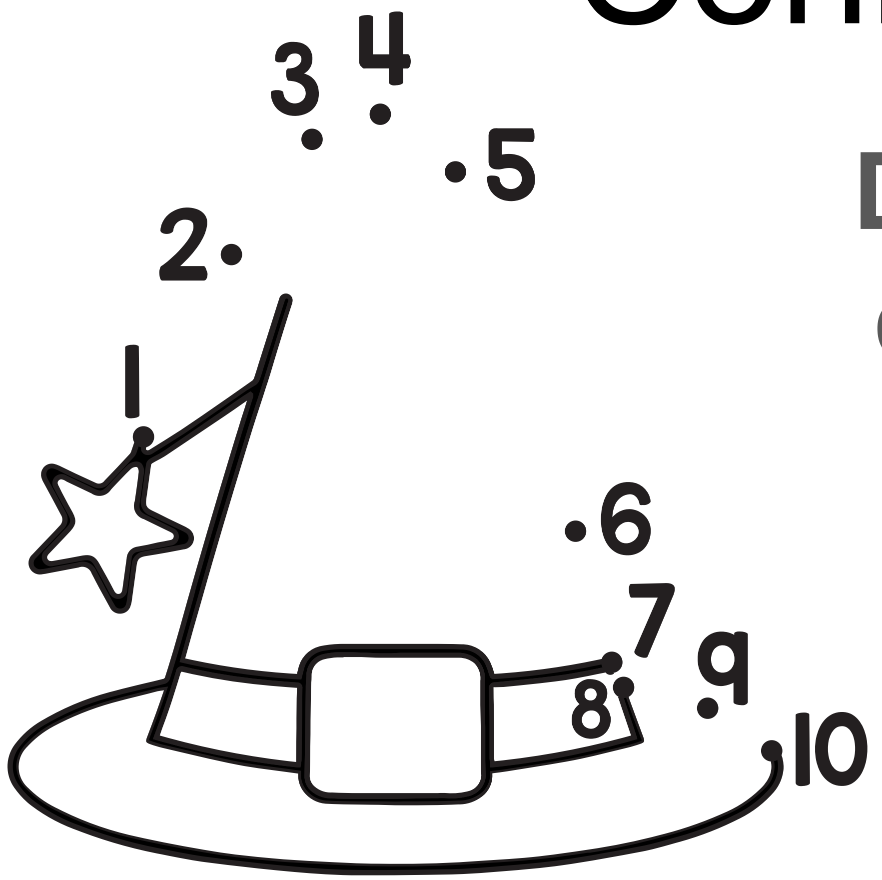
Pipeline composition via MLFlow

Connecting the dots



Diego Ciangottini
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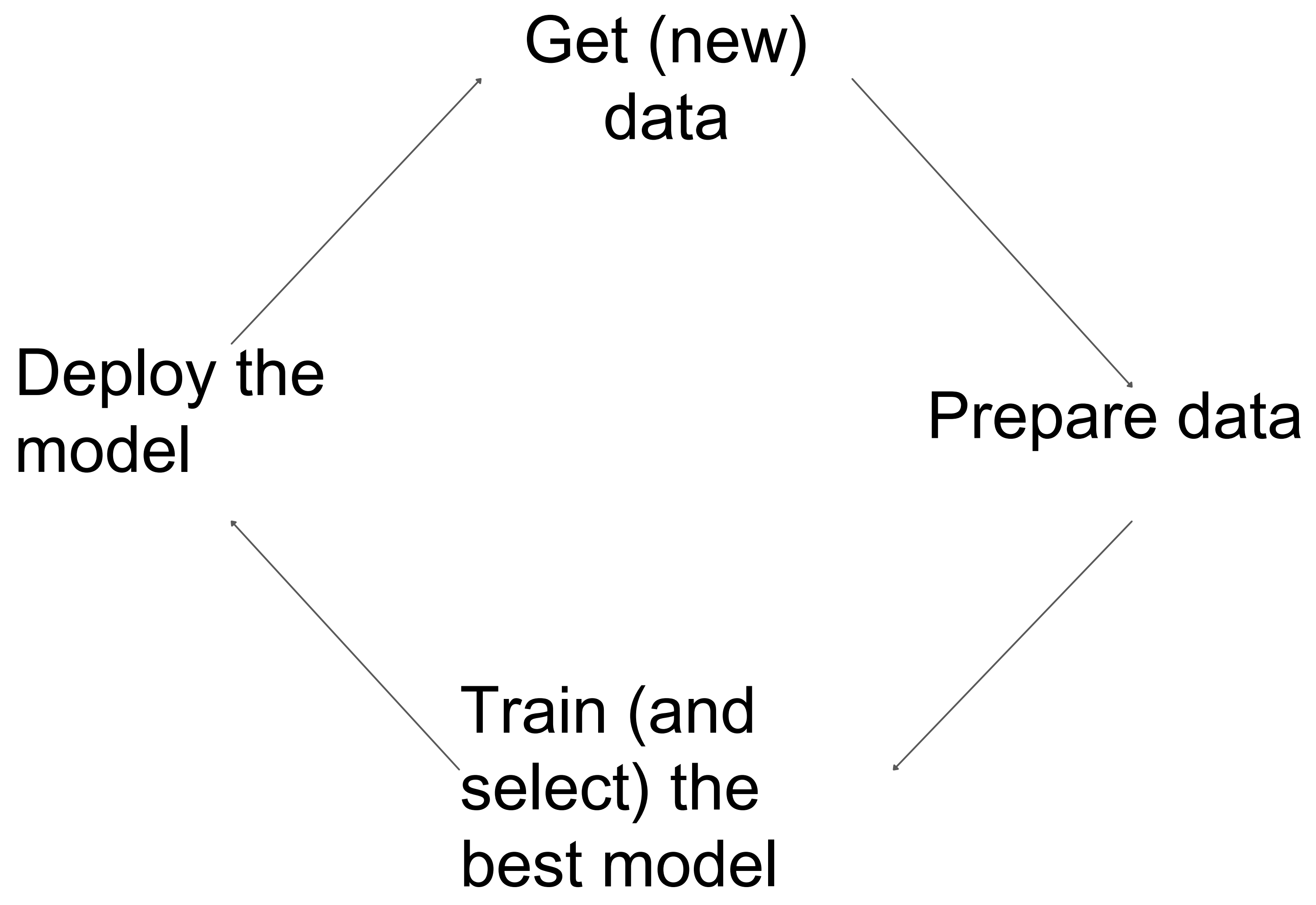
ICSC
Centro Nazionale di Ricerca in HPC,
Big Data and Quantum Computing

INFN
PERUGIA
Istituto Nazionale di Fisica Nucleare
Sezione di Perugia

Building a ML pipeline

Building machine learning pipeline is hard:

- 100s of software tools to leverage
- Hard to track and reproduce results: code, data, params, etc
- Hard to share models
- Hard to productionize models
- Needs large scale for best results



