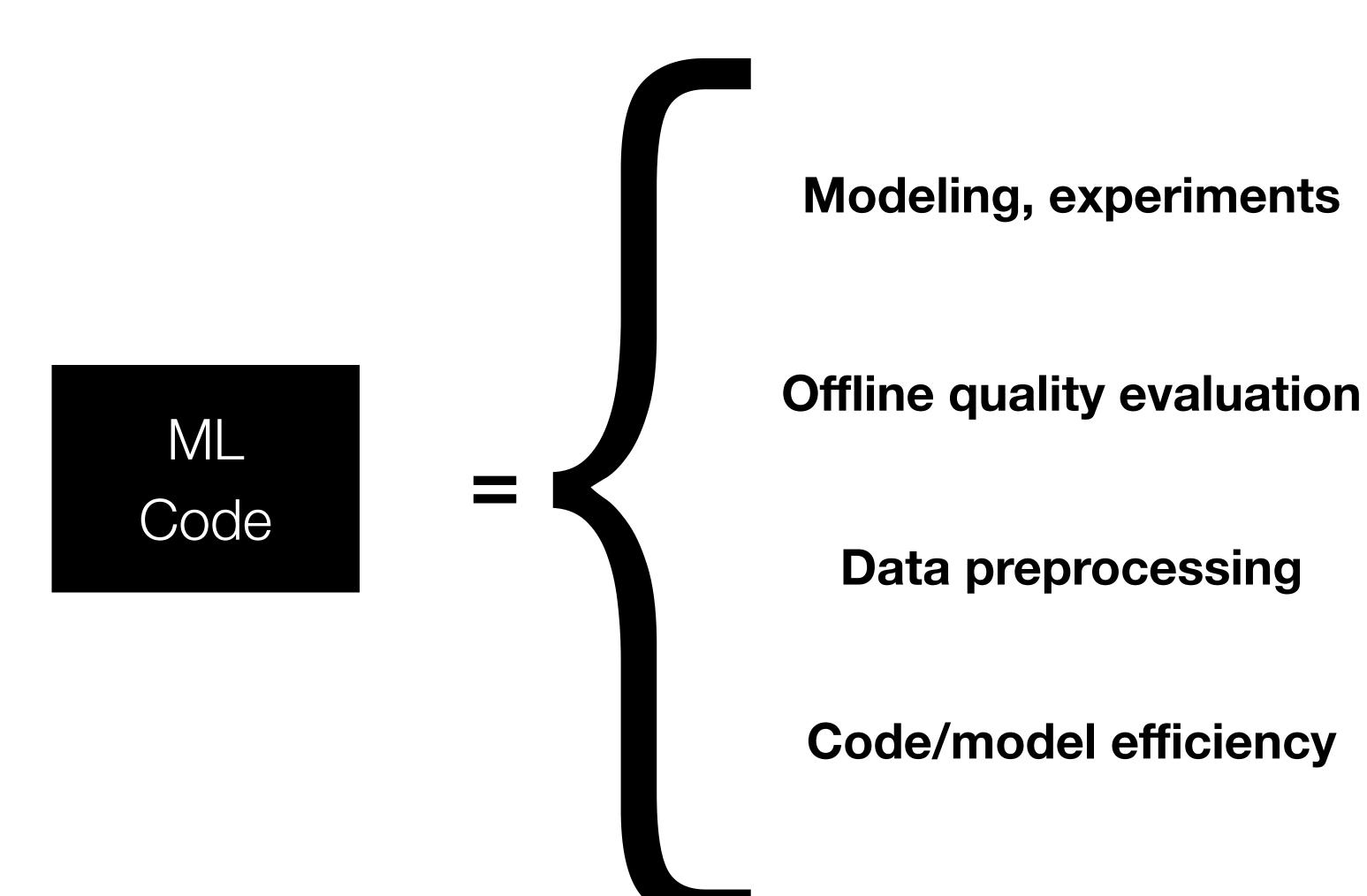
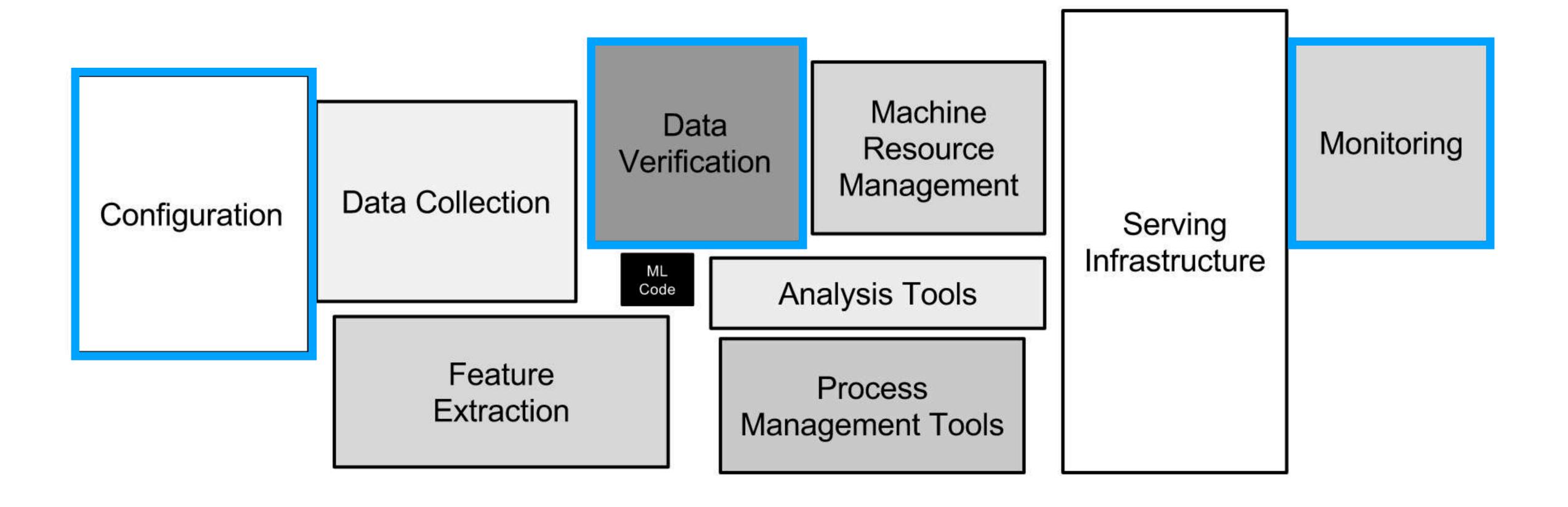
Efficient Deep Learning Systems Experiment management & ML code testing Max Ryabinin

