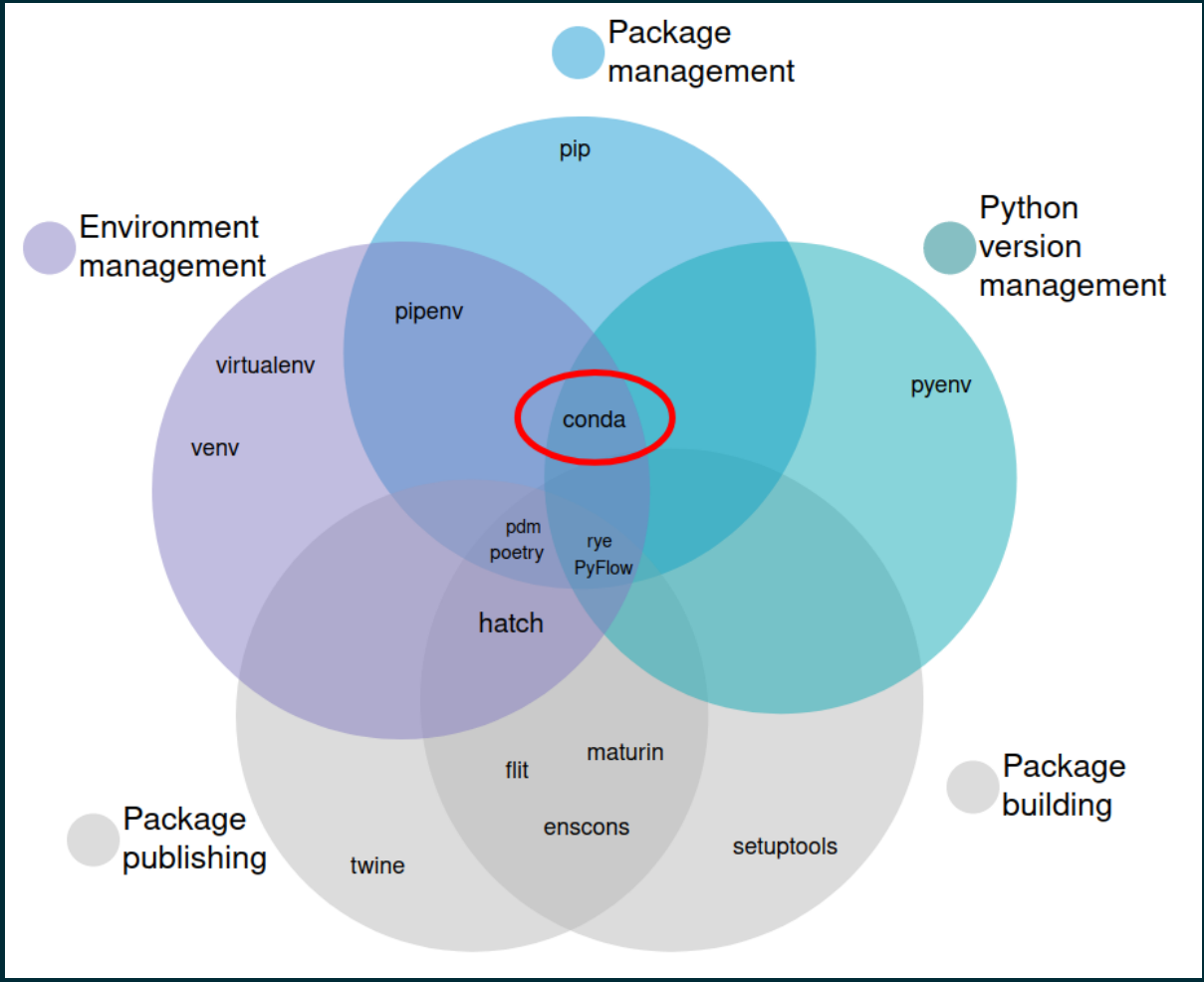
- Combines `pip` and `virtualenv`
- Introduces two additional files:
  - `Pipfile`
  - `Pipfile.lock` (replaces `requirements.txt`)
- Most important commands:

```
# Install package
pipenv install <package_name>

# Run Python script within virtual env
pipenv run <script_name.py>

# Activate virtual env
pipenv shell
```

