MLOps Engineering

Machine Learning Operations V2.0.0

Sessions 12 – 13 (WIP)

MsC in Business Analytics and Data Science

Madrid, Jun 2025

Agenda

- 1st Group exec summary (Q&A)
- CI/ CD with GitHub Actions
- FastAPI for model serving
- Docker for deployment

Preprocessing Performance vs. Data Validation

In your team's modular MLOps pipeline, during a code review, you notice the preprocessing step now takes twice as long due to extensive data validation checks, such as checking for missing values, data types, and outliers. Your junior insists these validations are critical for ensuring data quality. What decision do you make?

Set up the options. Choose one or multiple correct answers.

A Keep all validations; accuracy outweighs performance

B Move validation steps to a parallel process asynchronously. Leveragin cloud parallel processing

C Reduce validations only to those that protect data integrity, enhancing performance — Correct answer

D Remove most checks, and rely on the Pytest suit (that's what is there for)

Code Comments

In your team's modular MLOps pipeline, your junior has added extensive comments to the code, explaining what each function does, such as "this function loads the data." However, they haven't included comments explaining why certain strategies or parameters were chosen, like why a specific batch size was selected. How do you guide them to improve their documentation?

Set up the options. Choose one or multiple correct answers.

A Comments explaining "what" are sufficient for maintainability

B Replace code-level comments with a comprehensive README.md

C Emphasize adding brief but clear explanations of "why" key decisions were made — Correct answer

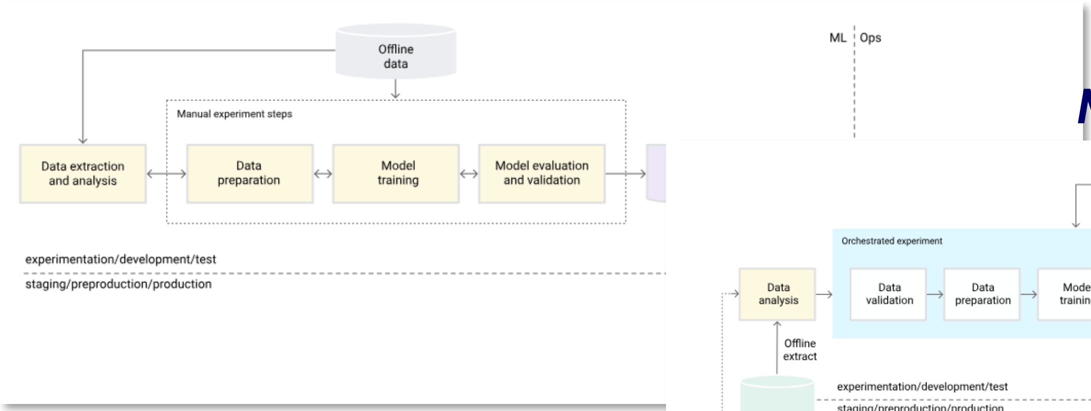
D Suggest adding links to external documentation for any unclear choices

Details for grading tests for 1st Group assignment

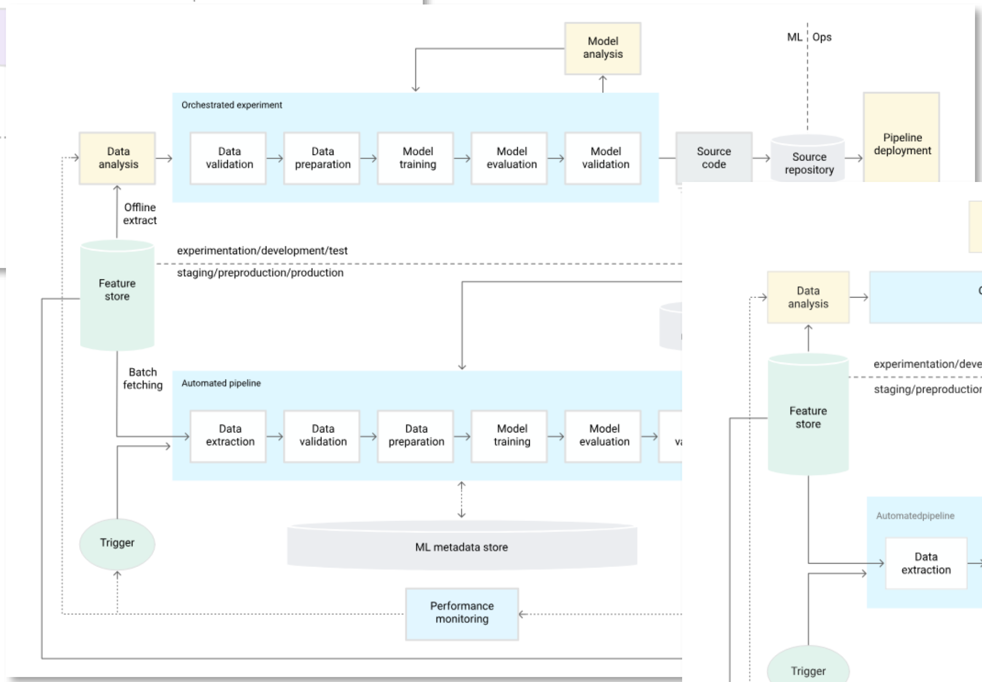
Test / Command	Purpose	Rubric dimension	Grading logic	Recommendation
black --check .	PEP 8 formatting	Code Quality & Efficiency	Score = (num_compliant_files / total_files) × 10	Run black . to auto-format the code
isort --check-only .	Import order style	Code Quality & Efficiency	Score = (num_compliant_files / total_files) × 10	Run isort . to auto-format all imports
flake8 .	Linting for style and simple bugs	Code Quality & Efficiency	Relative count of non-compliant across groups	Action on console feedback Use auto-formatters (black, isort)
flake8 --select=LOG <path>	Static check for correct logging usage (no f-strings, placeholders, etc.) ([github.com][1])	Logging & Monitoring	Relative count of non-compliant across groups	Action on console feedback
pylint src --score y	Advanced linting, docstrings score	Code Quality & Documentation	Direct pylint overall score	Action on console feedback
pytest --cov=src --cov-report=term-missing	Unit tests and coverage	Testing & Coverage	1. % number of tests that pass, vs. total 2. test coverage	Action on console feedback
radon cc -s -a src	Average cyclomatic complexity	Modularization & Code Quality	Map Radon average: A→10, B→8, C→6, D→4, E→2, F→0	Refactor high-complexity functions
detect-secrets scan --exclude-files '\.ipynb$'	Detect hard-coded secrets	Security	10/10 if no secrets on src code	Review and remove any secrets; use environment variables or .env files
pydocstyle src	Docstring presence and style	Documentation & Clarity	Violation/ files normalised x-groups	Action on console feedback
File presence check (custom Python)	Confirm key project files/folders exist (README.md, config.yaml, environment.yml, tests/, .gitignore, logs/, models/)	Documentation, Config & Artifacting	(files_found/expected) × 10	Ensure full config mgmt. logging and artifacting completeness
Config usage scan (custom Python)	Count hard-coded absolute paths vs use of os.environ / yaml configs	Config Mgmt	max(0, 10 – hardcoded_paths)	Ensure no paths are hard-coded
Error-handling scan (custom Python)	Count try: blocks and custom Exception subclasses	Error Handling & Validation	min(10, try_blocks ÷ 10 × 10)	If low, increase use of try/except blocks and define custom exceptions