Teaser



Teaser



Plan for today

- How (and why) to track your DL experiments
- Making your environment reproducible
- Versioning your data and models along with the code
- Flexible configuration of Python code
- Testing in general and for ML purposes

Tracking experiments: motivation

- Usually, training a model once is not enough:
 - The data gets updated
 - Hyperparameters need tuning
 - We want to modify the training code for better quality
- For all these cases, we need a way to keep track of our experiments
- Even more important in a <u>collaborative</u> setup

What to track

- Obviously, we want a table with run IDs and final metrics
- What else?
 - Plots with per-step/per-second metrics (convergence & performance)
 - Git commit hash for reproducibility (and diff for local changes!)
 - Visualizations of model inputs/outputs
 - Stdout/stderr of your training script (invest time in good logs)
 - In some cases, full info about the environment

How to track

- There are many tools for that [1,2,3,4,5]
- Range from "just upload the logs" to fullfledged tracking of the entire environment
- Self-hosted versions are available

- [1] https://www.wandb.com/
- [2] https://www.comet.ml/
- [3] https://neptune.ai/
- [4] https://tensorboard.dev/
- [5] https://clear.ml/

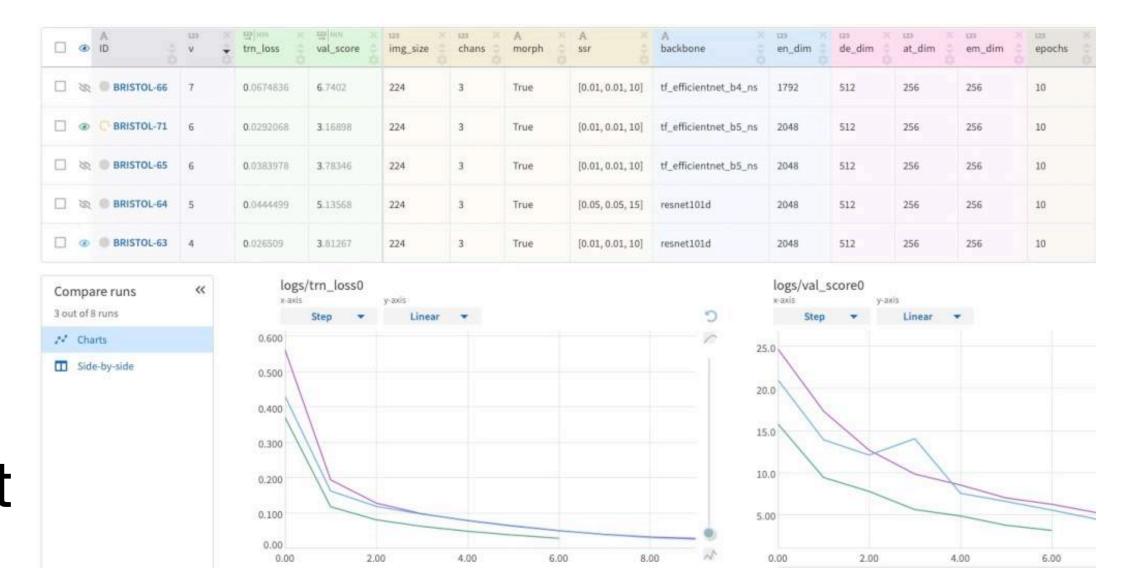


TABLE VIEW			PARALLEL COORDINATES VIEW		SCATTER PLOT MATRIX VIEW
Trial ID	Show Metrics	model	accuracy_test	lr	train_loss
1b2758da0f912		ViT-L_32	0.82009	1.9467e-10	0.42093
606b401e6f84		ViT-B_16	0.84609	1.9467e-10	1.0754
60c54527f120		ViT-L_16	0.85066	1.9467e-10	0.65612
6c5951c20e95		ViT-B_32	0.81788	1.9467e-10	1.3841
85c586a058ca		ViT-B_16	0.84621	1.9467e-10	0.45114
a2316e5f8b991		ViT-L_16	0.85050	1.9467e-10	0.40394
c32186203a97		ViT-B_32	0.81790	1.9467e-10	1.4536
f853f3481c8db		ViT-L_32	0.81780	1.9467e-10	0.81554

Dependency versioning

- Large Python projects involve numerous dependencies
- Over time, this presents multiple issues:

