HELMHOLTZ AI | ARTIFICIAL INTELLIGENCE COOPERATION UNIT

Introduction to machine learning operations

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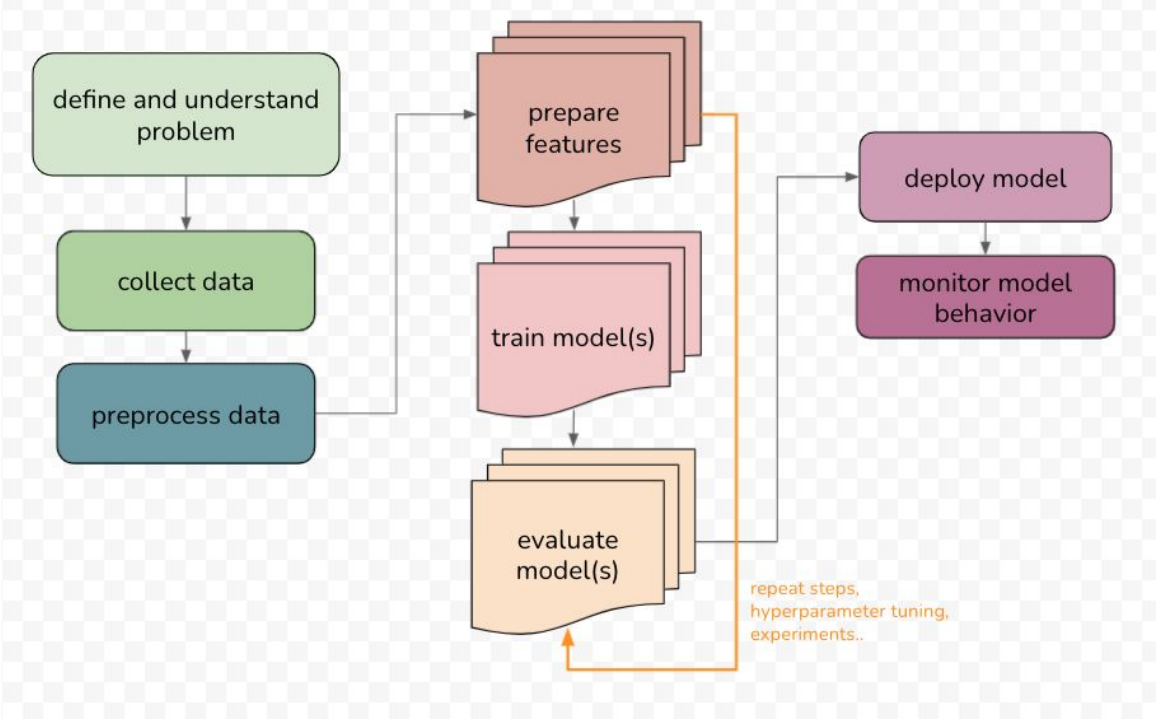
Introduction

- Goal:
  - Explore suitable tools for handling machine learning setups with focus on scientific usage
  - Draw a first conclusion and outlook
  - Provide a basis for further exploration
- Approach:
  - Define our use case
  - Gain understanding of emerging MLops landscape
  - Define comparison procedure
  - Examine a set of tools → Metaflow, MLflow, DVC

Use case

- Reproducibility
  - Crucial for research work → FAIR
- Exchangeable backend
  - Should be usable with custom computing infrastructure and HPC
- Workflow integration
  - Should be usable and comprehensible for people without computer science background
- Framework agnostic
  - Should work with various libraries and programming languages
- Open source
- Cost factor
  - We are on budget

Machine Learning Lifecycle



Comparison checklist

- General
- Version management and reproducibility
- Experiment tracking and comparison
- Pipeline execution and code invasiveness
- Scaling and backend
- Interaction with HPC
- Storage
- Logging and debugging
- Visualization
- Collaboration
- Compatibility
- Model serving
- Open source
- Costs
- Application to real world example

Short definitions

Metaflow

Metaflow is a python library, originally developed at Netflix, that helps building and managing data science projects.

MLflow

MLflow is an open source platform to manage machine learning life-cycles. The platform offers four distinct components, which can be used in either in stand-alone mode or together.

DVC

DVC is an open-source version control system for ML projects which is build around existing engineering toolsets and workflows

General

Comparison Factors

General

- design decisions
- emphasis
- components

Metaflow

Build around dataflow paradigm

High emphasis on seamless scalability and runtime agnostic (code can run on a laptop in parallel over multiple processes or in the cloud over multiple batch jobs)

Strong testing philosophy
Object Hierarchy:

Metaflow -> Flow -> Run -> Step -> Task -> Data Artifact

Flows: graph of operations
Steps: describe operations within the flow
Run: execution of flows

Workflow implemented via namespaces
Tightly coupled with Amazon Web Services
Designed around failure cases

MLflow

Organized into four components:

- Tracking
- Projects
- Models
- Model Registry

Components can be used on their own

Emphasis on maximum flexibility and customization

Out-of-the box with Microsoft Azure

Deployable on Amazon Sagemaker with one API call

DVC

Runs on top of any Git repository

Compatible with GitHub

Closely interacting with git (not necessary but recommended)

High emphasis on handling large datasets

Keep everything simple and accessible

Steps are connected into a DAG

Build around pipelines and stages

Minimal code invasiveness

Version management and reproducibility

Comparison Factors

Version management + reproducibility

- code
- model
- data

Metaflow

Built-in versioning via tags and namespaces

Production namespace and user namespace are separated (a bit like working on different branches)

Creates snapshots of runs

Environment is managed via conda(@conda decorator is implemented)

MLflow

Handled via MLflow projects
API and command-line tools for running projects, can be chained together to workflows

- build-in support of conda
- build-in support for docker-containers

Project: a directory with code/a git repository

- uses a descriptor file/ convention to specify dependencies/runs.