CONDA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CONDA

- General-purpose package management system
- Uses its own index for packages

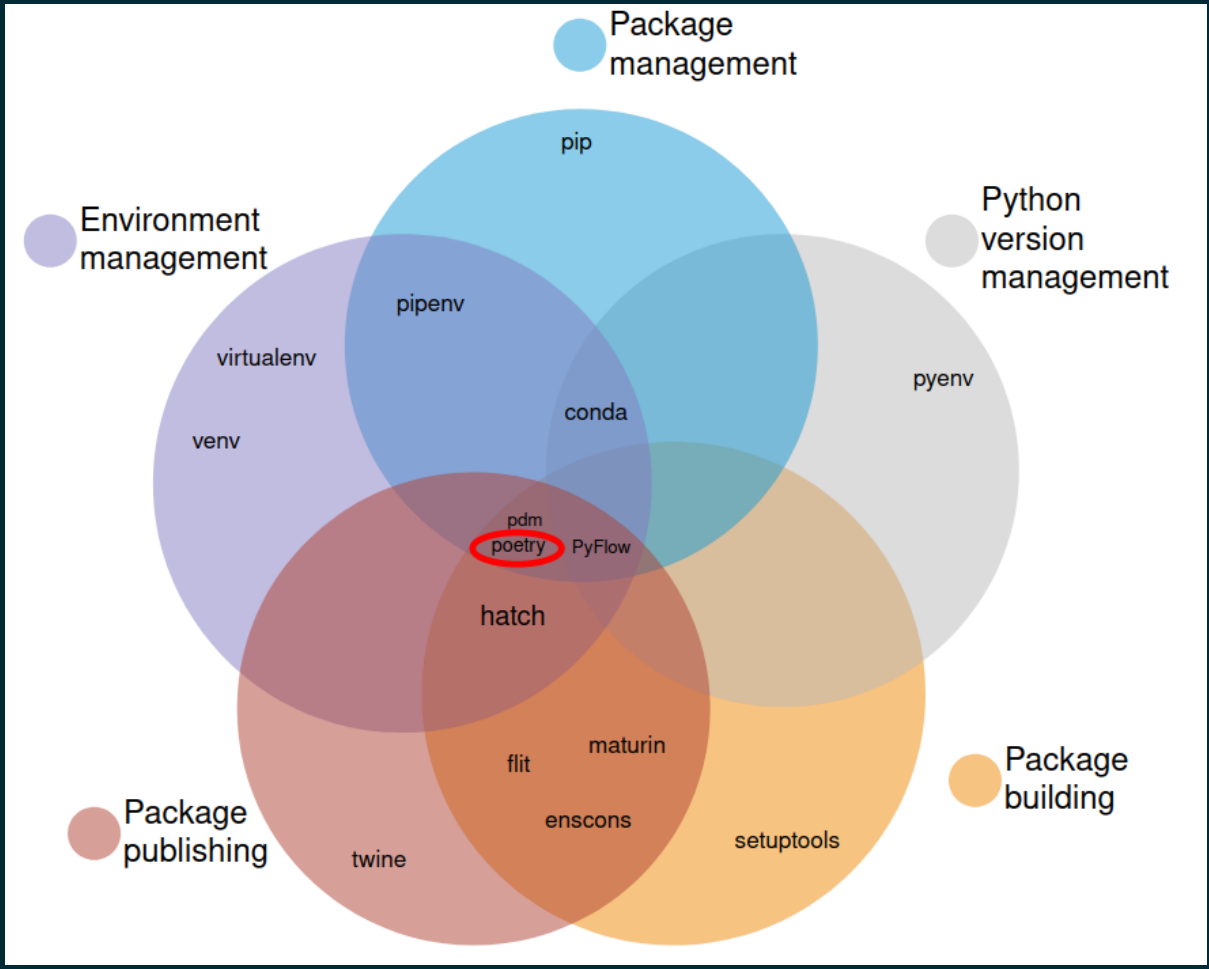
PACKAGING TOOLS

EVALUATION FEATURES

Manages dependencies	?
Resolves/locks dependencies	?
Clean build/publish flow	?
Allows to use plugins	?
Supports PEP 660 (editable installs)	?
Supports PEP 621 (project metadata)	?