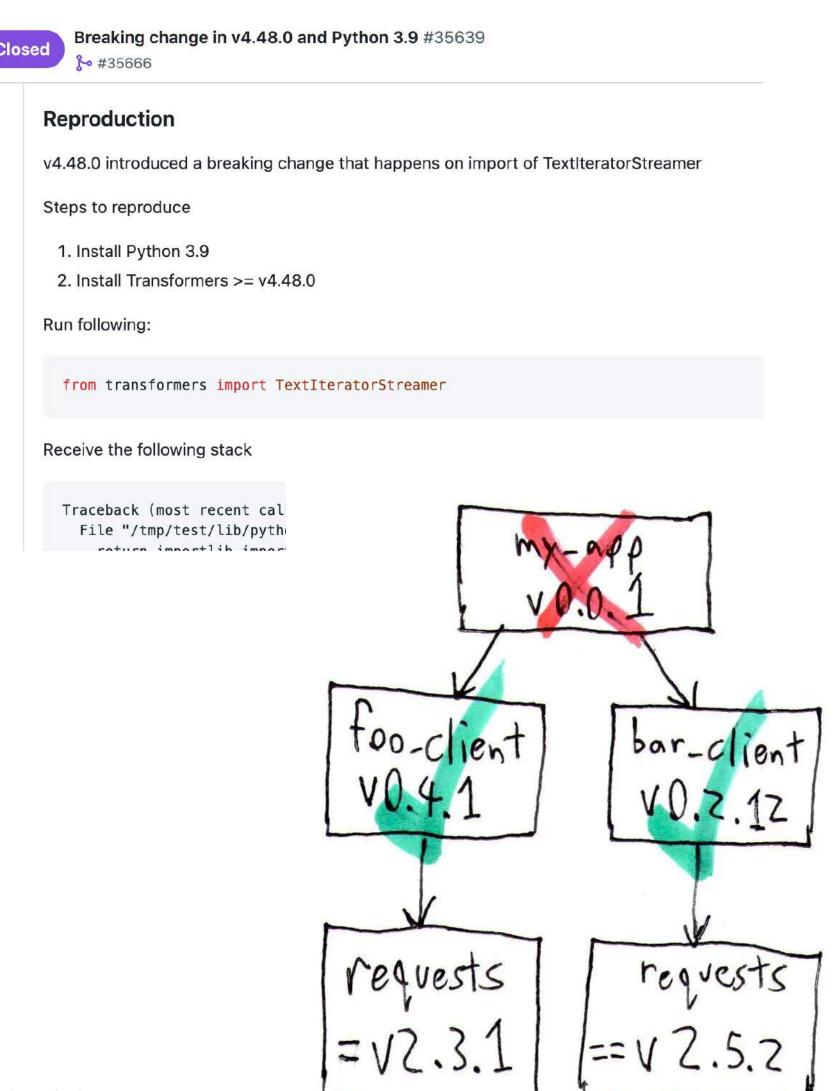
Summary: State-of-the-art Machine Learning for JAX, PyTorch and TensorFlow Latest version: 4.48.1

Required dependencies: filelock | huggingface-hub | numpy | packaging | pyyaml | regex | requests | safetensors | tokenizers | tqdm

Optional dependencies: accelerate | av | beautifulsoup4 | blobfile | codecarbon | cookiecutter | datasets | deepspeed | diffusers | dill | evaluate | faiss-cpu | fastapi | filelock | flax | ftfy | fugashi | gitpython | huggingface-hub | importlib-metadata | ipadic | isort | jax | jaxlib | kenlm | keras | keras-nlp | libcst | librosa | natten | nltk | numpy | onnxconverter-common | onnxruntime | onnxruntime-tools | opencv-python | optax | optimum-benchmark | optuna | packaging | parameterized | phonemizer | pillow | protobuf | psutil | pyctcdecode | pydantic | pytest | pytest-asyncio | pytest-rich | pytest-timeout | pytest-xdist | ray | regex | requests | rhoknp | rich | rjieba | rouge-score | ruff | sacrebleu | sacremoses | sagemaker | scikit-learn | scipy | sentencepiece | sigopt | starlette | sudachidict-core | sudachipy | tensorboard | tensorflow | tensorflow-cpu | tensorflow-probability | tensorflow-text | tf2onnx | tiktoken | timeout-decorator | timm | tokenizers | torch | torchaudio | torchvision | tqdm | unidic | unidic-lite | urllib3 | uvicorn

Dependency versioning

- Large Python projects involve numerous dependencies
- Over time, this presents multiple issues:
 - Version upgrades lead to breaking changes
 - Different libraries might have different transitive dependencies
 - Crucial dependencies are simply not specified



Img src: medium.com/knerd/the-nine-circles-of-python-dependency-hell-481d53e3e025

Dependency versioning tools

Several solutions for this exist:

- The simplest one: pip freeze>requirements.txt

 Works, but hard to upgrade + your project will be tough to depend on
- Better: <u>PEP 508</u> version constraints
 Upgrades are still hard, and transitive dependencies are not tracked

```
requirements.txt — Edited

contourpy==1.0.6

cycler==0.11.0

fonttools==4.38.0

joblib==1.2.0

kiwisolver==1.4.4

matplotlib==3.6.2

numpy==1.23.5

packaging==21.3

pandas==1.5.2

patsy==0.5.3

Pillow==9.3.0

plotly==5.11.0

pyparsing==3.0.9

python-dateutil==2.8.2
```

```
SomeProject
SomeProject == 1.3
SomeProject >= 1.2, < 2.0
SomeProject[foo, bar]
SomeProject ~= 1.4.2
SomeProject == 5.4; python_version < '3.8'
SomeProject; sys_platform == 'win32'
requests [security] >= 2.8.1, == 2.8.*; python_version < "2.7"</pre>
```

