

Software Design for Data Science

Virtual Environments

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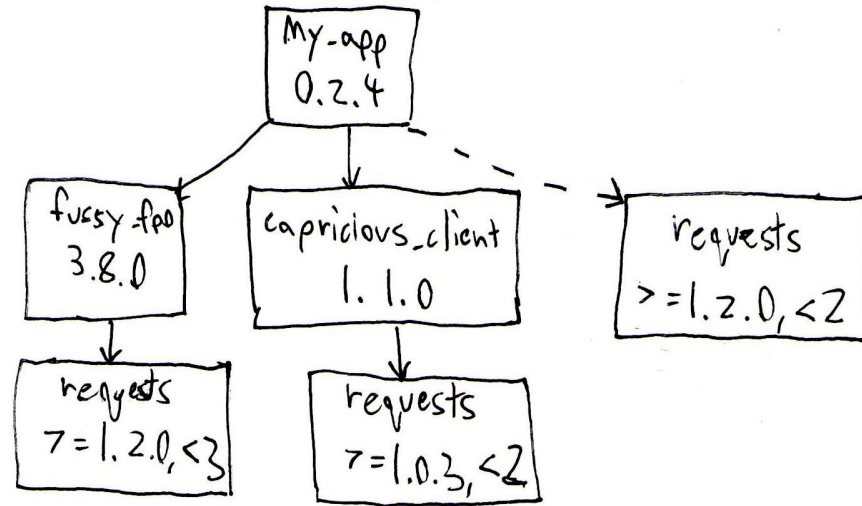


The problem

- Melissa is working on a project.
- Melissa installs scikit-learn to use in the project.
- Melissa writes great tests, which pass!
- Baisakhi wants to contribute to the GitHub repository
- Baisakhi clones the repository
- Nothing works for Baisakhi because she hasn't installed scikit-learn (or any other packages required by the project)!

The problem: dependency hell

- Dependency chains (A depends on B depends on C ...)
- Conflicting dependencies
- Circular dependencies (A depends on B depends on A)



The problem, continued

- Baisakhi and Melissa may be using different systems
 - Mac
 - Windows
- Baisakhi and Melissa may have different versions of Python
- Baisakhi and Melissa may have different Python packages installed

- We need a way so that the code will always work for both Baisakhi & Melissa
 - And for anyone else who wants to use the package!

Abstraction

Hiding the details of the implementation (ie the infrastructure)



Abstraction for Melissa & Baisakhi

We want to hide away the details of the underlying system and make it so that when Melissa & Baisakhi work on the project, they see the same things:

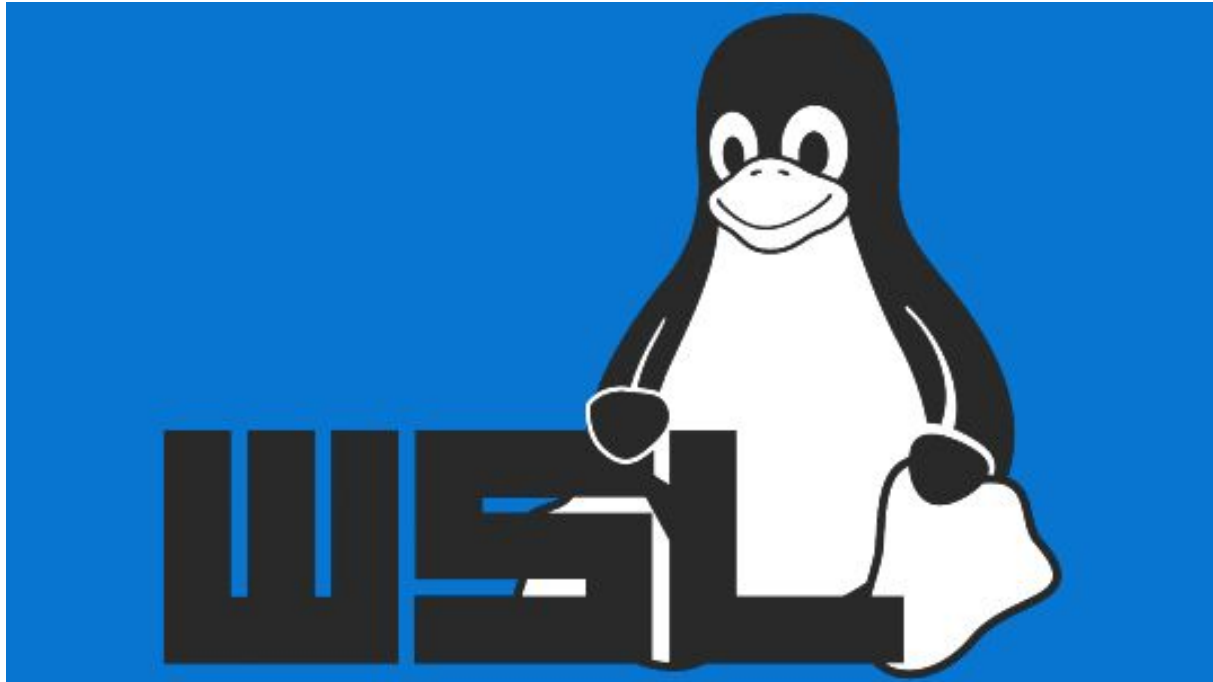
- The same Python version
- The same packages
- The same package versions
- etc