POETRY

POETRY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CAPABILITIES

- Python version management: ❌
- Package management: ✅
- Environment management: ✅
- Building a package: ✅
- Publishing a package: ✅

FEATURE EVALUATION

Manages dependencies	✅
Resolves/locks dependencies	✅
Clean build/publish flow	✅
Allows to use plugins	✅
Supports PEP 660 (editable installs)	✅
Supports PEP 621 (project metadata)	❌

MAIN COMMANDS

```
# Create directory structure and pyproject.toml
poetry new <project_name>

# Create pyproject.toml interactively
poetry init

# Install package from pyproject.toml
poetry install
```

DEPENDENCY MANAGEMENT

```
# Add dependency
poetry add <package_name>

# Display all dependencies
poetry show --tree
```

RUNNING CODE

```
# Activate virtual env
poetry shell

# Run script within virtual env
poetry run python <script_name.py>
```

LOCK FILE

- When installing package, poetry resolves its dependencies and creates `poetry.lock`
- Updating dependencies to latest versions with `poetry update`

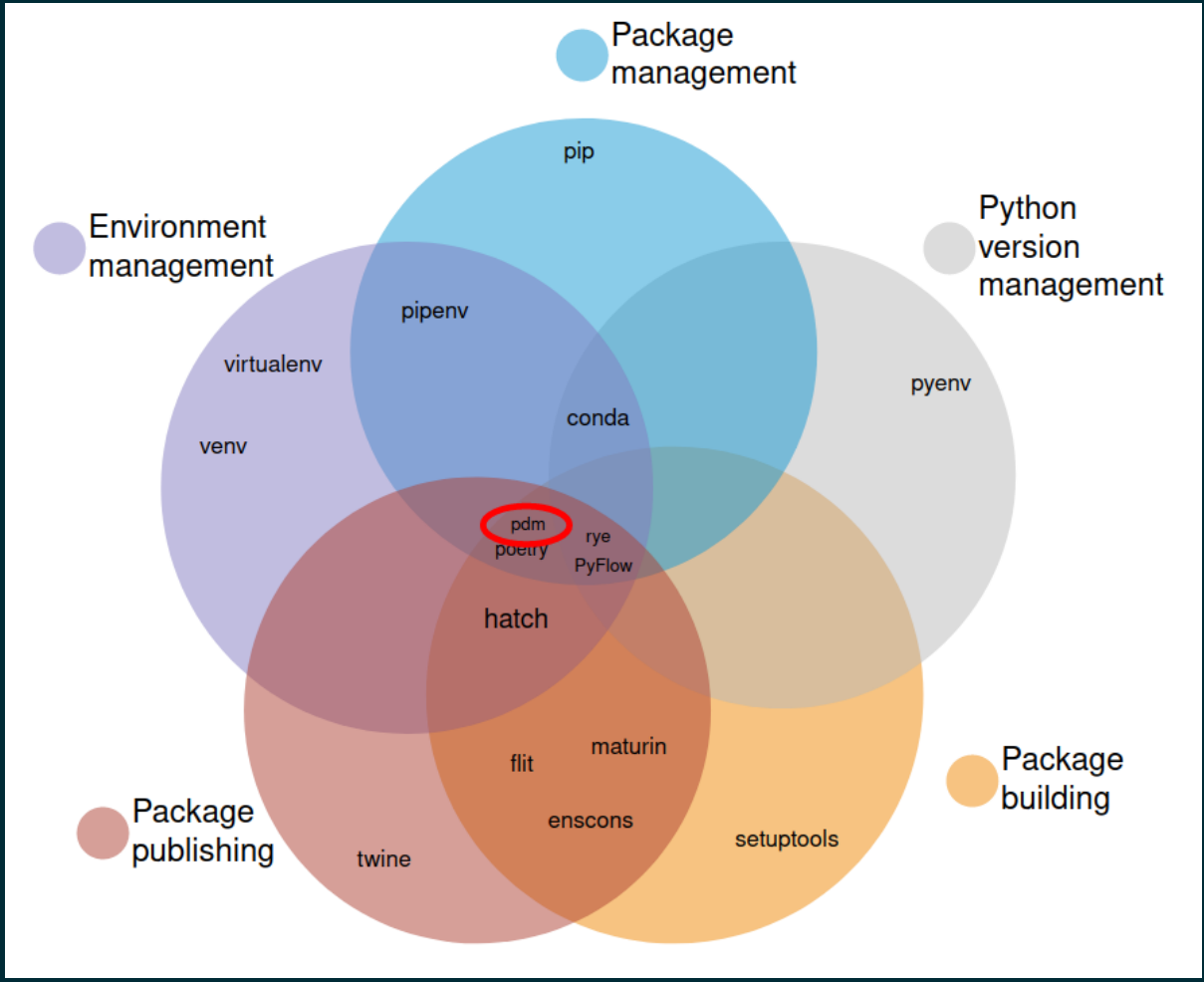
BUILD/PUBLISH FLOW

```
# Package code (creates `.tar.gz` and `.whl` files)
poetry build

# Publish to PyPi
poetry publish
```