Img src: <u>betterdatascience.com/python-pipreqs</u>

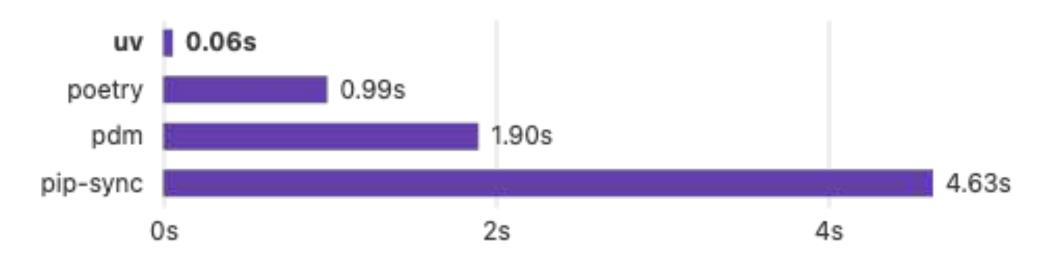
Dedicated versioning tools

- Poetry introduces a lockfile which specifies all permissible dependencies with their versions
 - Manages Python versions as well!

```
[metadata.files]
     astroid = [
         {file = "astroid-2.9.3-py3-none-an
825
         {file = "astroid-2.9.3.tar.gz", ha
826
827
     atomicwrites = [
         {file = "atomicwrites-1.4.0-py2.py
         {file = "atomicwrites-1.4.0.tar.gz
830
831
    attrs = [
         {file = "attrs-21.4.0-py2.py3-none
833
         {file = "attrs-21.4.0.tar.gz", has
834
835
     basedmypy = [
         {file = "basedmypy-1.2.2-py3-none-
837
         {file = "basedmypy-1.2.2.tar.gz",
838
839
     basedtyping = []
                           You, 3 days ago
     beautifulsoup4 = [
         {file = "beautifulsoup4-4.10.0-py3
842
         {file = "beautifulsoup4-4.10.0.tar
845 black = [
         {file = "black-21.12b0-py3-none-an
846
847 {file = "black-21,12b0,tar.gz", ha
```

Dedicated versioning tools

- Poetry introduces a lockfile which specifies all permissible dependencies with their versions
 - Manages Python versions as well!
- uv offers similar functionality while being a much faster replacement of pip



Creating virtual environments (replacing venv and virtualenv):

• uv venv: Create a new virtual environment.

See the documentation on using environments for details.

Managing packages in an environment (replacing pip and pipdeptree):

- uv pip install: Install packages into the current environment.
- uv pip show: Show details about an installed package.
- uv pip freeze: List installed packages and their versions.
- uv pip check: Check that the current environment has compatible packages.
- uv pip list: List installed packages.
- uv pip uninstall: Uninstall packages.
- uv pip tree: View the dependency tree for the environment.

See the documentation on managing packages for details.