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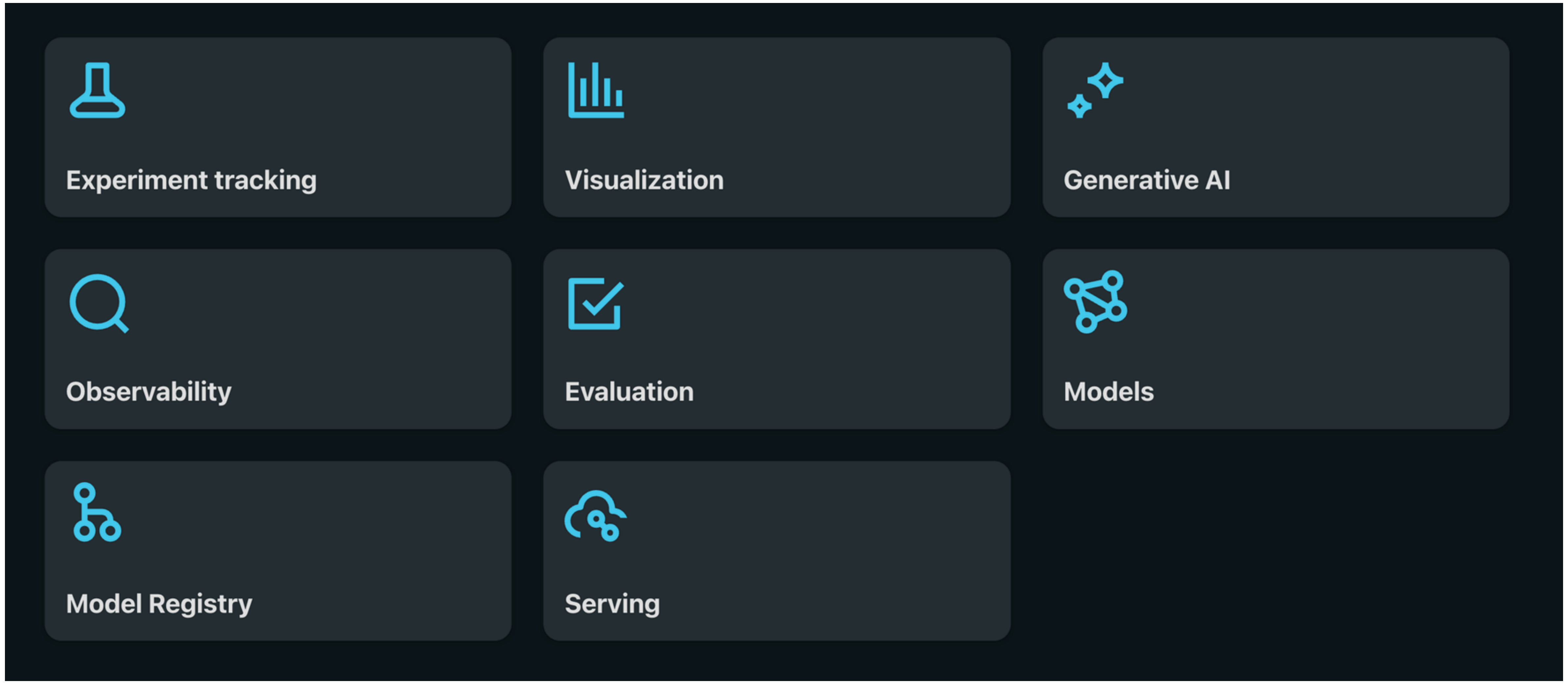
In most cases, you end up like this!

```
(base) ttedeschi@DESKTOP-GHVDTQ7:~/my_mlproject$ ls
mymodel_1.ipynb
mymodel_1_bis.ipynb
mymodel_1_bis_different_splitting.ipynb
mymodel_1_bis_lessfeatures.ipynb
mymodel_2.ipynb
mymodel_3.ipynb
mymodel_3_best.ipynb
mymodel_3_final.ipynb
mymodel_3_final_final.ipynb
mymodel_3_final_final_final.ipynb
```

What is MLFlow?

MLflow is a versatile, expandable, open-source platform for managing workflows and artifacts across the **machine learning lifecycle**

- Open and extensible
- Platform agnostic for maximum flexibility
  It has built-in integrations with many popular ML libraries, but can be used with any library, algorithm, or deployment tool. It is designed to be extensible, so you can write plugins to support new workflows, libraries, and tools.



mlflow™

https://mlflow.org/

PREFECT

dagster

Ship data pipelines with extraordinary velocity

Argo Workflows

Kubernetes-native workflow engine supporting DAG and step-based workflows.

Documentation

Kubeflow

A lot of options out there!

P R

dagster

Ship data pipelines with extraordinary velocity

Argo

Kubernetes-nati
and step-based

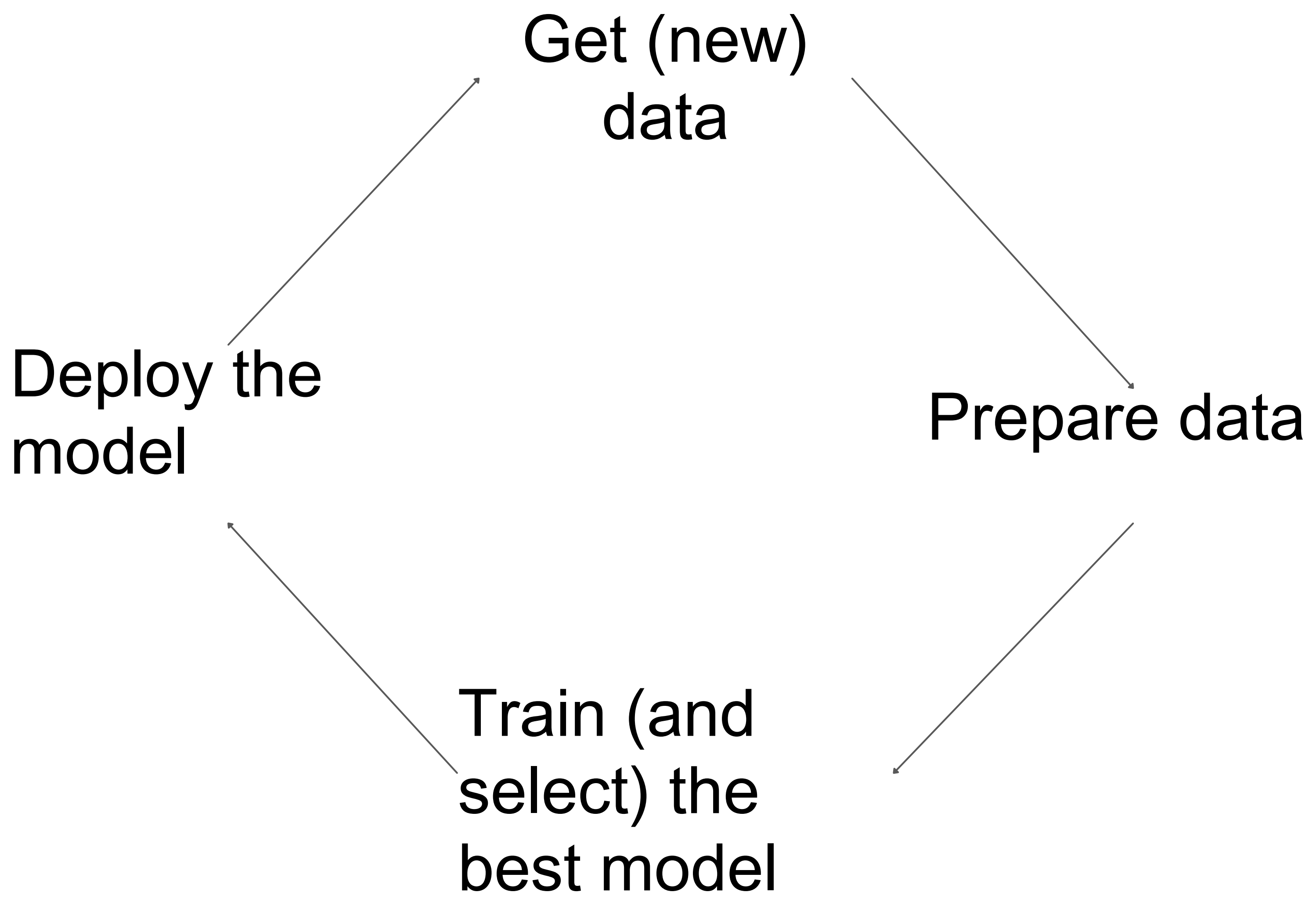
Documentat

Kubeflow

Main components

- **MLflow Tracking**:
  - Tracking ML experiments to record and compare model parameters, evaluate performance, and manage artifacts
- **MLflow Models**:
  - Packaging and deploying models from a variety of ML libraries to a variety of model serving and inference platforms
- **MLflow Model Registry**:
  - Collaboratively managing a central model store, including model versioning, stage transitions, and annotations
- **MLflow Projects**:
  - Packaging ML code in a reusable, reproducible form in order to share with other data scientists or transfer to production

How is each component mapped?