Virtualization

The act of creating a virtual (rather than actual) version of something at the same abstraction level, such as an environment, process, operating system, or hardware.

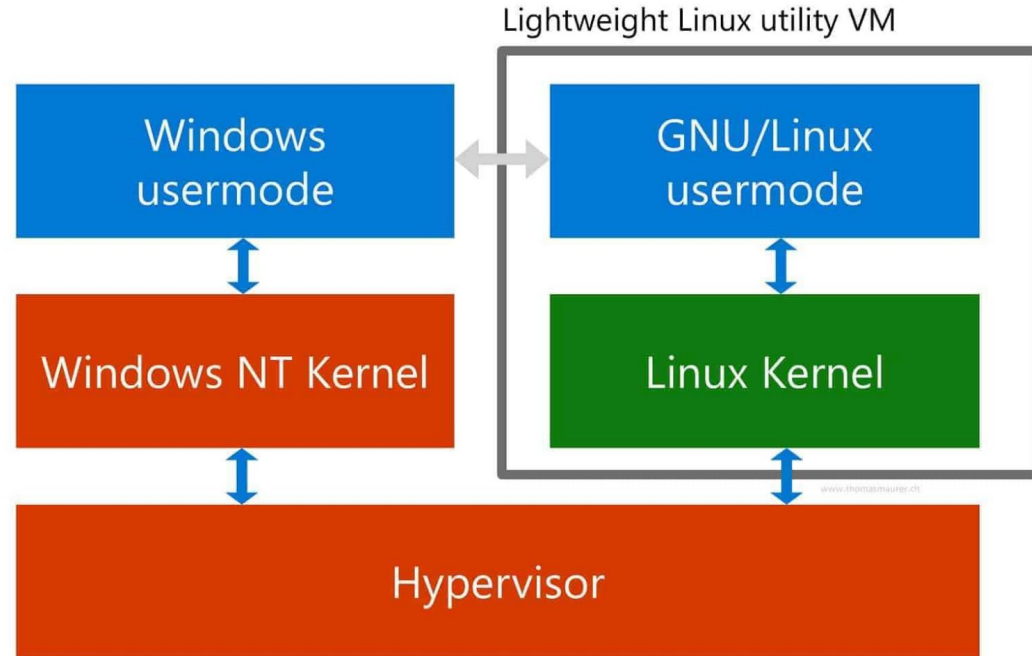
Virtualization example

Hardware, eg VirtualBox



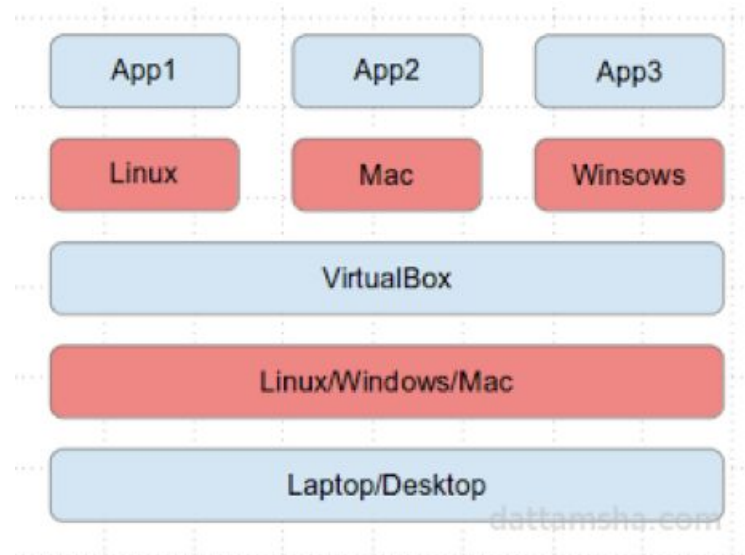
Virtual Machines - WSL

WSL 2 architecture overview



Virtual Machines - VirtualBox

- <https://www.virtualbox.org>
- Open source, free, and just works
- Uses processor level virtualization instructions to operate guest operating system
- Choose the right guest type
- Allocate enough resources
- Always install guest additions



Virtual Machines - EC2

- Start with a base operating system image
- Install software you want
- Create any data volumes, etc. you want
- Halt the instance
- Make an Amazon Machine Image
- Publish
- Pay for S3 storage, use a paid AMI model...