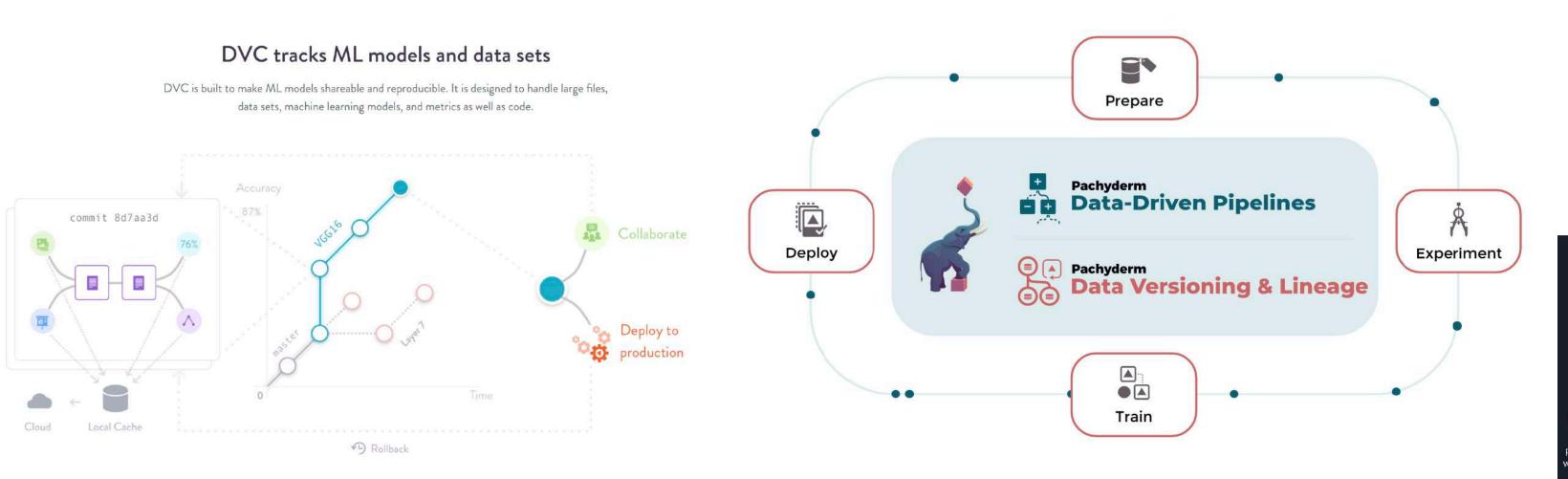
python-poetry.org
docs.astral.sh/uv

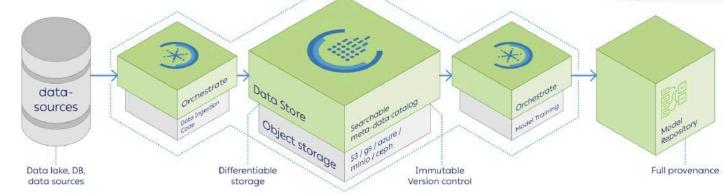
Data versioning

- Code is not the only component in your system
- Data is a crucial dependency, especially in complicated pipelines
- Tracking changes in it is equally important
- Pinning each experiment to its data enhances reproducibility

Solutions

- Several existing projects allow to integrate artifact versioning into pipelines
- Support external storage, matching with commits, metric comparison
- Possible to rerun specific parts of the pipeline on data/config change







Configuration

- As your project grows, the number of "moving parts" increases
 - Infrastructure: API endpoints, data URLs, etc.
 - Model hyperparameters and components
- Changing them manually across the entire repo is not sustainable
- argparse/click-based solutions are hard to write and properly version
- Hardcoding values in dedicated Python files is not flexible enough