PDM

PDM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PDM - CAPABILITIES

- Python version management: ❌
- Package management: ✅
- Environment management: ✅
- Building a package: ✅
- Publishing a package: ✅

PDM

- Strongly inspired by `poetry` and `pyflow`
- Requires Python 3.7 or higher
- Implements PEP 582 (local packages)
- Allows users to choose build backend

PDM - FEATURE EVALUATION

Manages dependencies	✅
Resolves/locks dependencies	✅
Clean build/publish flow	✅
Allows to use plugins	✅
Supports PEP 660 (editable installs)	✅
Supports PEP 621 (project metadata)	✅

MAIN COMMANDS

```
# Create pyproject.toml interactively
pdm init

# Install package from pyproject.toml
pdm install
```

DEPENDENCY MANAGEMENT

```
# Add dependency
pdm add <package_name>

# Display all dependencies
pdm list --graph
```

RUNNING CODE

```
# No pdm shell command

# Run script within env
pdm run python <script_name.py>
```

LOCK FILE

- Similar to poetry
- When installing package, pdm resolves its dependencies and creates `pdm.lock`
- Updating dependencies to latest versions with `pdm update`

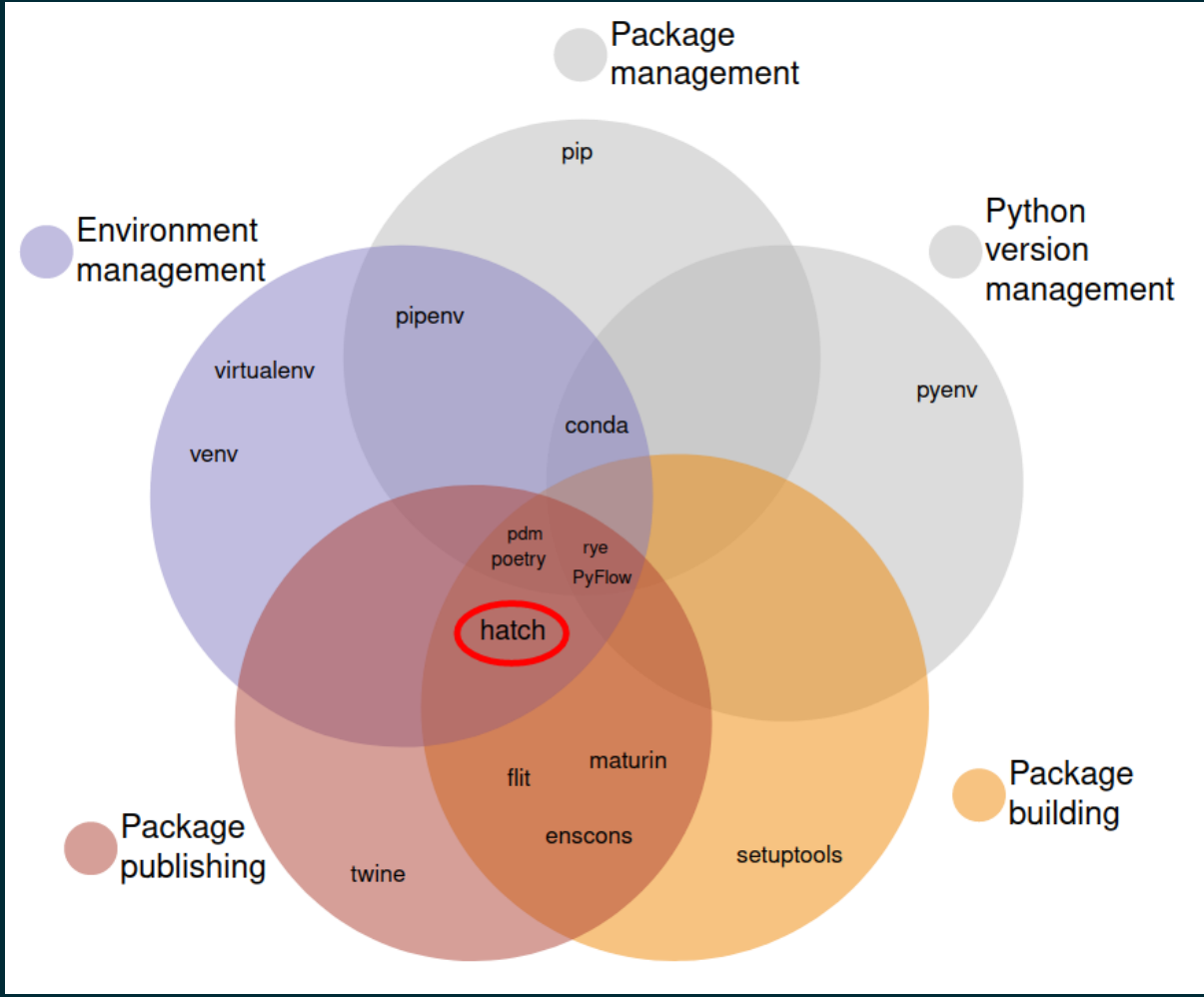
BUILD/PUBLISH FLOW

```
# Package code (creates `.tar.gz` and `.whl` files)
pdm build

# Publish to PyPi
pdm publish
```