MLOps is a journey - involving people, processes, tools and data transformation

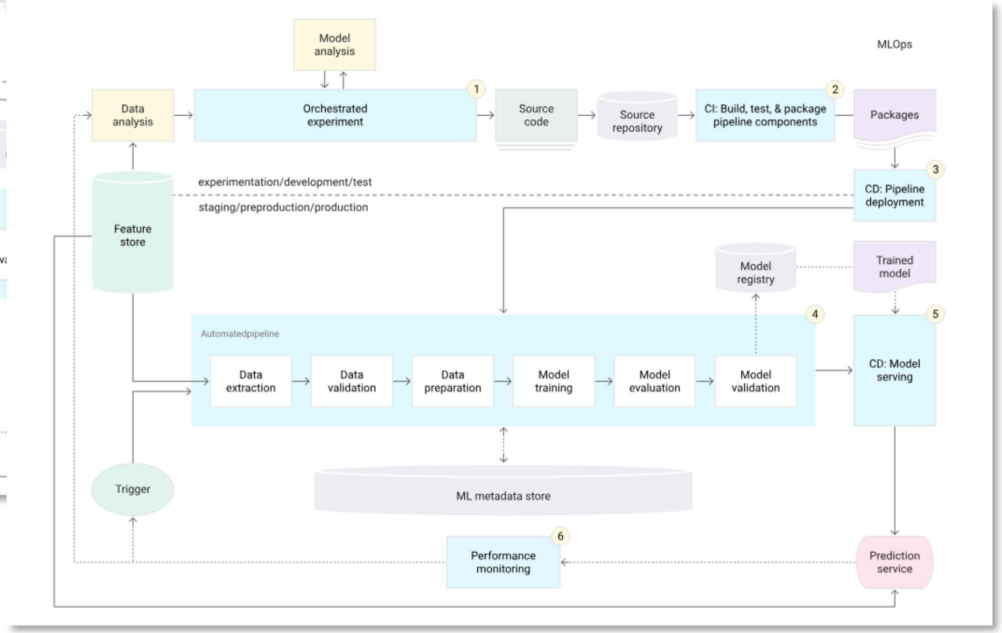
MLOps level 0: Manual process



MLOps level 1: ML pipeline automation



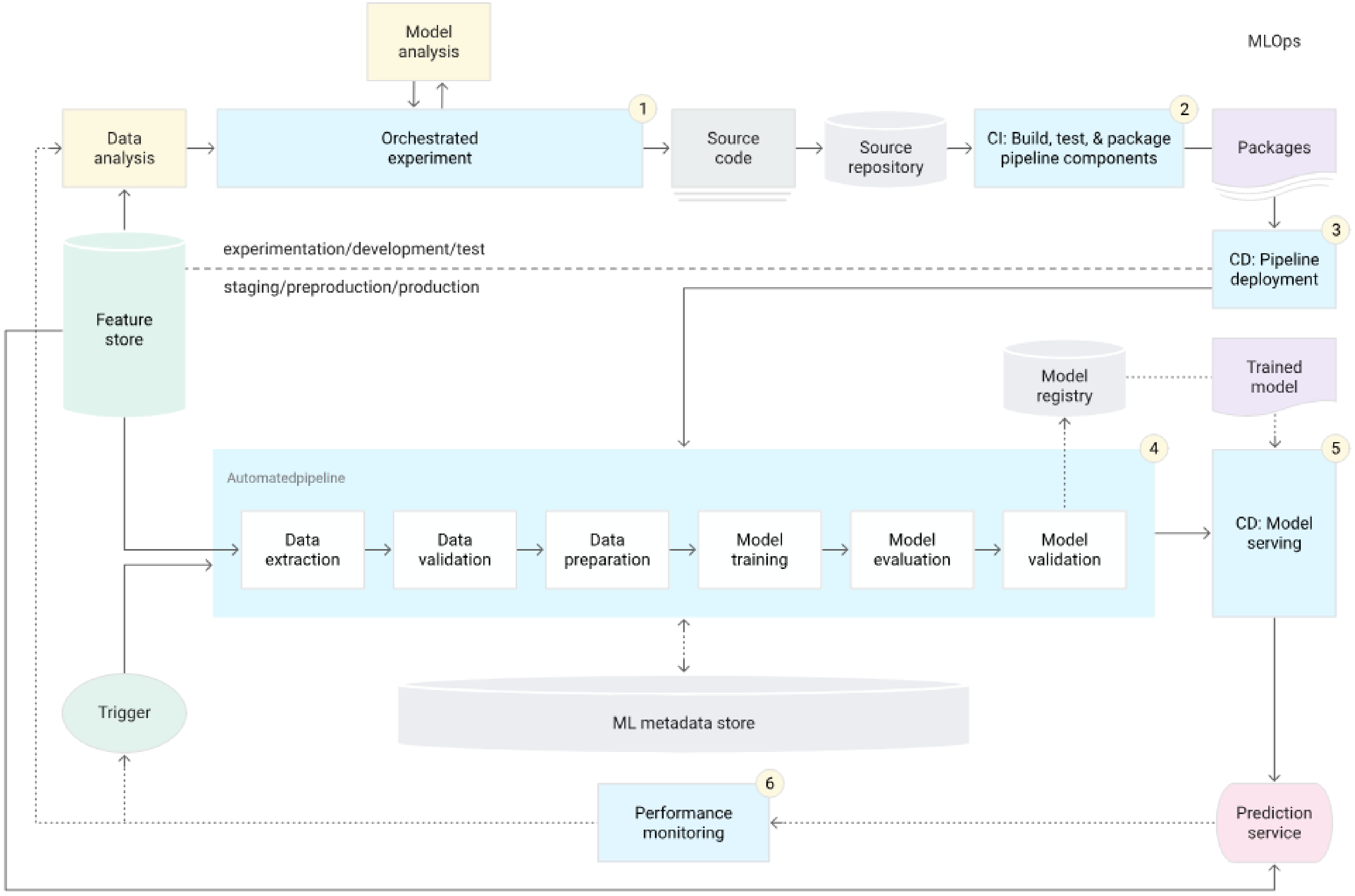
MLOps level 2: CI/CD pipeline automation



Source: Google

Level 2

Automate CI/CD pipelines to reliably retrain and deploy ML models as data and business needs evolve fast



Source: Google

Continuously integrate and verify code to catch errors early, then deliver **only tested, deployable builds** to production

Continuous Integration (CI)

Refers to continuous building of the code/ model. Automatically triggered when:

- New code is pushed (or committed)
- Runs the test suit (Unit and Integration)
- Compiles the code after pushing the changes
- Builds packages, containers, executables, etc.
- Delivers the code to the CD pipeline

Continuous Delivery (CD)

Ensures the code is "always" deployable:

- Code/ model is verified by the CI tasks
- Ensures compatibility of code/ models with target environment
- Checks model performance before deploying
- Code is verified by a Human
- Code/ models are pushed into the production environment

From Software Dev CI/CD to MLOps + CT/CM

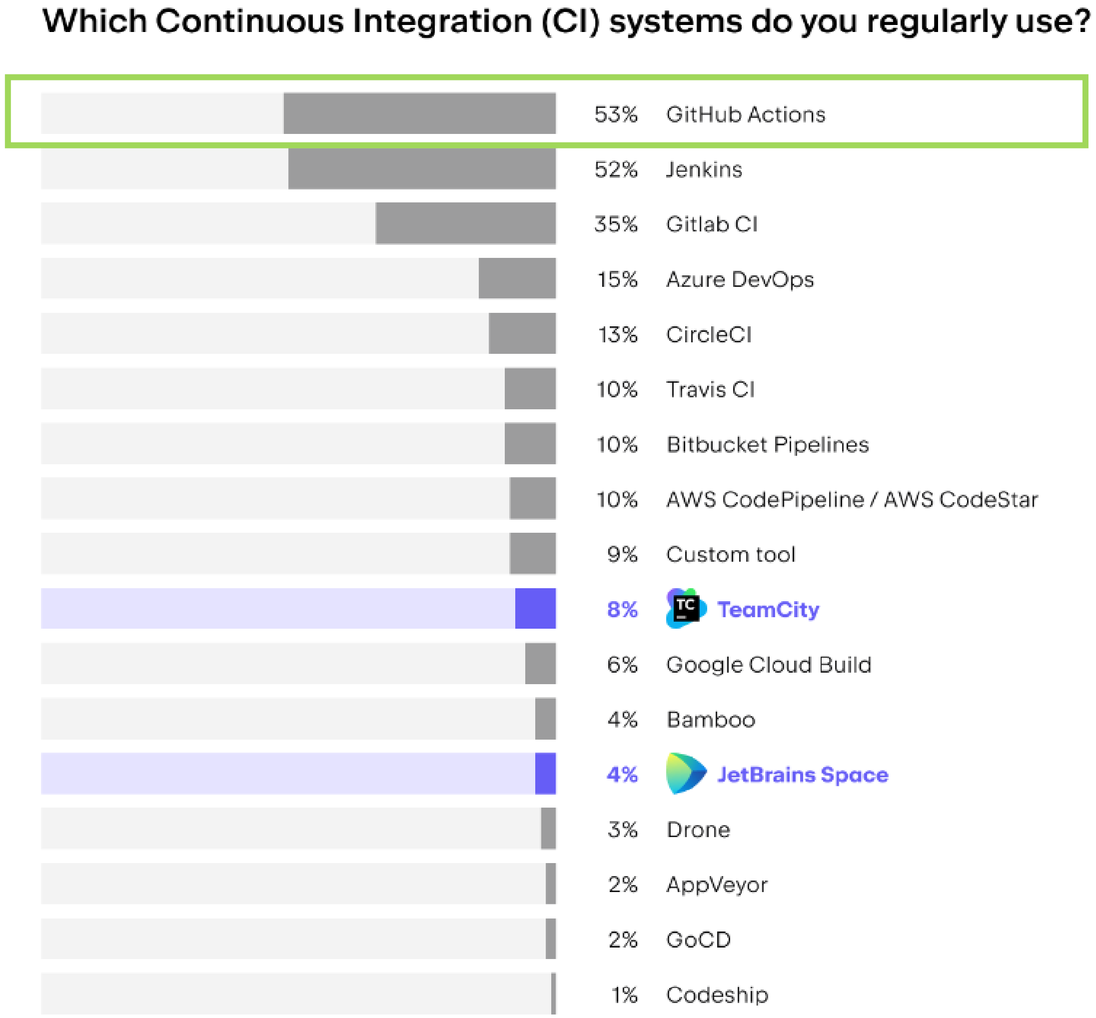
- **Continuous Integration (CI)** is not only about testing and validating code and components, but also **testing and validating data, data schemas, and models**
- **Continuous Delivery (CD)** is not only about a single software package or a service, but a system (an ML training pipeline) that **should automatically deploy another service** (model prediction service)
- **Continuous Training (CT)** is a new property, unique to ML systems, that's concerned with **automatically retraining candidate models** for testing and serving

Can be trigger w/ GitHub Actions

- **Continuous Monitoring (CM)** is not only about catching errors in production systems, but also about **monitoring production inference data and model performance metrics** tied to business outcomes

Using WandB

CI/CD in MLOps (via Github Actions) accelerates release frequency, enhancing user value and feedback collection



Source: Jet Brains

1. **Automated Workflows**: Streamlines CI/CD processes for machine learning models efficiently
2. **Easy Integration**: Seamlessly integrates with existing GitHub repositories and tools
3. **Customizable Pipelines**: Offers flexibility in designing tailored MLOps workflows
4. **Community-Driven Actions**: Access to a vast repository of pre-built actions for varied tasks
5. **Enhanced Security**: Provides built-in security features for secure MLOps operations.