Hydra

- One of the most popular solutions for handling configuration
- Uses YAML configs, allows overriding values from the command line
- Simple type checking via Structured Configs
- Grouped configs offer easy switching between groups of presets



```
Basic example

Config:

conf/config.yaml

db:
    driver: mysql
    user: omry
    pass: secret

Application:

my_app.py

import hydra
    from omegaconf import DictConfig, OmegaConf

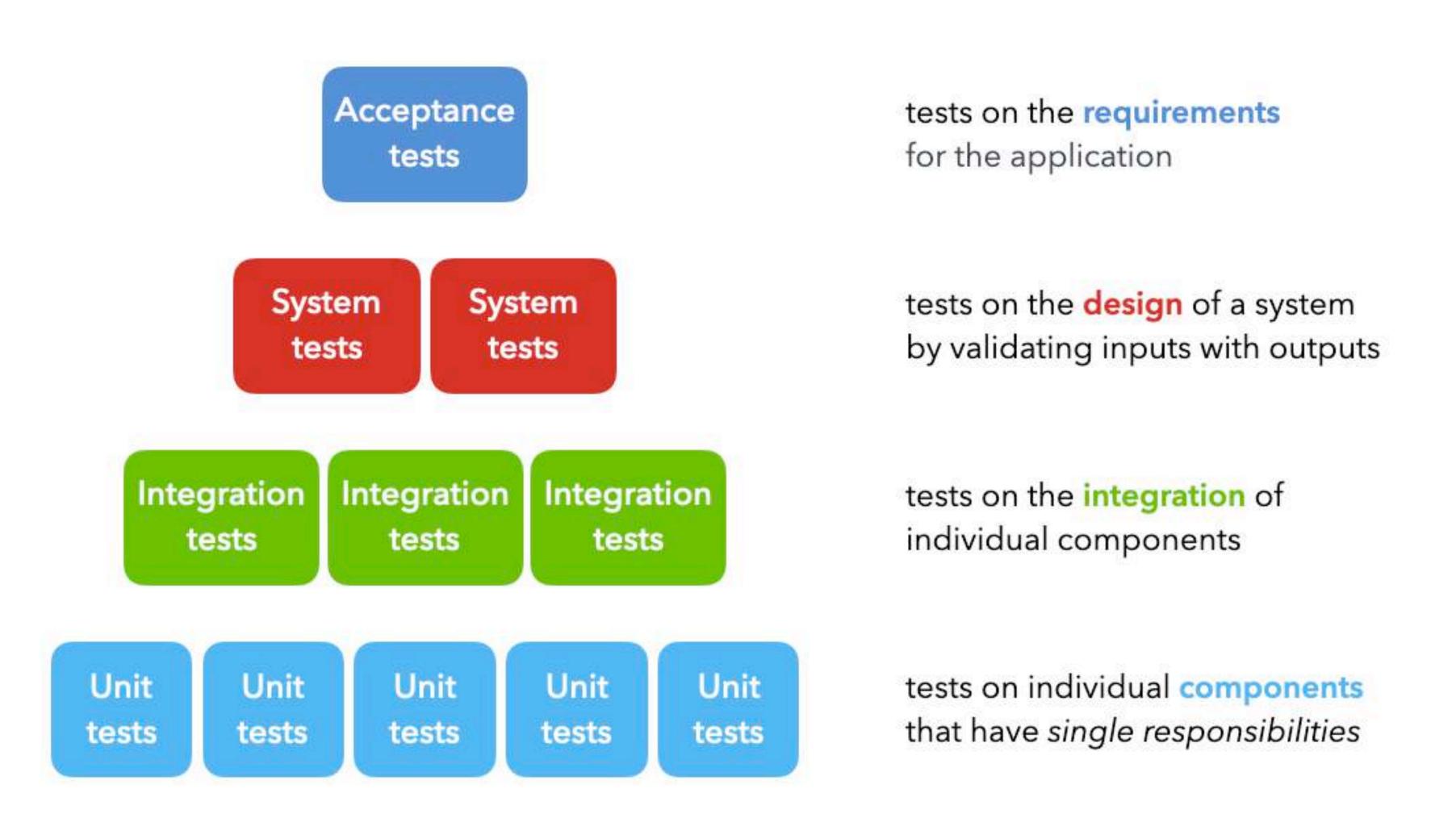
@hydra.main(config_path="conf", config_name="config")
    def my_app(cfg: DictConfig) -> None:
        print(OmegaConf.to_yaml(cfg))

if __name__ == "__main__":
        my_app()
```

Testing

- In general, testing refers to verifying the intended code properties:
 - Not only correctness, but also performance, handling inputs, etc.
- Why should we test our code?
 - It helps avoid the bugs (both now and when refactoring)
 - But it does not prevent them! Treat tests like classifiers applied to your code
 - It improves the overall code quality by decoupling
 - Essentially, you get self-documented code for free

Types of software tests



Types of software tests

- There are many kinds and typologies, e.g.:
 - 1. Unit tests verify the correctness of a single component
 - 2. Integration tests ensure that modules work together
 - 3. End-to-end tests verify that the entire application is correct
 - 4. Stress/load/performance tests check the speed of code under load
- We'll focus on 1 and 2: they are the easiest to write and cover most cases