HATCH

HATCH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HATCH - CAPABILITIES

- Python version management: ❌
- Package management: ❌
- Environment management: ✅
- Building a package: ✅
- Publishing a package: ✅

HATCH - FEATURE EVALUATION

Manages dependencies	❌
Resolves/locks dependencies	❌
Clean build/publish flow	✅
Allows to use plugins	✅
Supports PEP 660 (editable installs)	✅
Supports PEP 621 (project metadata)	✅

CREATING A NEW PROJECT

```
# Create directory structure and pyproject.toml
hatch new <project_name>

# Interactive mode
hatch new -i <project_name>

# Initialize existing project / create pyproject.toml
hatch new --init
```

DEPENDENCY MANAGEMENT

```
# Packages are added manually to pyproject.toml
hatch add <package_name> # This command doesn't exist!

# Display dependencies
hatch dep show table
```

RUNNING CODE

```
# Activate virtual env
hatch shell

# Run script within virtual env
hatch run python <script_name.py>
```

BUILD/PUBLISH FLOW

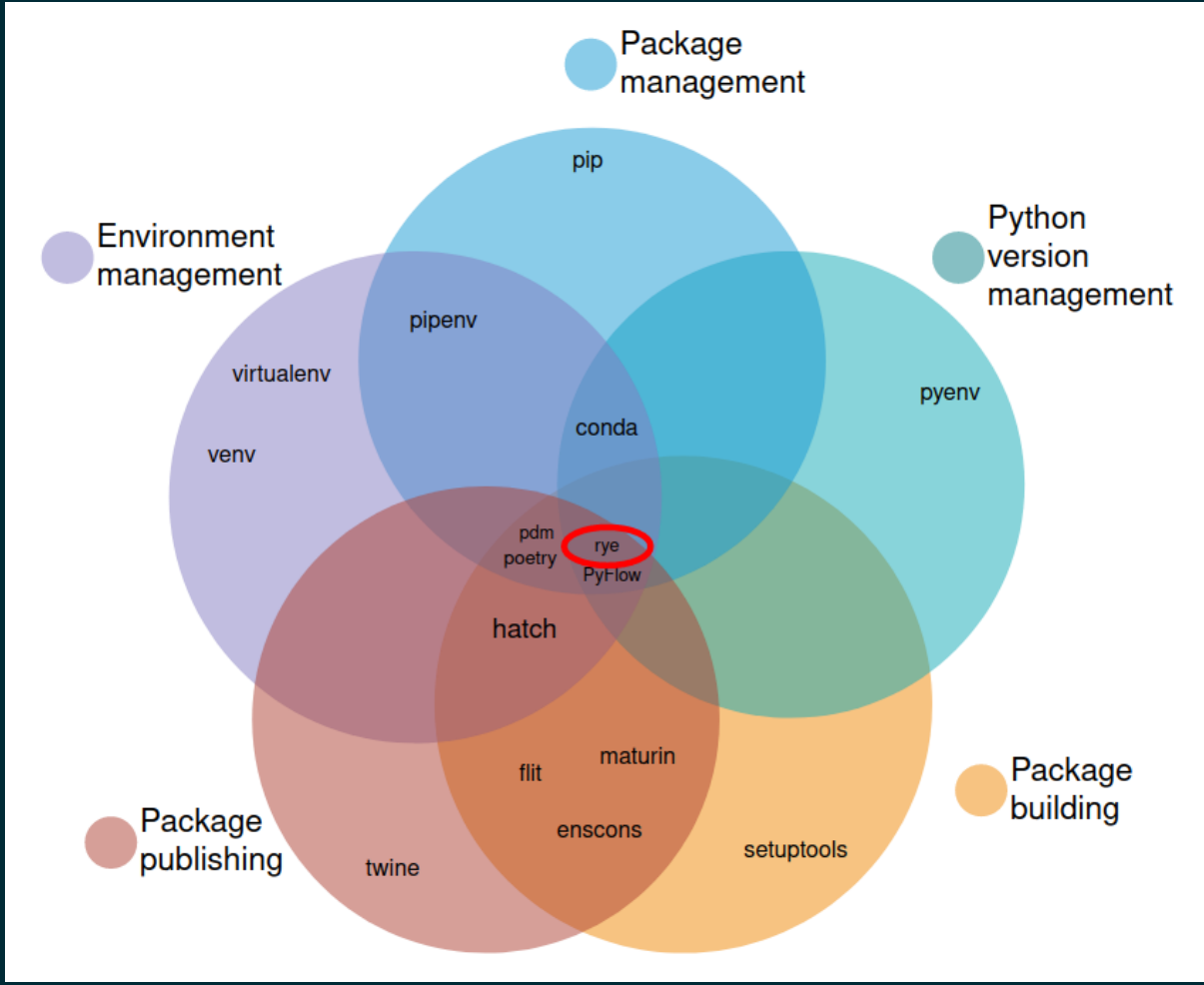
```
# Package code (creates `.tar.gz` and `.whl` files)
hatch build

# Publish to PyPi
hatch publish
```

DECLARATIVE ENVIRONMENT MANAGEMENT

- Environments can be configured within `pyproject.toml`
- We can define scripts for an environment
- Example use case: code formatting

RYE