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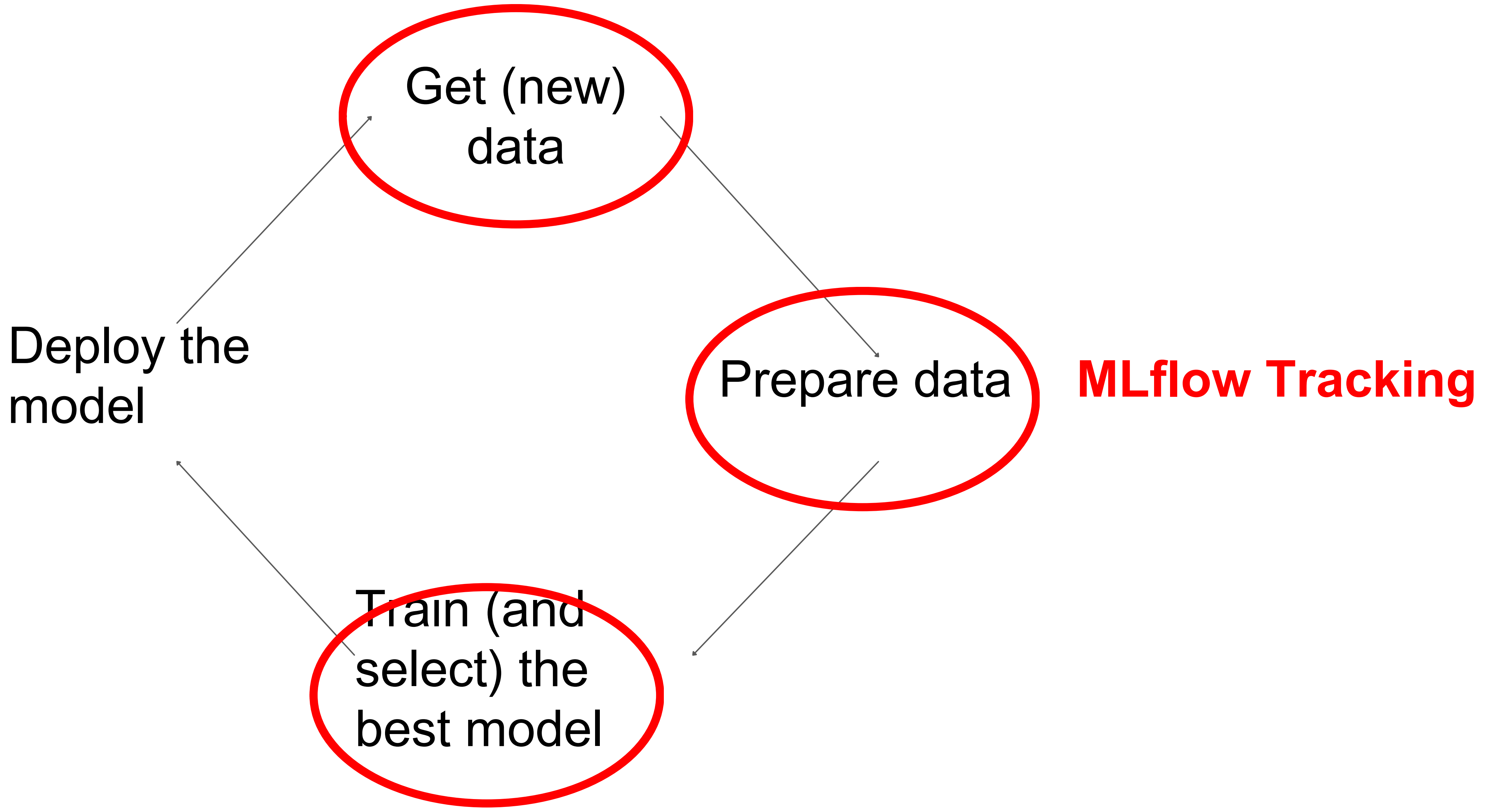

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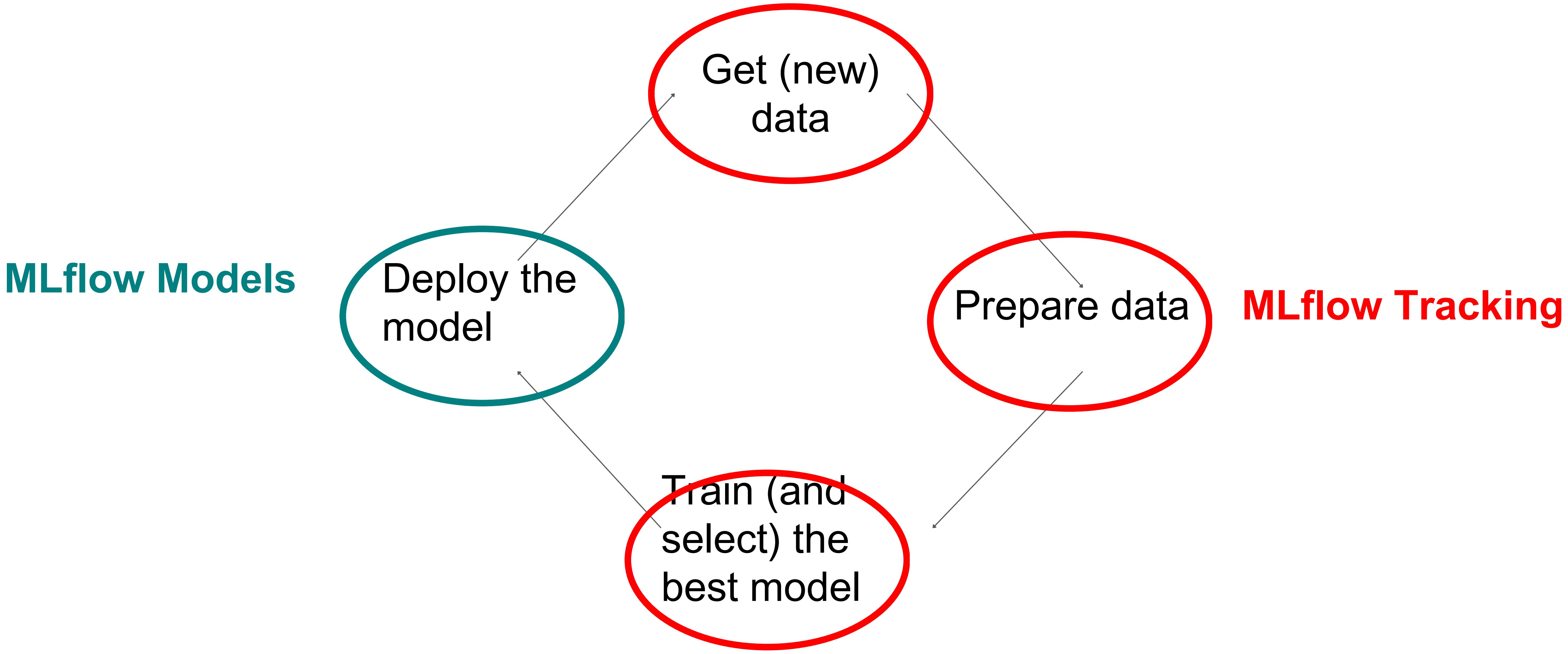