How to test Python code

- Python built-in: unittest
 - Quite simple, ready to use
 - Cons: has its own syntax, not that flexible

```
import unittest
class TestStringMethods(unittest.TestCase):
    def test_upper(self):
        self.assertEqual('foo'.upper(), 'F00')
    def test_isupper(self):
        self.assertTrue('F00'.isupper())
        self.assertFalse('Foo'.isupper())
    def test_split(self):
        s = 'hello world'
        self.assertEqual(s.split(), ['hello', 'world'])
        # check that s.split fails when the separator is not a string
        with self.assertRaises(TypeError):
            s.split(2)
if __name__ == '__main__':
                                                           Ran 3 tests in 0.000s
    unittest main()
                                                           0K
```

How to test Python code

- Python built-in: unittest
 - Quite simple, ready to use
 - Cons: has its own syntax, not that flexible
- Better: pytest
 - Flexible, works with assert statements, has plenty of integrations via plugins

```
# content of test_sample.py
def func(x):
    return x + 1

def test_answer():
    assert func(3) == 5
```



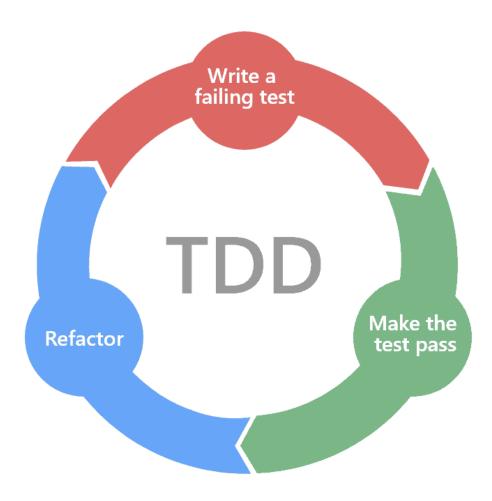
```
Ran 3 tests in 0.000s

OK
```

```
$ pytest
platform linux -- Python 3.x.y, pytest-6.x.y, py-1.x.y, pluggy-1.x.y
cachedir: $PYTHON_PREFIX/.pytest_cache
rootdir: $REGENDOC_TMPDIR
collected 1 item
                                                  [100%]
test_sample.py F
  def test_answer():
     assert func(3) == 5
     assert 4 == 5
      + where 4 = func(3)
test_sample.py:6: AssertionError
============== short test summary info ======================
FAILED test_sample.py::test_answer - assert 4 == 5
```

Test-driven development in ML context

- We can start from end-goal (aka "business") requirements
- Keep tests a natural part of your workflow!
 This means getting a convenient setup both locally and in CI
- Leverage TDD for your ML code as well
- Test the expected changes in behavior of your model



Property-based testing

- How do we generate test cases?
 - Coming up with our own inputs is not exhaustive
 - Basically, we only test that the code works for given inputs
 - Furthermore, our requirements become unclear
- Property-based testing aims to solve this problem
 - Instead of specifying exact inputs, we tell what they should be
 - The framework tests the code on many inputs and tries to simplify failing cases

Hypothesis

- A Python framework for propertybased-testing
- Integrates with pytest
- Has strategies for generating NumPy arrays (which generalizes to PyTorch tensors)

```
from hypothesis import given, strategies as st
@given(st.integers(), st.integers())
def test_ints_are_commutative(x, y):
    assert x + y == y + x
@given(x=st.integers(), y=st.integers())
def test_ints_cancel(x, y):
    assert (x + y) - y == x
@given(st.lists(st.integers()))
def test_reversing_twice_gives_same_list(xs):
   # This will generate lists of arbitrary length (usually between 0 and
   # 100 elements) whose elements are integers.
    ys = list(xs)
    vs.reverse()
   ys.reverse()
    assert xs == ys
@given(st.tuples(st.booleans(), st.text()))
def test_look_tuples_work_too(t):
    # A tuple is generated as the one you provided, with the corresponding
   # types in those positions.
    assert len(t) == 2
    assert isinstance(t[0], bool)
   assert isinstance(t[1], str)
```

```
>>> import numpy as np
>>> from hypothesis.strategies import floats
>>> arrays(np.float, 3, elements=floats(0, 1)).example()
array([ 0.88974794,  0.77387938,  0.1977879 ])
```

Takeaways

- Invest time in good and convenient logging
- Make sure to keep track of your data and models
- Flexible configuration makes it easy to alter your experiment setups
- Good tests simplify debugging and maintenance