Code can be published on GitHub in the MLflow Project format

MLflow Model Registry manages model lifecycles. (especially build for large collaborations and many models from many teams involved)

DVC

Version management works together with git

- like a distributed version control system
- lock-free, local branching, versioning

Can be used together with CML for further improving CI/CD

Dvc manages the remote storage of data and creates files which then can be tracked via git

Due to its structure one can use different virtual environments as with other code projects, but no special integration (found so far)

Experiment tracking and comparison

Comparison Factors

Experiment tracking + comparison

parameter handling
metadata
data artifacts

Metaflow

client API is used to inspect results of past runs and some other parameters

Can be used within code and notebooks

data artifacts: container object, produced by runs. Contains actual value + metadata

MLflow

Realized with MLflow Tracking API+UI

Can be used within code and notebooks

Automatically keeps track of parameters, metrics, code, and models from each experiment

DVC

Realized with DVC Experiments

Designed for exploration of many different configurations and scenarios

Organize experiments and keep only the best ones

Tracking, scheduling, comparison integrated

Run experiments via `dvc exp run`

Known cases where experiment data has been fed into external tools (weights&biases)

Pipeline execution and code invasiveness

Comparison Factors	Metaflow	MLflow	DVC
Pipeline execution + code invasiveness	Integration: - form the ML-Process code into Flows - a flow is implemented by subclassing FlowSpec and implementing steps as methods Run: - execution of user-defined flows - also executable via CLI	Integration: - mlflow via the Python API into existing code Run : - via CLI tool, or via mlflow.projects.run() Python API	Integration: - as underlying mechanism, (no code needs to be altered), or via Python API - (it can be helpful to structure code around input/output paradigms) Run: - via execution of `dvc run` and/or `dvc repro`

Scaling and backend

Comparison Factors

Scaling + Backend

Metaflow

Integrates with Batch from AWS
- directly accessible via @ressources decorator

Languages such as C++ can be called from within a step for direct performance tuning

Can work with Amazon Sagemaker

Works well with meson (workflow orchestration + scheduling)

Also mention of scaling up on larger machines but no further specs

The foreach branch offers a mechanism for independent/parallel executions

MLflow

Integrates with Databricks as Managed MLflow, Kubernetes, Spark

Custom backends and needs can be implemented and integrated via mlflow community plugins

DVC

Integrates with Spark, Hive

Heavy cluster jobs can be decomposed into smaller DVC pipeline steps (parallel execution)

Interaction with HPC cluster

Comparison Factors	Metaflow	MLflow	DVC
Interaction with HPC cluster • installation • requirements • challenges	To be tested	To be tested	Work in progress

Storage

Comparison Factors	Metaflow	MLflow	DVC
Storage	Local file path Amazon S3	MLflow Tracking Server offers two types of storage - database-backed store: experiment and run metadata as well as params, metrics, and tags for runs - file store: large data, log of artifact output (eg models). supports: - local file paths, NFS, SFTP - Amazon S3, Azure Blob Storage, Google Cloud Storage	Local file path, SH/SFTP, HDFS, HTTP, NFS, disc to store data Amazon S3, Microsoft Azure Blob Storage, Google Drive, Google Cloud Storage, Aliyun OSS ..

Logging and debugging

Comparison Factors

Logging and debugging

what
where
how

Metaflow

Persists all runs + resulting data artifacts

Results can be accessed via unique run ID

Retrieval generally via namespaces + tags via Client API, see debugging

Resume execution of a past run at a failed step. Iterate quickly on step code

Python stack trace available

Plugin for VScode

..some other IDE's also work (PyCharm)

Explicit Metaflow Test Suite for test-driven development

MLflow

MLflow Tracking

Automatic logging via mlflow.autolog()

Library-specific autolog calls available (eg pytorch, fastai, scikit-learn..)