Virtualization of Python environments

- For Melissa & Baisakhi, we need to virtualize *environment*
 - Python version
 - Package dependency versions
- Separate your *computer's* Python/packages from the *project's* Python/packages
- Multiple options
 - venv
 - virtualenv
 - conda

Conda Virtual Environments

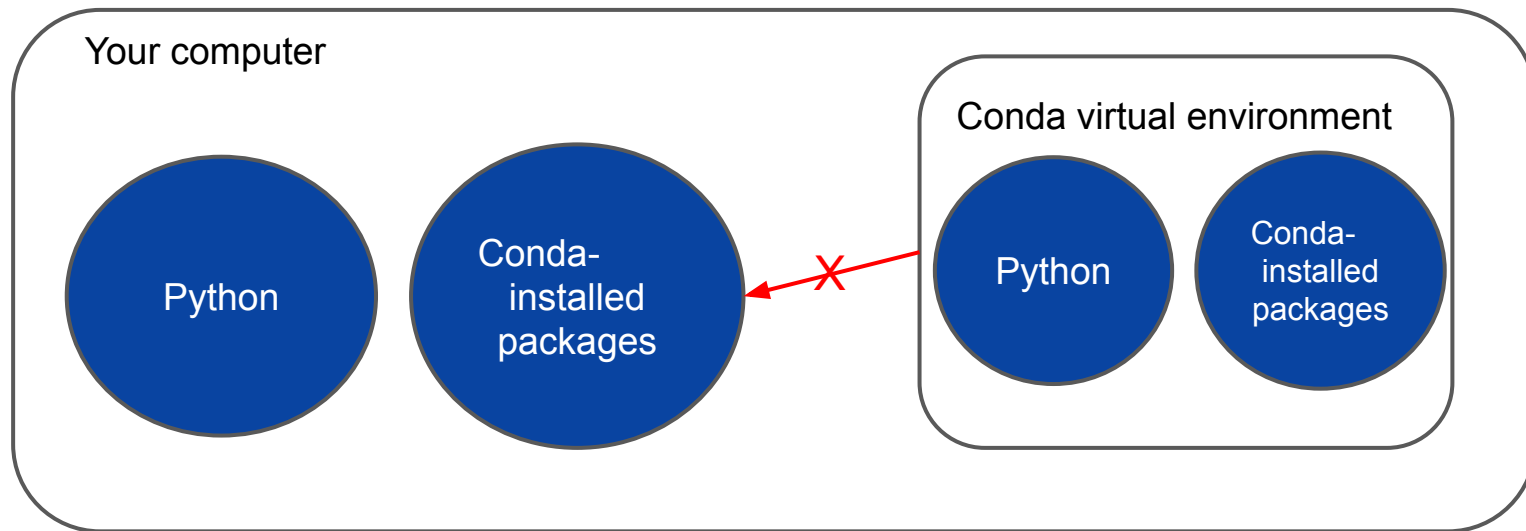
- `conda create -n <name> <options>`
 - Creates a new environment with the given name
- `conda activate <name>`
 - “Activates” the environment (“switches into it”, like a git branch)
- Anything you do now will affect only the *current* environment
 - Installing packages
 - Updating package versions
- `conda deactivate`
 - “Deactivates” the environment (“switches off of it”, like switching back to git’s main branch)
- `conda remove --name <name> --all`
 - Deletes the environment
- `conda info --envs`
 - Lists all the environments that exist

Exercise: Create a Python Virtual Environment

- Create a conda environment for SPECIFICALLY Python 3.8.15
 - Hint: use `conda create`
 - Hint: don't forget to activate the environment!
 - Hint: check the options on the `conda create` command to see how to set Python version
- Start up a Jupyter notebook and prove that it's Python 3.8.15
 - Hint: remember that the new environment doesn't have access to your global packages!
 - Hint: check out the `platform` module for how you might access the Python version

Python Virtual Environments

What just happened?