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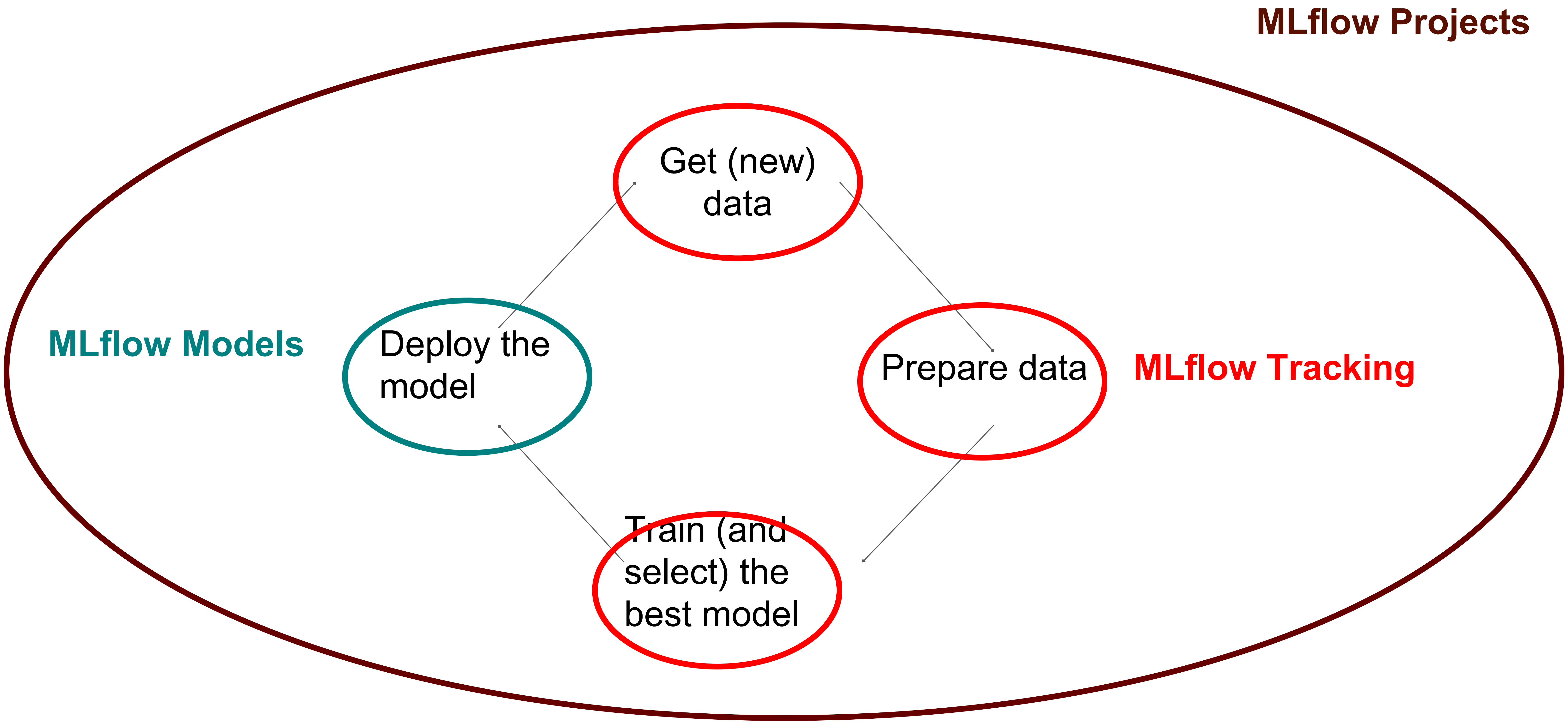
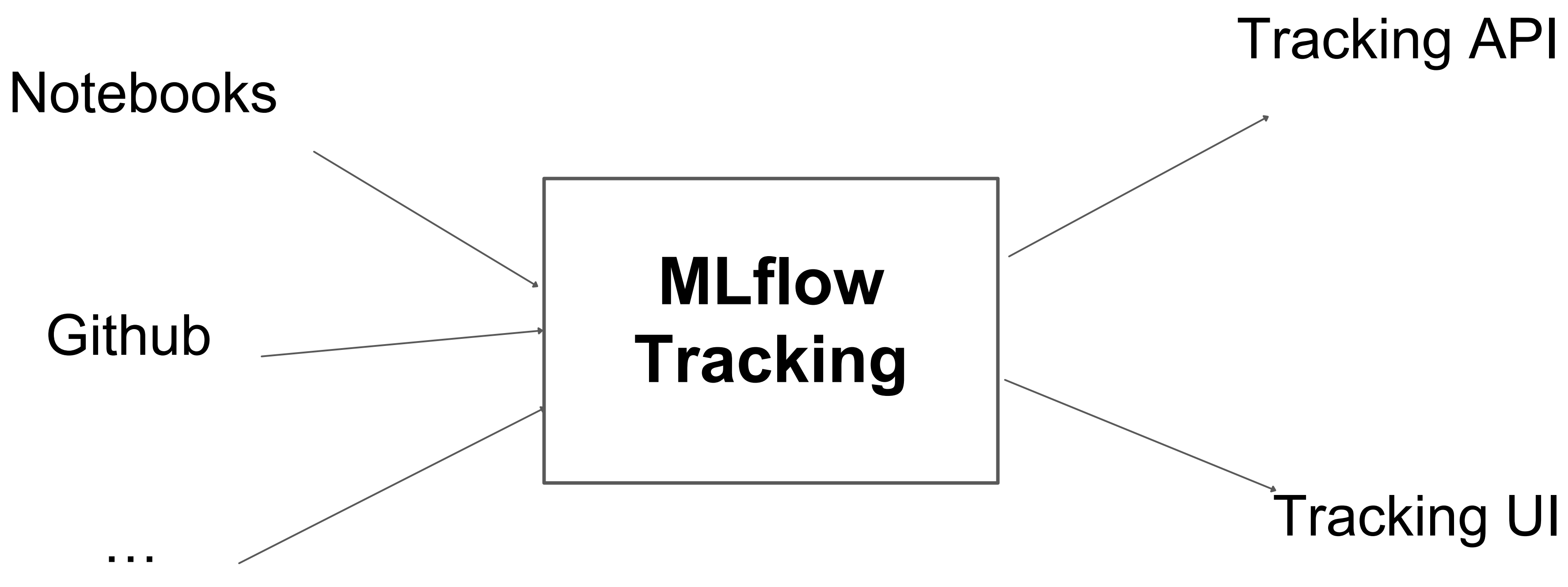


MLFlow tracking

The **MLflow Tracking** component is an **API and UI for logging** parameters, code versions, metrics, and output files when running your machine learning code and **for later visualizing** the results.
MLflow Tracking lets you log and query experiments using Python, REST, R API, and Java API APIs.

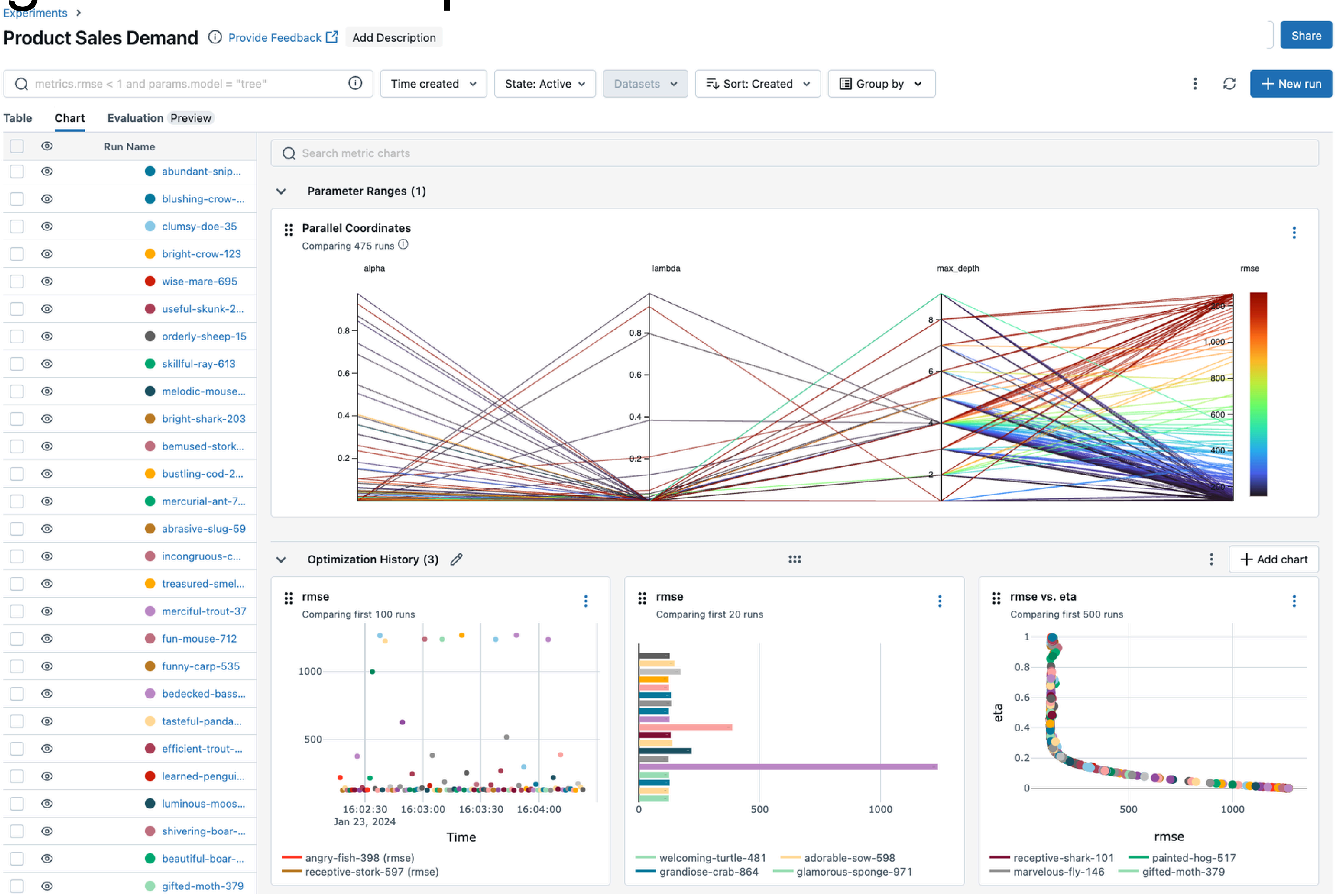
https://mlflow.org/docs/latest/tracking.html