Runs can be annotated via tags

No specific debugging information found

DVC

Realized via Checkpoints (checkpoints can be registered during your code or script runtime (similar to a logger) to track successive steps in a longer experiment)

Automatic log of stage runs (run cache)

VScode plugin currently in development

Visualization

Comparison Factors	Metaflow	MLflow	DVC
Visualization of results	flow graphs are visualized	MLflow Tracking UI	DVC Studio
Graphical user interface	Didn't find anything comparable for specific parameters or trainings	Good GUI to compare and select models	As it just launched (as of this writing) yet to be tested
		Experiment-based run listing and comparison	Seems to offer similar functionality to MLflows GUI
		Searching for runs by parameter or metric value	Plotting of metrics and results can be handled via `dvc plots`
		Visualizing run metrics	
		Downloading run results	

Collaboration

Comparison Factors	Metaflow	MLflow	DVC
Collaboration with others	Collaboration is enabled and achieved by using tags and namespaces People create different flows in their user namespaces, results can be accessed by other members	MLflow supports git, collaborative work on MLflow Projects workflows possible Collaboration via Model Registry possible (suitable for large scale setups) Community efforts to add collaboration possibilities: combining MLflow with neptune -> WIP	Achievable by utilizing remote storage capabilities, also similar to collaboration in github/gitlab DVC Studio also seems to offer some collaboration specific functionalities

Compatibility

Comparison Factors	Metaflow	MLflow	DVC
Compatibility • Pytorch • Keras • other languages	Different python libraries are supported Languages such as C++ can be called within a step Jupyter notebooks are supported	Different python libraries are supported Languages such as C++ can be called within a step	Pipelines are defined around input/output, thus language-agnostic, support for Python, R, Julia, Scala Spark, custom binary,TensorFlow, PyTorch, etc Jupyter notebooks are supported

Model serving

Comparison Factors	Metaflow	MLflow	DVC
Model serving	pickle for object serialization/deserialization as default Others possible	MLflow Models Served via concept of flavors, thus models can be processed by different downstream tools Variety of tools to deploy models (eg. a TensorFlow model can be loaded as a TensorFlow DAG, or as a Python function to apply to input data.) Tools to deploy many common model types to diverse platforms: e.g model supporting the “Python function” flavor can be deployed to a Docker-based REST server or to cloud platforms such as Azure ML and AWS	No concrete defaults as dvc is mainly concerned with the data storage/retrieval part Get models via `dvc get` or dvc.api.open()

Open source

Comparison Factors	Metaflow	MLflow	DVC
Open Source version available?	Yes	Yes	Yes

Costs

Comparison Factors	Metaflow	MLflow	DVC
Costs	No entreprise plan or anything, usage of metaflow itself is free You pay for the AWS service in case of usage	No entreprise plan or anything, usage of MLFlow itself is free You pay for additional services in case of usage (Managed MLflow, Cloud storage..)	Usage of DVC itself is free DVC studio free up to 5 team members

Real world application

Comparison Factors	Metaflow	MLflow	DVC
Tested with real-world example?	To be tested	To be tested	Work in progress (see Interaction with HPC)

Wrap up

- This was a lot…
- Table and code available at https://gitlab.hzdr.de/haicu/vouchers/desy/ml_ops_exploration

Conclusion

- Metaflow
  - Build with scaling and collaboration in mind
  - Code structured as graph flow, features controlled via decorators, iterators for chaining everything together
  - Powerful approach
  - requires sufficient familiarity with programming
  - Strong reliance on amazon products in order to function optimally
- Mlflow
  - Very diverse functionality
  - Highly customizable
  - Well developed GUI
  - Detailed documentation
  - Vast framework
  - Requires a lot of time and aimed at advanced users
  - No emphasis on collaboration
  - Initial code investment (writing plugins) for integrating custom backends
- DVC
  - Build upon existing and well-known tools, especially git
  - Least code-invasiveness
  - Pipelines and stages are extremely useful
  - Lightweight compared to the other tools
  - Accessible documentation
  - (offers GUI now)
  - Less features
  - Has a smaller focus, does not handle model specifics

Conclusion

- Metaflow → great for large in-production use cases and large teams but not for our use-case

- MLflow → should be seriously considered if HelmholtzAI is planning to standartize and scale up, developing and maintaining a full machine learning lifecycle infrastructure. Can be used by single researchers if they only focus on MLflow Tracking and run experiments locally.

- DVC → smaller compared to the other tools but easier in implementation and usage, has best balance between advantages and disadvantages for our use-case

Outlook

- Either a boiled-down usage of MLflow or going with DVC
  - In both cases the usage of custom backend, remote storage and a more throughout examination of the UI is yet to be estimated (coming soon, experiments with a real voucher are on their way)

- In terms of community support, all three tools offer some ways to interact and get help.
  - DVCs discord server has been proved to be very active and welcoming when addressed with questions, also regarding usage together with SLURM (Yet to be tested for the others)

- Use cases and requirements will change over time and this work might and ***should*** be re-evaluated

Discussion

Questions? :)

Glossary

FAIR: Findable Accessible Interoperable Reproducible
Data Artifacts: results from a flow, usually model + metadata
CLI: command line interface - a text-based interface that is used to operate software and operating systems
Dataflow paradigm: Programming paradigm that models programs as directed graphs of the data flowing between operations
API: application programming interface - a set of commands, functions, protocols], and objects that programmers can use to create software or interact with an external system
Namespace: like scope for variables, but for functions and classes. It allows you to use the same function or class name in different parts of the same program without causing a name collision.
Data pipeline: a set of data processing elements connected in series, where the output of one element is the input of the next one. The elements of a pipeline are often executed in parallel or in time-sliced fashion.