Sharing your virtual environment

- `conda env export > environment.yml`
 - Encodes all of the Python and package information in your environment to `environment.yml`
 - Format is [YAML](#), a human-readable data serialization language
- `conda env create -f environment.yml`
 - Creates a new environment from a file, with all of its specified packages
- `conda env update -f environment.yml`
 - Updates your environment to match the `environment.yml` file
 - Useful if your teammates are adding packages - do it after you pull
 - Useful to upgrade packages
- Always commit the `environment.yml` file to the repository!

Exercise: Create an environment.yml file

For your Python 3.8.15 environment:

1. Create an environment.yml file:

```
conda env export > environment.yml
```

2. Delete the existing environment so that we can practice creating from yml:

```
conda deactivate  
conda remove --name <name> --all
```

3. Recreate the environment from the yml file:

```
conda env create -f environment.yml
```

4. Prove that it works - start up your Jupyter notebook again.

Generated environment.yml

```
name: py3815
channels:
  - defaults
```

← Name for the environment
← Where Conda can find packages (default location)

```
dependencies:
  - anyio=3.5.0=py38hca03da5_0
  - appnope=0.1.2=py38hca03da5_1001
  - argon2-cffi=21.3.0=pyhd3eb1b0_0
  - argon2-cffi-bindings=21.2.0=py38h1a28f6b_0
  - asttokens=2.0.5=pyhd3eb1b0_0
  - attrs=22.1.0=py38hca03da5_0
  - babel=2.11.0=py38hca03da5_0
  - backcall=0.2.0=pyhd3eb1b0_0
  - beautifulsoup4=4.11.1=py38hca03da5_0
  - bleach=4.1.0=pyhd3eb1b0_0
  - brotli=0.7.0=py38h1a28f6b_1002
```

All the packages that conda has installed in this environment

This includes transitive dependencies (ie the packages that Jupyter depends on)

Not necessary for other people

```
prefix: /Users/melissawinstanley/opt/miniconda3/envs/py3815
```

Simpler environment.yml

```
name: py3815
channels:
  - defaults
dependencies:
  - jupyter=1.0.0
  - notebook=6.5.2
  - python=3.8.15
```

- No prefix
- Only explicitly needed dependencies



What does this number mean?

Semantic Package Versioning

Also known as “semver”

NOT ALL PACKAGES ADHERE TO THIS THOUGH! Do your research.

Extra stuff

Extra info about release or build (eg for specifying “pre-release” or beta release)

6.5.2

Major version number

This changes when the package has
BREAKING CHANGES

Minor version number

This changes when the package has new
backwards-compatible
features

Patch version number

This changes when the package has bug fixes

What I would probably do

```
name: py3815
channels:
  - defaults
dependencies:
```

```
- jupyter=1
- notebook=6
- python=3.8
```

These two packages adhere to semantic versioning.

This way I automatically get any new versions just by doing
`conda env update`

Python doesn't adhere to semantic versioning

You don't HAVE to do it this way - use more specific package versions if you like!
You can also omit package versions (everything after the "="), although it's less safe.

What about pip?

If you use pip to manage packages:

- `environment.yml => requirements.txt`
 - Looks similar!
- Can create from the environment in a similar way

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

- Can reinstall all the requirements into the current environment

```
pip install -r requirements.txt
```

- This does NOT create a new environment
- You can combine `environment.yml` (for the environment) with `requirements.txt` (for managing packages with pip) if you like


Adding pip to environment.yml

```
name: py3815
channels:
  - defaults
dependencies:
  - jupyter=1
  - notebook=6
  - python=3.8
  - pip
  - pip:
    - matplotlib
    - pandas
```

Add pip dependencies by adding a
color after another "pip", then
indenting an extra level, then
adding the pip dependencies

Or with requirements.txt

```
name: py3815
channels:
  - defaults
dependencies:
  - jupyter=1
  - notebook=6
  - python=3.8
  - pip
  - pip:
    - -r requirements.txt
```



Tell conda to load pip
dependencies from
requirements.txt

Exercise: Simplify your environment.yml

For your Python 3.8.15 environment:

1. Simplify your environment.yml file.
 - Remove any unnecessary packages.
 - Simplify the version numbers if you like.
2. Update your environment.

```
conda env update -f environment.yml
```

3. Prove that it works - start up your Jupyter notebook again.

What about other dependencies?

- Conda environments are for Python & Python packages
- If you need to download other tools or infrastructure, you'll have to do that in a separate script or with a different version manager.

Exercise: create a virtual environment for your project

1. Create an environment for your team's project.
2. Create an `environment.yml` file for the environment.
Include any packages that you need to make your code work.
3. Commit, create a PR, and merge the change.
4. Make sure everyone on the team can create the environment from the file.
5. Include instructions for how to use the environment file in your documentation (`README` or somewhere in the `docs` folder).