MLFlow tracking - main concepts

MLFlow tracking is organized around the concept of **runs**

like executions of some piece of data science code, collected in **experiments** (useful for comparing runs intended to tackle a particular task).



Tracking UI

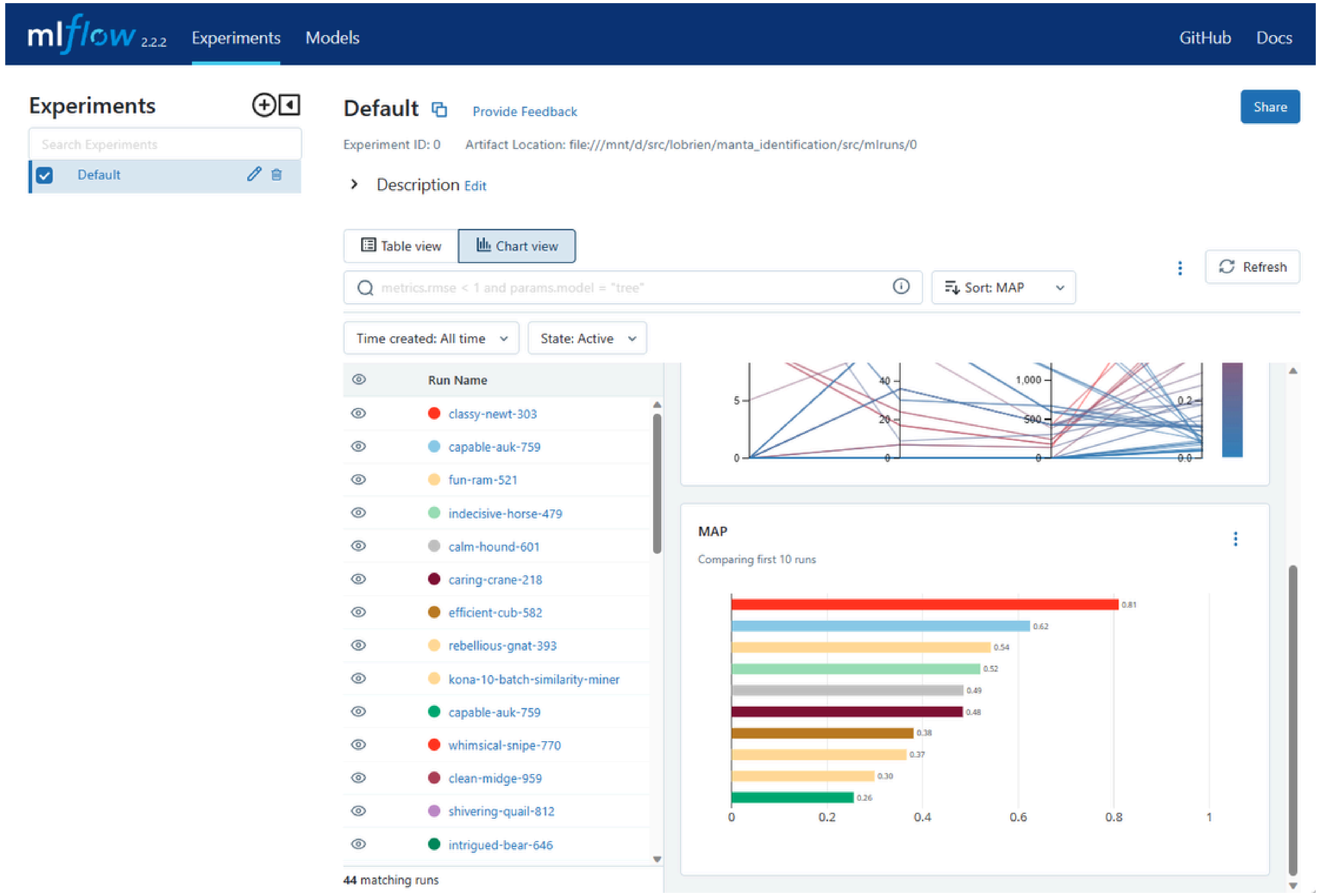
The Tracking UI lets you visualize, search and compare runs, as well as download run artifacts or metadata for analysis in other tools.

- If you log runs to a **local mlruns directory**, run mlflow ui in the directory above it, and it loads the corresponding runs.
- Alternatively, the **MLflow tracking server** serves the same UI and enables remote storage of run artifacts.
    - You run an MLflow tracking server using mlflow server
    - In that case, you can view the UI using URL http://<ip address of your MLflow tracking server>:5000 in your browser from any machine, including any remote machine that can connect to your tracking server.
    - To log to a tracking server, set the MLFLOW_TRACKING_URI environment variable to the server's URI, along with its scheme and port (for example, http://10.0.0.1:5000) or call mlflow.set_tracking_uri()