Integrating GitHub Actions with MLflow & WandB automates workflows, ensures model consistency, and streamlines artifact management

1. **CI/CD**: Automates ML model testing, building, and deployment with each **code change** via Actions

2. **Automated Experiment Tracking**: Actions **triggers** MLflow experiments **automatically** on new code pushes, ensuring consistent experiment logging

3. **Automated Model Testing and Validation**: **New ML models** are automatically tested and validated in the Actions workflow

4. **Version Control for Models and Artifacts**: **Ensures** every model and artifact version is controlled and recorded

5. **Workflow Automation for Data Preparation and Processing**: **Triggers** data preparation and processing workflows, ensuring MLflow has **ready-to-use data** for model training

6. **Notifications and Reporting**: Set up Actions for proactive **notifications and reports** on ML experiment and model deployment statuses

GitHub Actions

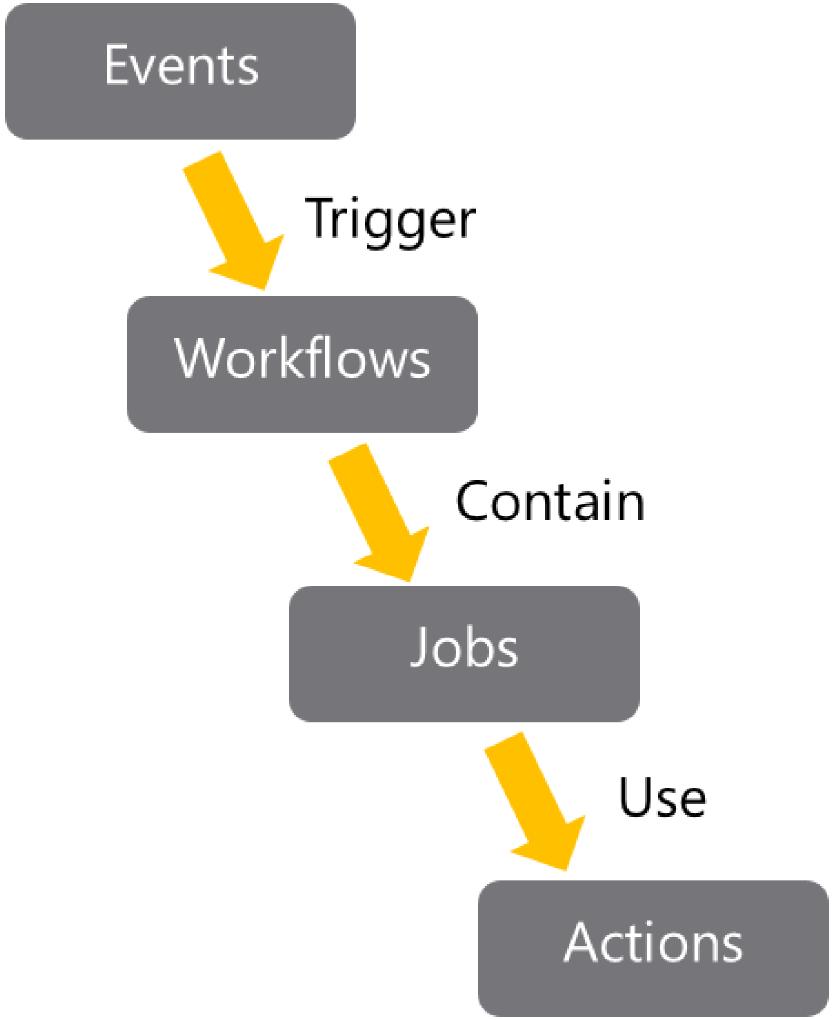
W&B

mlflow

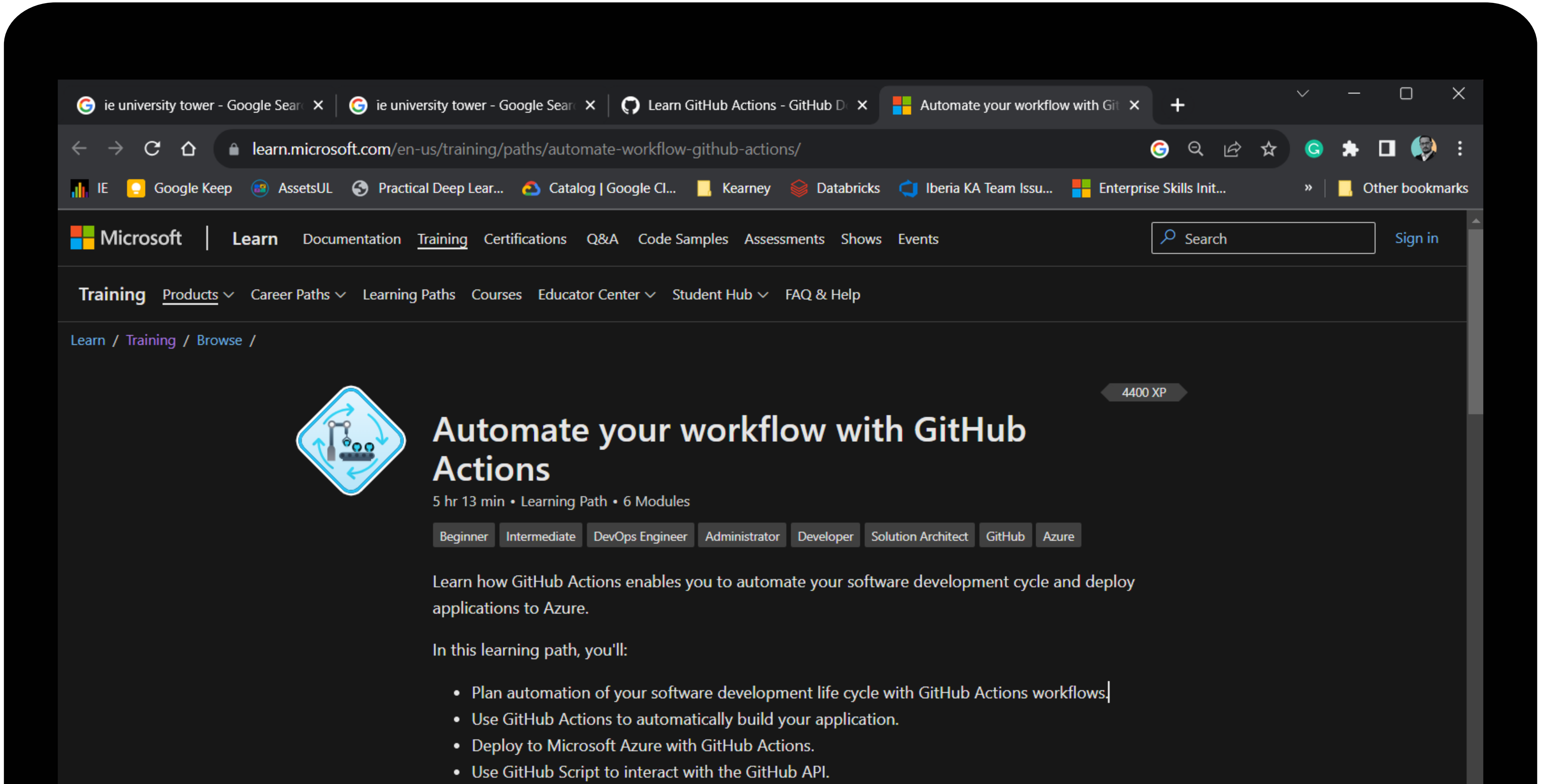
GitHub ACTIONS can do more than CI/CD !