RYE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RYE - CAPABILITIES

- Python version management: ✅
- Package management: ✅
- Environment management: ✅
- Building a package: ✅
- Publishing a package: ✅

RYE

- Very new (first release May 2023)
- Inspired by rustup and cargo from Rust
- Written in Rust

RYE - FEATURE EVALUATION

Manages dependencies	✅
Resolves/locks dependencies	✅
Clean build/publish flow	✅
Allows to use plugins	❌
Supports PEP 660 (editable installs)	✅
Supports PEP 621 (project metadata)	✅

CREATING A NEW PROJECT

```
# Create directory structure and pyproject.toml
rye init <project_name>

# Pin a Python version
rye pin 3.10
```

DEPENDENCY MANAGEMENT

```
# Add dependency - this does not install the package!
rye add <package_name>

# Synchronize virtual envs, lock file, etc.
# This install packages and Python versions
rye sync
```

RUNNING CODE

```
# Activate virtual env
rye shell

# Run script within virtual env
rye run python <script_name.py>
```

BUILD/PUBLISH FLOW

```
# Package code (creates `.tar.gz` and `.whl` files)
rye build

# Publish to PyPi
rye publish
```

SUMMARY - PACKAGING TOOLS

	poetry	pdm	hatch	rye
Manages dependencies	✅	✅	❌	✅
Resolves/locks dependencies	✅	✅	❌	✅
Clean build/publish flow	✅	✅	✅	✅
Supports plugins	✅	✅	✅	❌
PEP 660 (editable installs)	✅	✅	✅	✅
PEP 621 (project metadata)	❌	✅	✅	✅

THE END