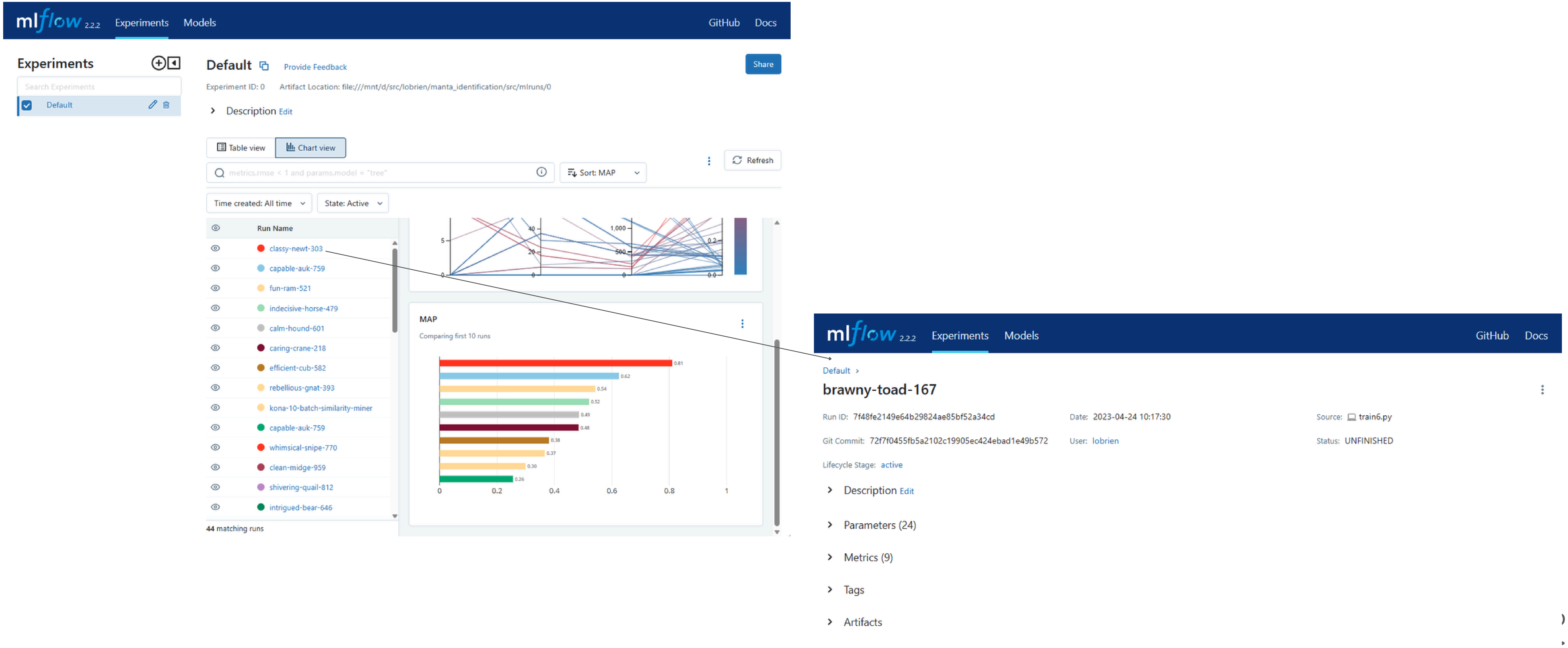
The UI contains the following key features:

- Experiment-based run listing and comparison (including run comparison across multiple experiments)
- Searching for runs by parameter or metric value
- Visualizing run metrics
- Downloading run results

Tracking UI


mlflow 2.2.2
Experiments
Models
GitHub
Docs
Experiments
Search Experiments
Default
Default
Provide Feedback
Share
Experiment ID: 0
Artifact Location: file:///mnt/d/src/lobrien/manta_identification/src/mlruns/0
Description Edit
Table view
Chart view
Refresh
metrics.rmse < 1 and params.model = "tree"
Sort: MAP
Time created: All time
State: Active
Run Name
classy-newt-303
capable-auk-759
fun-ram-521
indecisive-horse-479
calm-hound-601
caring-crane-218
efficient-cub-582
rebellious-gnat-393
kona-10-batch-similarity-miner
capable-auk-759
whimsical-snipe-770
clean-midge-959
shivering-quail-812
intrigued-bear-646
44 matching runs
MAP
Comparing first 10 runs

Tracking UI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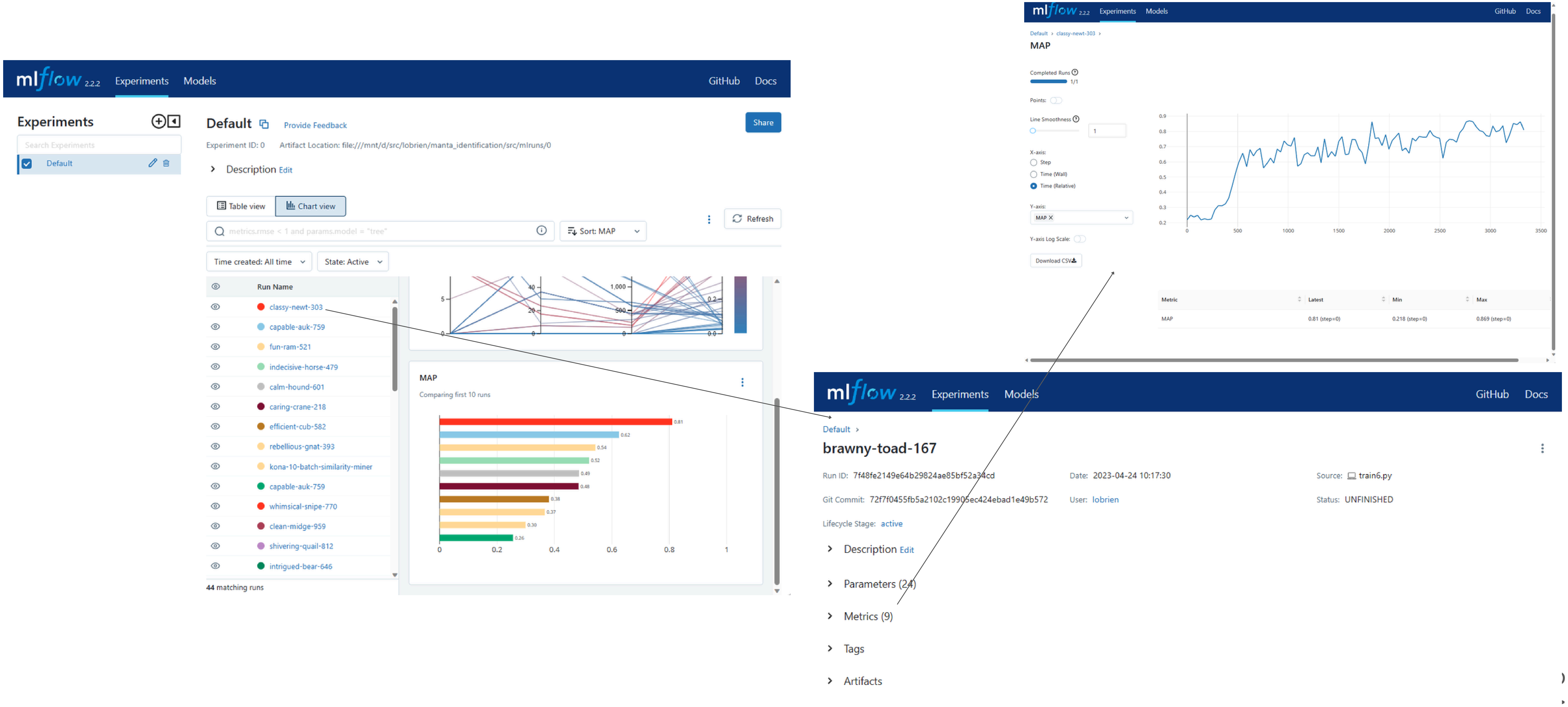
44 matching runs
MAP
Comparing first 10 runs
0.81
0.62
0.54
0.52
0.49
0.48
0.38
0.37
0.30
0.26
0
0.2
0.4
0.6
0.8
1
mlflow 2.2.2
Experiments
Models
GitHub
Docs
Default
brawny-toad-167
Run ID: 7f48fe2149e64b29824ae85bf52a34cd
Date: 2023-04-24 10:17:30
Source: train6.py
Git Commit: 72f7f0455fb5a2102c19905ec424ebad1e49b572
User: lobrien
Status: UNFINISHED
Lifecycle Stage: active
Description Edit
Parameters (24)
Metrics (9)
Tags
Artifacts

Tracking UI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0.26
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0.2
0.4
0.6
0.8
1
Default › classy-newt-303 ›
MAP
Completed Runs
1/1
Points:
Line Smoothness
X-axis:
Step
Time (Wall)
Time (Relative)
Y-axis:
MAP
Y-axis Log Scale:
Download CSV
Metric
Latest
Min
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Default ›
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Where is data recorded?

- **MLflow runs** can be recorded to local files, to a SQLAlchemy-compatible database, or remotely to a tracking server.
- **MLflow artifacts** can be persisted to local files and a variety of remote file storage solutions.
  For storing runs and artifacts, MLflow uses two components for storage: backend store and artifact store.
- **backend store** persists MLflow entities (runs, parameters, metrics, tags, notes, metadata, etc)
- **artifact store** persists artifacts (files, models, images, in-memory objects, or model summary, etc)

How to log?