- Automated testing
- Automatically responding to new issues, mentions
- Triggering code reviews
- Handling pull requests
- Branch management

Actions are executed on "runners," either hosted by GitHub or self-hosted



Optional: Introduction to GitHub Actions



1 Start with pure CI (pytest only)

Running unit tests on every push gives immediate feedback and locks basic quality

Tasks

1. Add .github/workflows/ci.yml
2. Install deps, cache pip to speed repeats
3. Run pytest -q for Python 3.10 (or matrix e.g. 3.8-3.11)

```yaml
name: CI

on:
  push:
    branches: [main]
  pull_request:
    branches: [main]

jobs:
  test:
    runs-on: ubuntu-latest
    strategy:
      matrix:
        python-version: ['3.10', '3.11']
    steps:
      - uses: actions/checkout@v4
      - name: Set up Python
        uses: actions/setup-python@v5
        with:
          python-version: ${{ matrix.python-version }}
      - name: Cache pip
        uses: actions/cache@v3
        with:
          path: ~/.cache/pip
          key: ${{ hashFiles('requirements*.txt') }}
      - name: Install dependencies
        run: pip install -r requirements.txt -r
requirements-dev.txt
      - name: Run tests
        run: pytest -q
```

Canonical directory and updated files (illustrative)

```
my_project/
│
├── .github/
│    └── workflows/
│         └── ci.yml
├── tests/
│    └── test_api.py
├── environment.yml
├── requirements.txt
├── requirements-dev.txt
└── README.md
```

Anatomy of .github/workflows/ci.yml

```yaml
name: CI

on:
  push:
    branches: [main]
  pull_request:
    branches: [main]

jobs:
  test:
    runs-on: ubuntu-latest
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        python-version: ['3.10', '3.11']
    steps:
      - uses: actions/checkout@v4
      - name: Set up Python
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        with:
          python-version: ${{ matrix.python-version }}
      - name: Cache pip
        uses: actions/cache@v3
        with:
          path: ~/.cache/pip
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Anatomy of .github/workflows/ci.yml

```yaml
name: CI

on:
  push:
    branches: [main]
  pull_request:
    branches: [main]

jobs:
  test:
    runs-on: ubuntu-latest
    strategy:
      matrix:
        python-version: ['3.10', '3.11']
    steps:
      - uses: actions/checkout@v4
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          path: ~/.cache/pip
          key: ${{ hashFiles('requirements*.txt') }}
      - name: Install dependencies
        run: pip install -r requirements.txt -r
requirements-dev.txt
      - name: Run tests
        run: pytest -q
```

Triggers ("on:") Runs the workflow on every push and every pull request (PR) to the main branch.
Purpose: Ensures tests always run before code is merged to your main development branch

Job definition: Defines a job e.g. test
runs-on: Specifies the virtual machine OS e.g. Ubuntu (most common for Python CI)

Matrix strategy: Runs the same set of steps in parallel for different Python versions
Purpose: Catches compatibility issues with multiple Python versions (or any other SW)

Set up Python interpreter: Installs and sets the active Python version for the job
Purpose: Ensures correct Python version for each run

Steps: Defines each action/ command run in the job
Checkout code: Downloads the repo to the CI environment so it can be tested

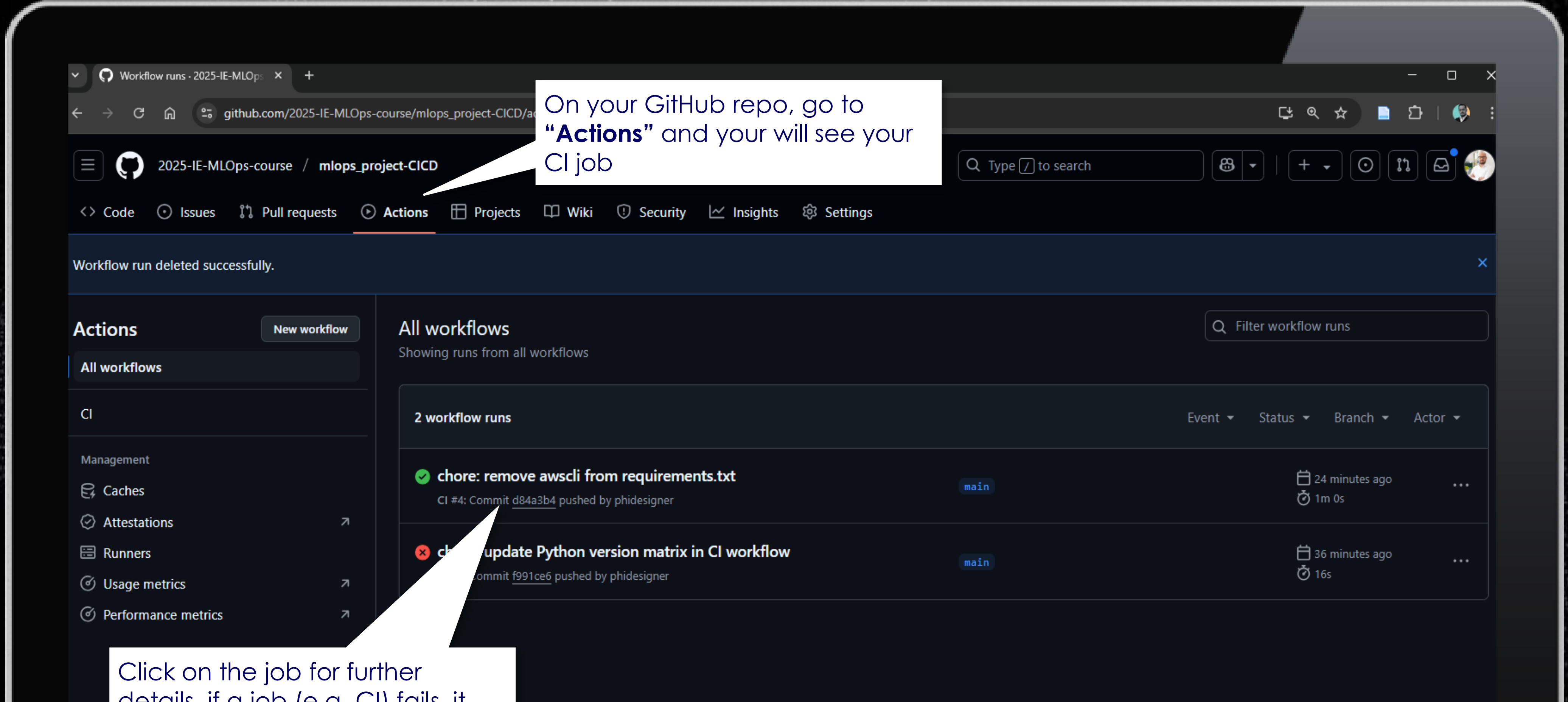
Cache dependencies: Uses the actions/cache to store (and later retrieve) downloaded Python packages
path: specifies what to cache i.e. ~/.cache/pip is pip's default download cache
key: Unique ID that updates whenever 'requirements.txt' change
Purpose: Speeds up repeated workflow runs

Install dependencies: Installs all runtime (**requirements**.txt) and dev/test (**requirements-dev**.txt)
Purpose: Ensures the test environment matches the local dev setup

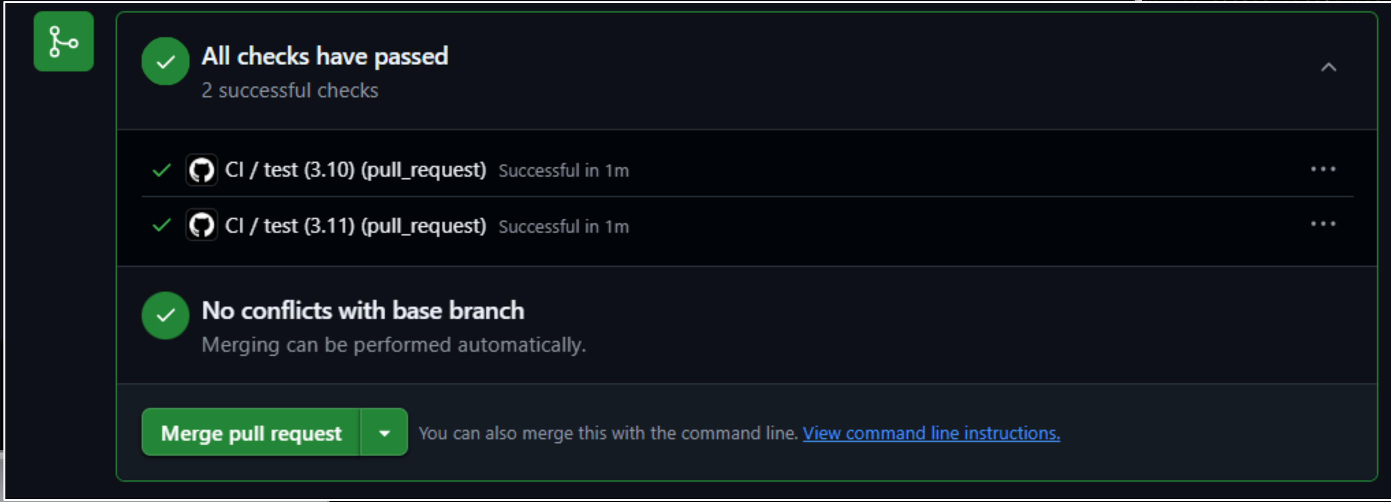
Run tests: Executes pytest (or any other command)
Purpose: Fails the job if any test fails

ie UNIVERSITY

On your GitHub repo, go to "**Actions**" and your will see your CI job



Click on the job for further details, if a job (e.g. CI) fails, it won't let you merge to your branch



2

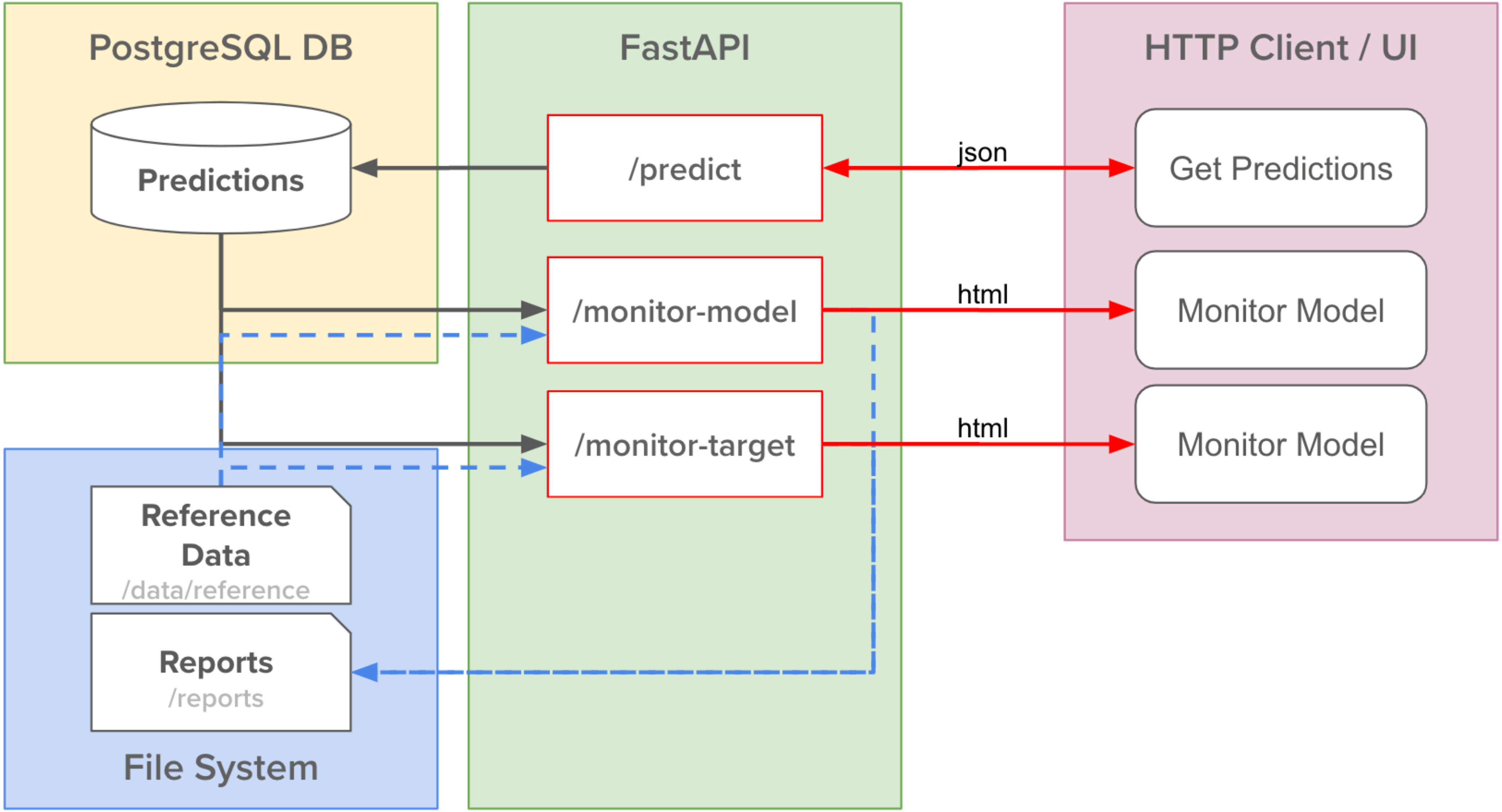
Exposing your learner with a high-performance, easy-to-use API using FastAPI

FastAPI for MLOps

- **FastAPI** is a tool to let apps talk to your ML model using standard web methods (verbs)
- **RESTful API** means using simple web commands (GET, POST…) to manage model services
- **HTTP endpoint** is the web address where you "ask" the model questions
- **Pydantic** checks and converts data to correct format automatically
- **OpenAPI docs** give interactive interface, so users test model calls in browser
- **Async I/O (Starlette + Uvicorn)** lets many users talk to the model at once
- REST API uses HTTP methods (verbs) to manage resources:
  - **GET** → Ask model a question, e.g. "What's today's temperature?"
  - **POST** → Send data to model, e.g. "Analyse this photo"
  - **PUT/PATCH** → Update model settings, e.g. "Change performance metric"
  - **DELETE** → Remove a model or its data, e.g. "Erase old version"

Typical FastAPI ML flow: import FastAPI > define endpoints > load model > handle predict route

Simple architecture schema



Source: https://medium.com/data-science/step-by-step-approach-to-build-your-machine-learning-api-using-fast-api-21bd32f2bbdb

2 Add FastAPI service

Exposing a lightweight API before containerising and deploy on a remote server

Tasks

1. Create app/main.py with FastAPI()
2. Include /health returning {"status": "ok"} for probes
3. Add requirements-api.txt with fastapi uvicorn

```
my_project/
├── app/
│   ├── __init__.py
│   ├── main.py
├── tests/
│   ├── test_api.py
├── scripts/
│   ├── call_api.py
├── .env
├── pytest.ini
├── environment.yml
├── requirements.txt
├── requirements-dev.txt
└── README.md
```

Anatomy of */app/main.py*

```
(…)
RAW_FEATURES = CONFIG.get("raw_features",
[])
ENGINEERED = CONFIG.get("features",
{}).get("engineered", [])

app = FastAPI()


class PredictionInput(BaseModel):
    rx_ds: int = Field(..., alias="rx ds")
    A: int
    B: int
    C: int
    …
    class Config:
        allow_population_by_field_name =
True
        schema_extra = {
            "example": {
                "rx_ds": 100,
                "A": 0,
                "B": 1,
                "C": 0,
                 … }}
(…)
```

```
(…)

@app.get("/")
def root():
    return {"message": "Welcome to the
opioid abuse prediction API"}

@app.get("/health")
def health():
    return {"status": "ok"}

@app.post("/predict")
def predict(payload: PredictionInput):
    data = payload.dict(by_alias=True)
    df = pd.DataFrame([data])
    X_raw = df[RAW_FEATURES]
    X_proc = PIPELINE.transform(X_raw)
    if ENGINEERED:
        feature_names =
get_output_feature_names(
            preprocessor=PIPELINE,
            input_features=RAW_FEATURES,
            config=CONFIG,
        )
        indices = [feature_names.index(f)
for f in ENGINEERED if f in feature_names]
        X_proc = X_proc[:, indices]
    pred = MODEL.predict(X_proc)[0]
    proba = MODEL.predict_proba(X_proc)[0,
1] if hasattr(MODEL, "predict_proba") else
None
    return {"prediction": int(pred),
"probability": float(proba) if proba is
not None else None}
```

Initialize our **FastAPI**

Defines the input data schema using ***Pydantic***

- Each feature as a type-checked field
- *rx_ds* is mapped to/from "*rx ds*" for alias support
- *Class Config* enables field aliases and provides an example payload for docs

Anatomy of */app/main.py*

```python
(…)
app = FastAPI()

class PredictionInput(BaseModel):
    rx_ds: int = Field(..., alias="rx ds")
    A: int
    B: int
    C: int
    …
    class Config:
        allow_population_by_field_name =
True
        schema_extra = {
            "example": {
                "rx_ds": 100,
                "A": 0,
                "B": 1,
                "C": 0,
                 … }}
(…)
```

Prediction endpoint:

- Accepts a POST request with validated input data
- Converts input to a DataFrame, applies the preprocessing pipeline
- Optionally selects engineered features
- Uses the loaded ML model to predict the outcome and probability
- Returns prediction and probability as JSON.

```python
(…)

@app.get("/")
def root():
    return {"message": "Welcome to the
opioid abuse prediction API"}

@app.get("/health")
def health():
    return {"status": "ok"}

@app.post("/predict")
def predict(payload: PredictionInput):
    data = payload.dict(by_alias=True)
    df = pd.DataFrame([data])
    X_raw = df[RAW_FEATURES]
    X_proc = PIPELINE.transform(X_raw)
    if ENGINEERED:
        feature_names =
get_output_feature_names(
            preprocessor=PIPELINE,
            input_features=RAW_FEATURES,
            config=CONFIG,
        )
        indices = [feature_names.index(f)
for f in ENGINEERED if f in feature_names]
        X_proc = X_proc[:, indices]
    pred = MODEL.predict(X_proc)[0]
    proba = MODEL.predict_proba(X_proc)[0,
1] if hasattr(MODEL, "predict_proba") else
None
    return {"prediction": int(pred),
"probability": float(proba) if proba is
not None else None}
```

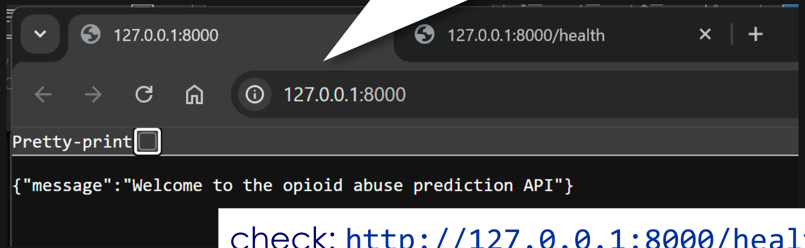
Root endpoint with simple message

Check endpoint

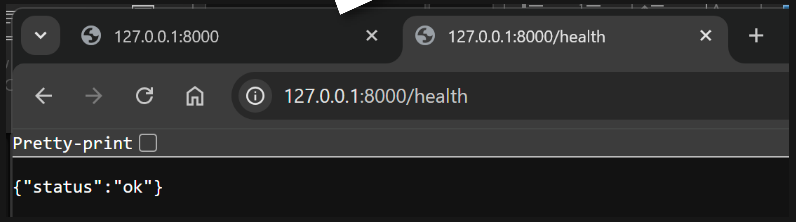
Run, test, and validate your FastAPI prediction service **locally** using scripts, browser endpoints, and interactive docs