"Manual" logging:

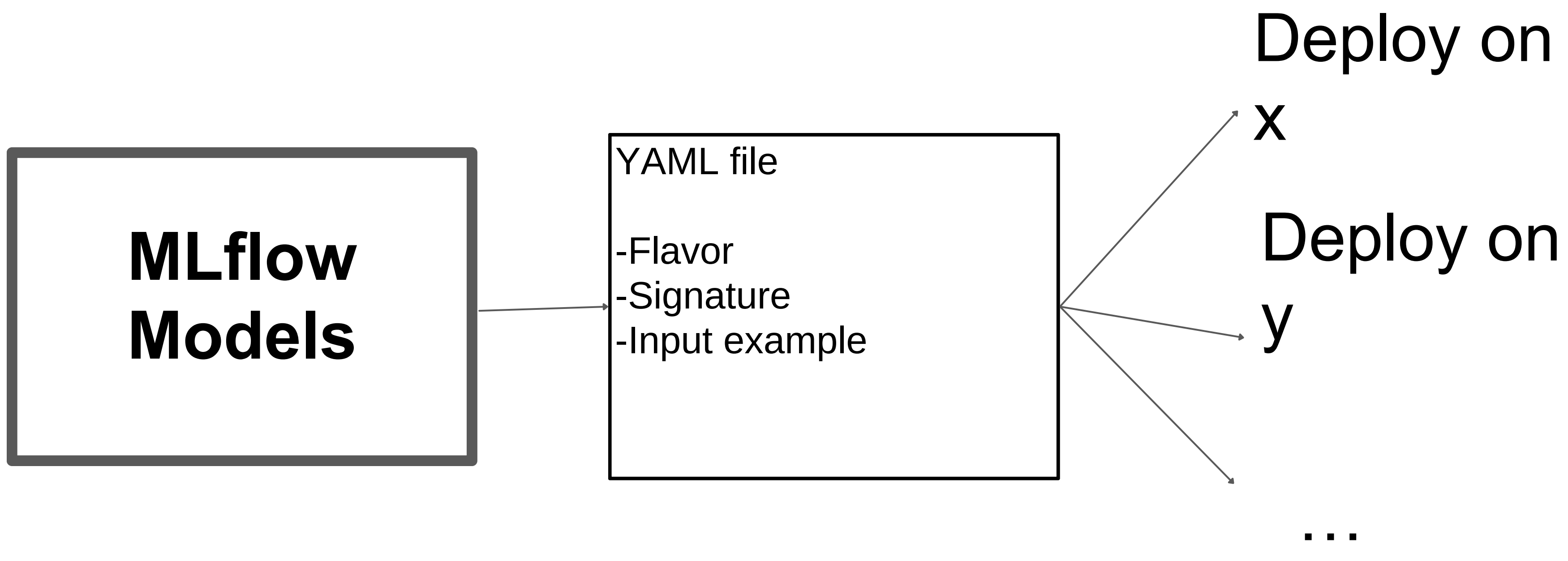
- **mlflow.log_param()/mlflow.log_params()**
  - logs a single key-value param in the currently active run. The key and value are both strings.
  - Use mlflow.log_params() to log multiple params at once.
- **mlflow.log_metric() / mlflow.log_metrics()**
  - logs a single key-value metric. The value must always be a number.
  - MLflow remembers the history of values for each metric (supports two alternative methods for distinguishing metric values on the x-axis: timestamp and step)
  - Use mlflow.log_metrics() to log multiple metrics at once.
- **mlflow.log_input()**
  - logs a single mlflow.data.dataset.Dataset object corresponding to the currently active run.
  - You may also log a dataset context string and a dict of key-value tags.
- **mlflow.log_artifact()/ mlflow.log_artifacts()**
  - logs a local file or directory as an artifact, optionally taking an artifact_path to place it in within the run's artifact URI.
  - Run artifacts can be organized into directories, so you can place the artifact in a directory this way.
  - mlflow.log_artifacts() logs all the files in a given directory as artifacts, again taking an optional artifact_path.

Autolog:

- Automatic logging allows you to log metrics, parameters, and models without the need for explicit log statements.
- There are two ways to use autologging:
  - Call mlflow.autolog() before your training code. This works for each supported library you have installed as soon as you import it.
  - Use library-specific autolog calls for each library you use in your code
    - available: Scikit-learn, Keras, Gluon, XGBoost, LightGBM, Statsmodels, Spark, Fastai, Pytorch

MLflow Models

https://mlflow.org/docs/latest/models.html



A standard format for **packaging machine learning models that can be used in a variety of downstream tools**

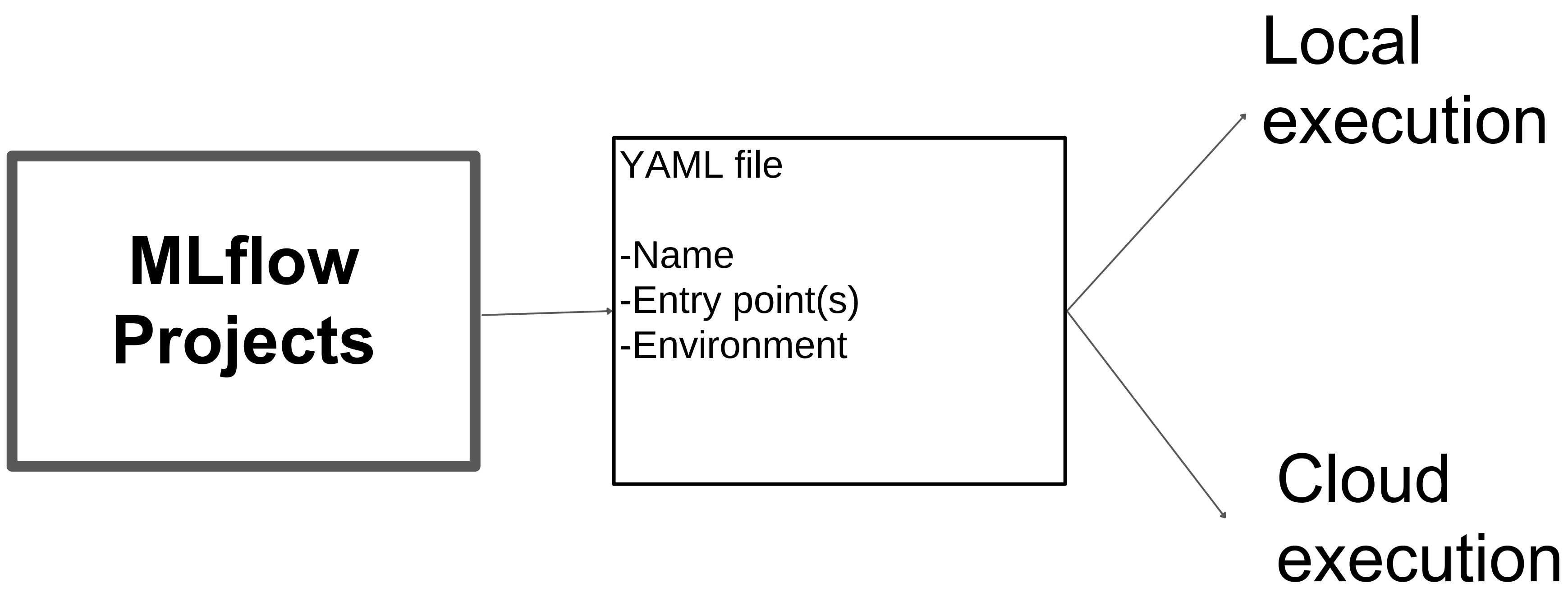
- Each MLflow Model is a directory containing arbitrary files, together with an ML model file in the root of the directory that can define multiple flavors that the model can be viewed in

MLflow Projects

MLflow Projects are just a convention for organizing and describing your code (packaging it in a reusable and reproducible way) to let other data scientists (or automated tools) run it
A project is simply a directory of files, or a Git repository, containing your code + conventions for placing files in this directory and a MLproject file (YAML formatted). Each project can specify several properties:

- **Name**: A human-readable name for the project.
- **Entry Points**: Commands that can be run within the project, and information about their parameters. If you list your entry points in a MLproject file, however, you can also specify parameters for them, including data types and default values.
- **Environment**: The software environment that should be used to execute project entry points. This includes all library dependencies required by the project code (local, Conda, Virtualenv, and Docker)

https://mlflow.org/docs/latest/projects.html



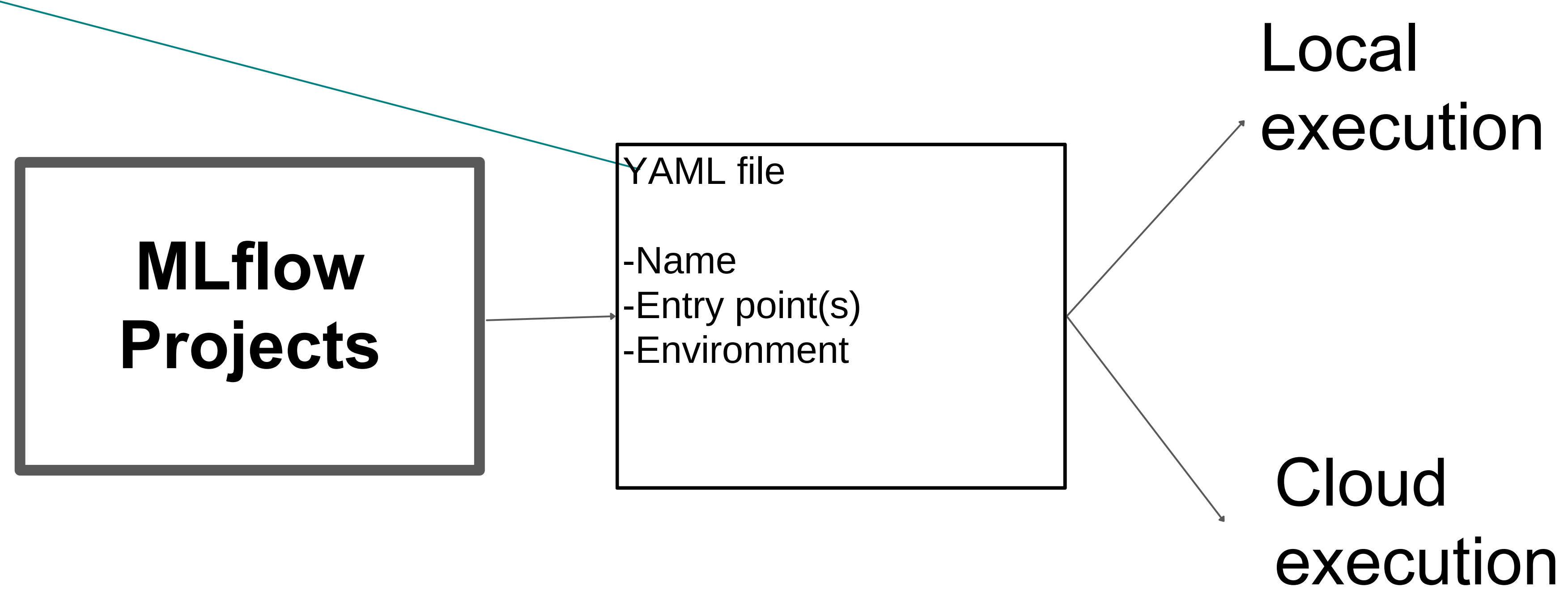
MLflow Projects

```yaml
name: My Project

python_env: python_env.yaml

entry_points:
  main:
    parameters:
      data_file: path
      regularization: {type: float, default: 0.1}
    command: "python train.py -r {regularization} {data_file}"
  validate:
    parameters:
      data_file: path
    command: "python validate.py {data_file}"
```

https://mlflow.org/docs/latest/projects.html



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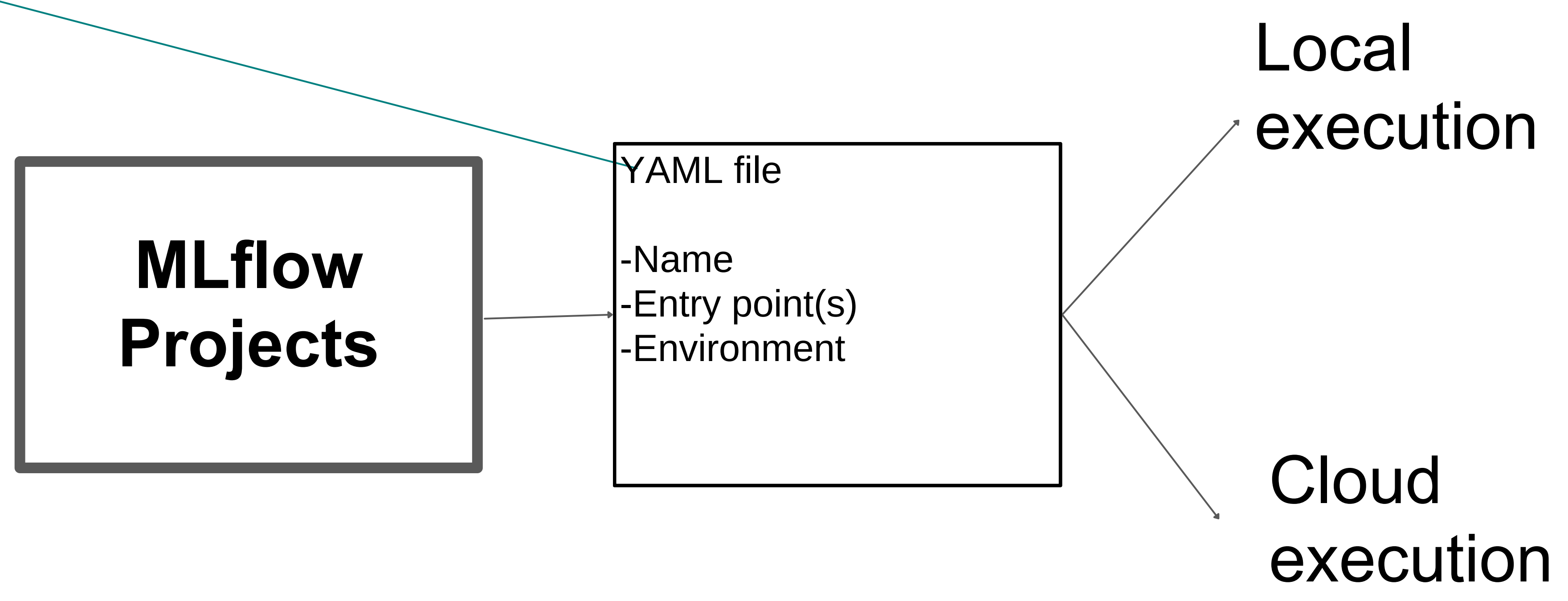
      data_file: path
    command: "python validate.py {data_file}"
```

```yaml
# Python version required to run the project.
python: "3.8.15"
# Dependencies required to build packages. This field is optional.
build_dependencies:
  - pip
  - setuptools
  - wheel==0.37.1
# Dependencies required to run the project.
dependencies:
  - mlflow==2.3
  - scikit-learn==1.0.2
```

https://mlflow.org/docs/latest/projects.html



Building pipelines with MLflow Projects

The mlflow.projects.run() API, combined with other functions, makes it possible to build multi-step workflows with separate projects (or entry points in the same project) as the individual steps.

- Each call to mlflow.projects.run() returns a run object, that you can use with mlflow.client to determine when the run has ended and get its output artifacts
- These artifacts can then be passed into another step that takes path or uri parameters.
- You can coordinate all of the workflow in a single Python program that looks at the results of each step and decides what to submit next using custom code.
  - Modularizing Your Data Science Code
  - Hyperparameter Tuning

Integration/adoption

- MLflow is well integrated with most of the Machine Learning ecosystem:
  - Tensorflow
  - Pythorch
  - Keras
  - Scikit-learn
  - XGBoost
  - Onnx
  - …
- Also integrated with different computing environments: docker, kubernetes, commercial clouds…
- Adopted by 80+ companies

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- More sophisticated example: https://github.com/mlflow/mlflow/tree/master/examples/hyperparam