```
# Running your app locally
> uvicorn app.main:app --reload

# Test via script
>  python scripts/call_api.py --url http://127.0.0.1:8000/predict --input /home/idiazl/2025_MLOps/mlops_project-CICD/data/inference/new_data.csv

> python scripts/call_api.py --url http://127.0.0.1:8000/predict_batch --input /home/idiazl/2025_MLOps/mlops_project-CICD/data/inference/new_data.csv
```

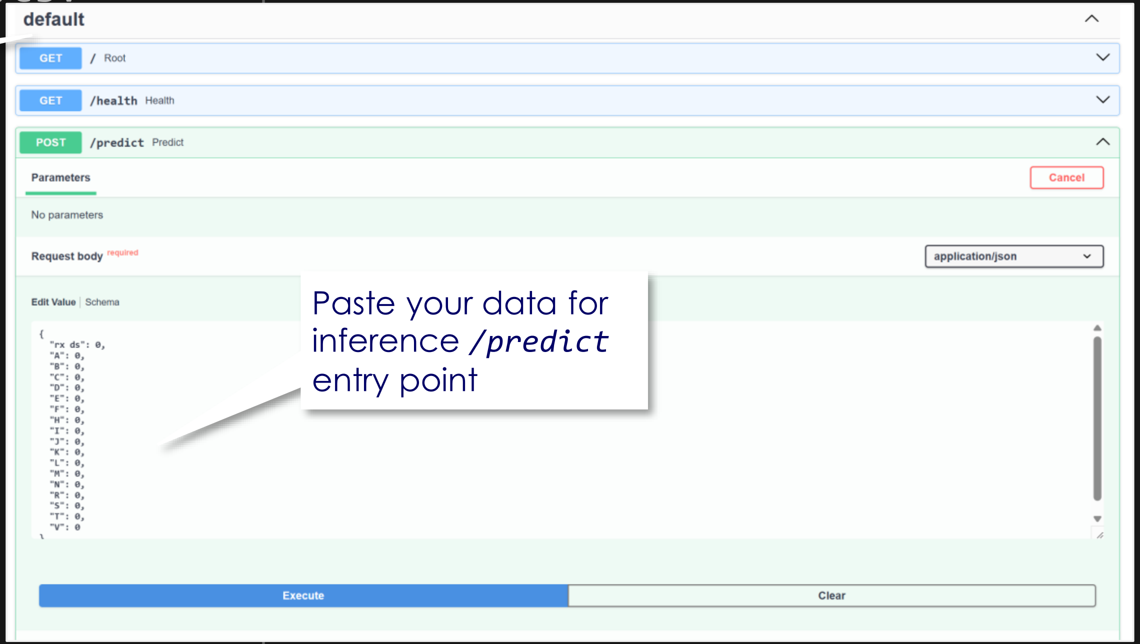
- Starts your API on http://127.0.0.1:8000
- *--reload* auto-restarts when you change code



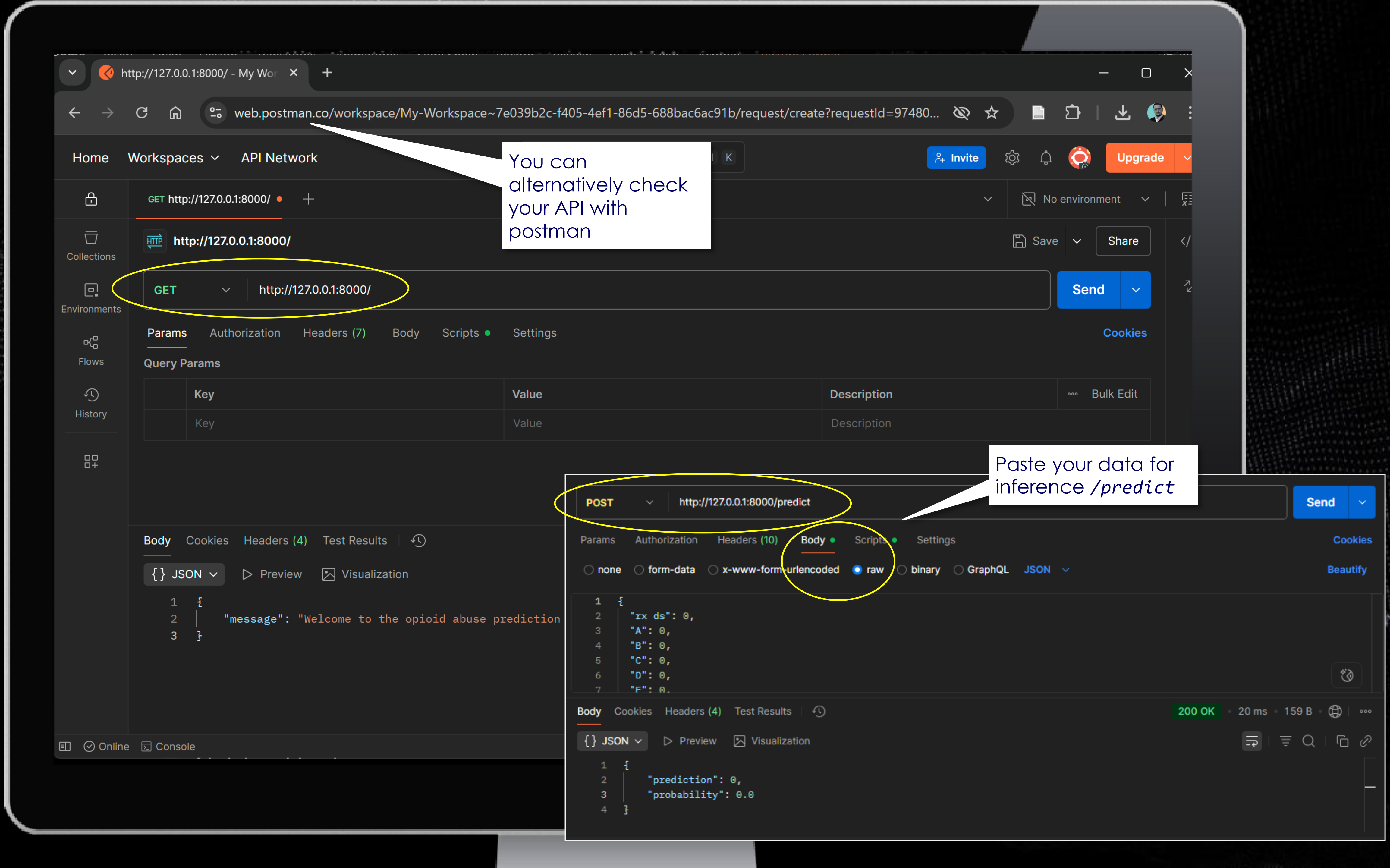
check: http://127.0.0.1:8000/health



- check: http://127.0.0.1:8000/docs
- Interactive docs at */docs* to try your /predict endpoint with sample data



Paste your data for inference */predict* entry point


You can alternatively check your API with postman
Paste your data for inference /predict
GET http://127.0.0.1:8000/
"message": "Welcome to the opioid abuse prediction
POST http://127.0.0.1:8000/predict
"rx ds": 0,
"A": 0,
"B": 0,
"C": 0,
"D": 0,
200 OK
"prediction": 0,
"probability": 0.0

3 Dockerise the project

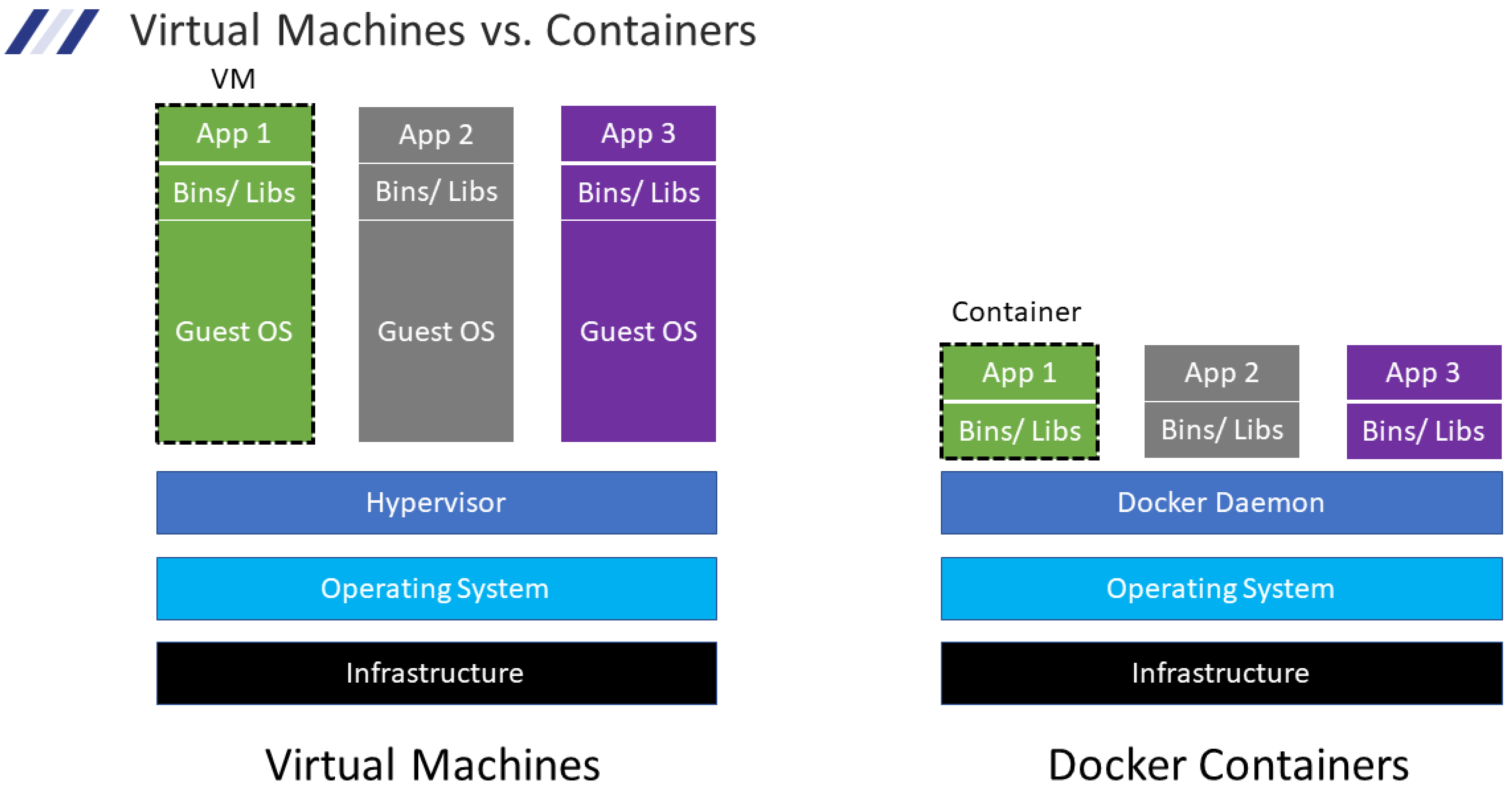
The Docker image isolates runtime and eases deployment to remote servers e.g. Render, Railway, etc.

Tasks

1. Install Docker desktop
2. Create Dockerfile
3. .dockerignore
4. Configure render.yaml
5. Add requirements (-api).txt
   1. /app
   2. /inference
   3. config, .env, scripts and models

```
my_project/
├── app/
│    ├── __init__.py
│    ├── main.py
├── Dockerfile
├── .dockerignore
├── render.yml
├── requirements.txt
├── requirements-dev.txt
└── README.md
```

Different to VMS, Docker images don't run on their own OS



Anatomy of */Dockerfile*

```
FROM python:3.10-slim

WORKDIR /code
ENV PYTHONPATH=/code/src

# install dependencies first to leverage
layer caching
COPY requirements.txt requirements-dev.txt
./
RUN pip install --no-cache-dir -r
requirements.txt -r requirements-dev.txt

# copy application code
COPY app ./app
COPY src ./src
COPY config.yaml ./
COPY main.py ./
COPY MLproject ./
COPY scripts ./scripts

EXPOSE 8000

HEALTHCHECK CMD curl --fail
http://localhost:${PORT:-8000}/health ||
exit 1

CMD ["sh", "-c", "python
scripts/download_from_wandb.py && uvicorn
app.main:app --host 0.0.0.0 --port ${PORT:-
8000}"]
```

Uses a lightweight **Python** image as base, to minimize image size

- Sets **working directory** inside the container to */code*, so all following commands run from there
- **ENV** tells Python where to find your custom modules in */code/src*

Copies dependency files from the local machine into the container (Dev and Prod)

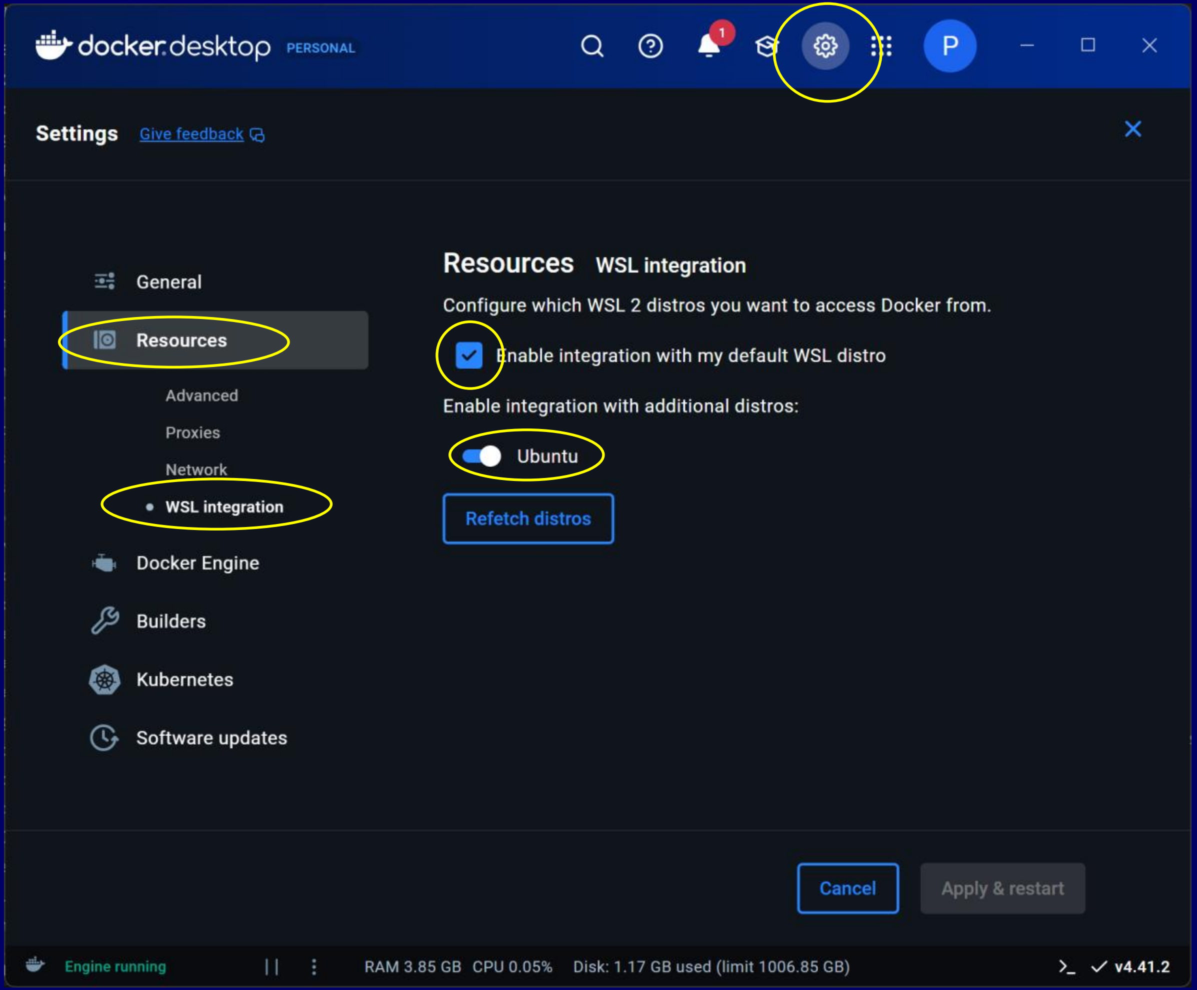
- Installs all Python dependencies
- *--no-cache-dir* keeps the image size smaller by not saving pip's download cache

Copies the app code and configs into the image.Eensuring all required source files and configs are available for the app to run (together with *.dockerignore*)

Defines a simple check to see if the app is healthy. If it fails, marks the container as unhealthy

- Runs a script to download artifacts from Weights & Biases
- Launches the FastAPI app with Uvicorn on port 8000 (or default)

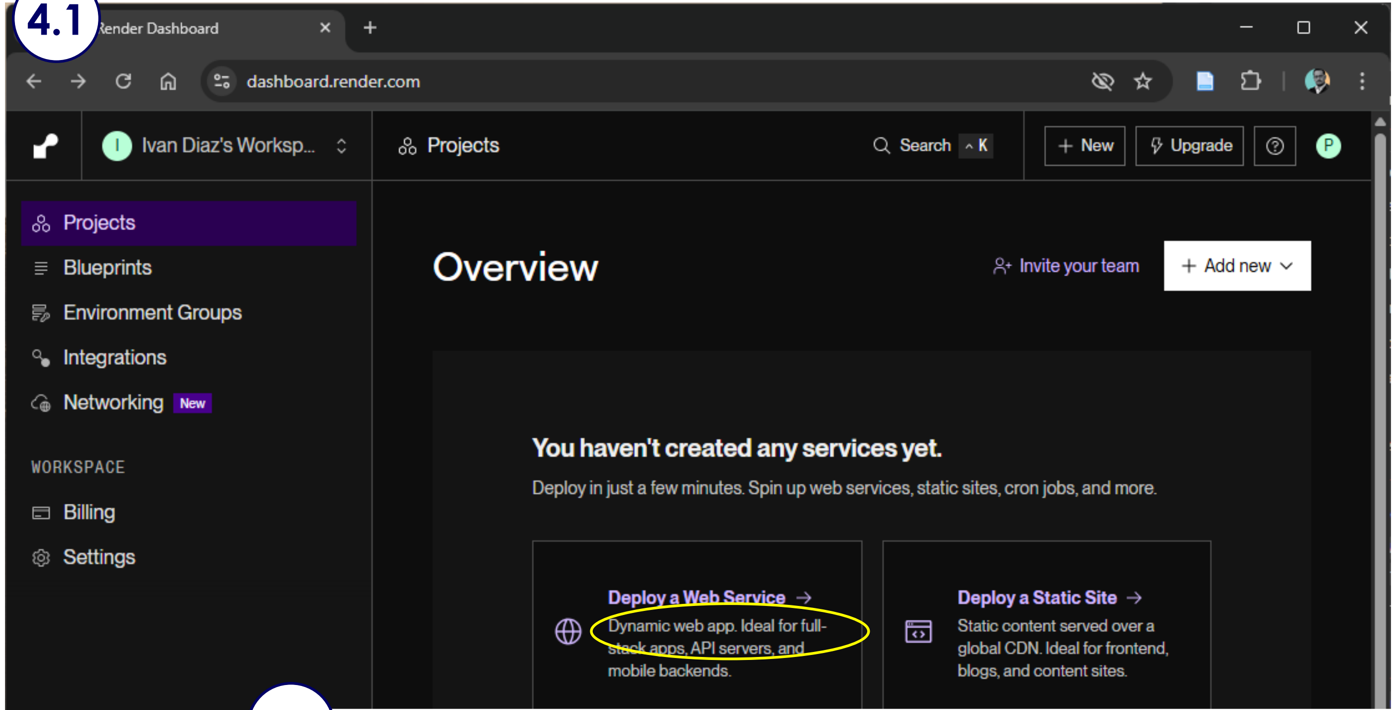
For WSL users make sure WSL is integrated



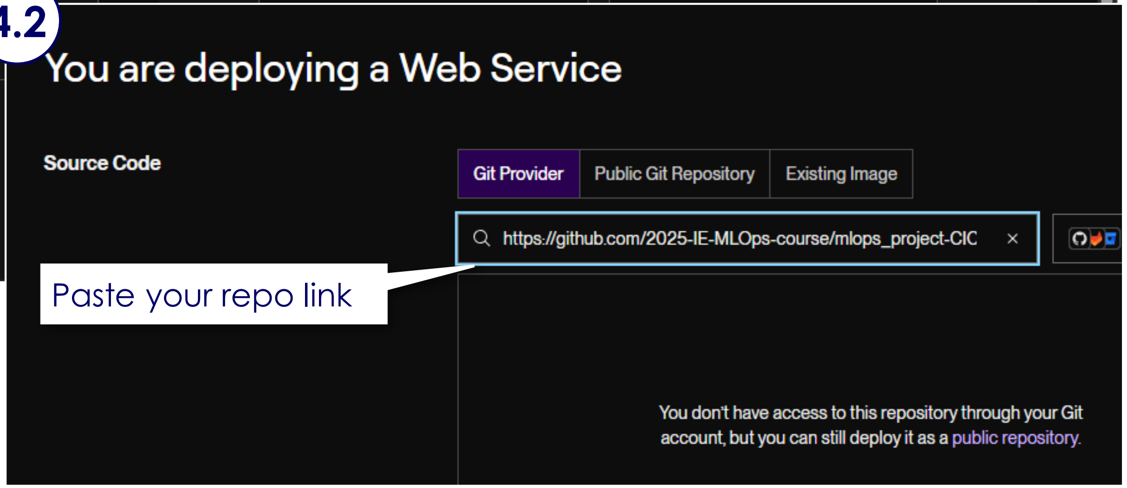

```
# Docker set up checks

> docker version
> Docker run hello-world

# 1. Set/ update WANDB credentials on your .env
WANDB_PROJECT=opioid_mlops_project_CICD
WANDB_ENTITY=idiazl
WANDB_API_KEY=xxxx

# 2. Build the image
> docker build -t <opioid-api> .

# Check for created images
> docker images

# 3. Run the container
> docker run --env-file .env -p 8000:8000 opioid-api

# 4. Check status via app, docs, or terminal
> curl http://localhost:8000/health

# 5. Submit a local testing batch (via script)
> python scripts/call_api.py --url
http://localhost:8000/predict_batch --input
data/inference/new_data.csv
```

4 Deploying on Render.com (remote)

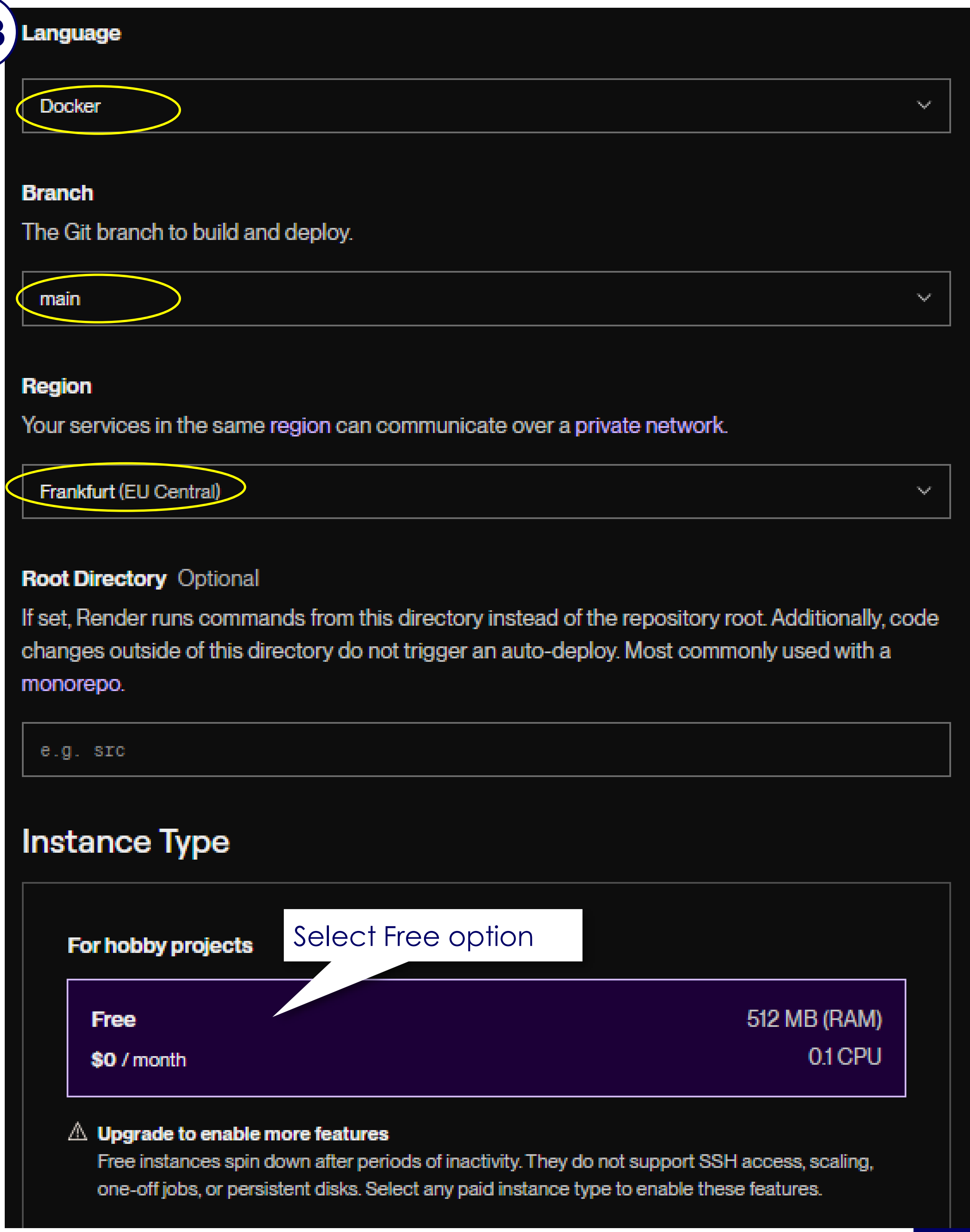
4.1



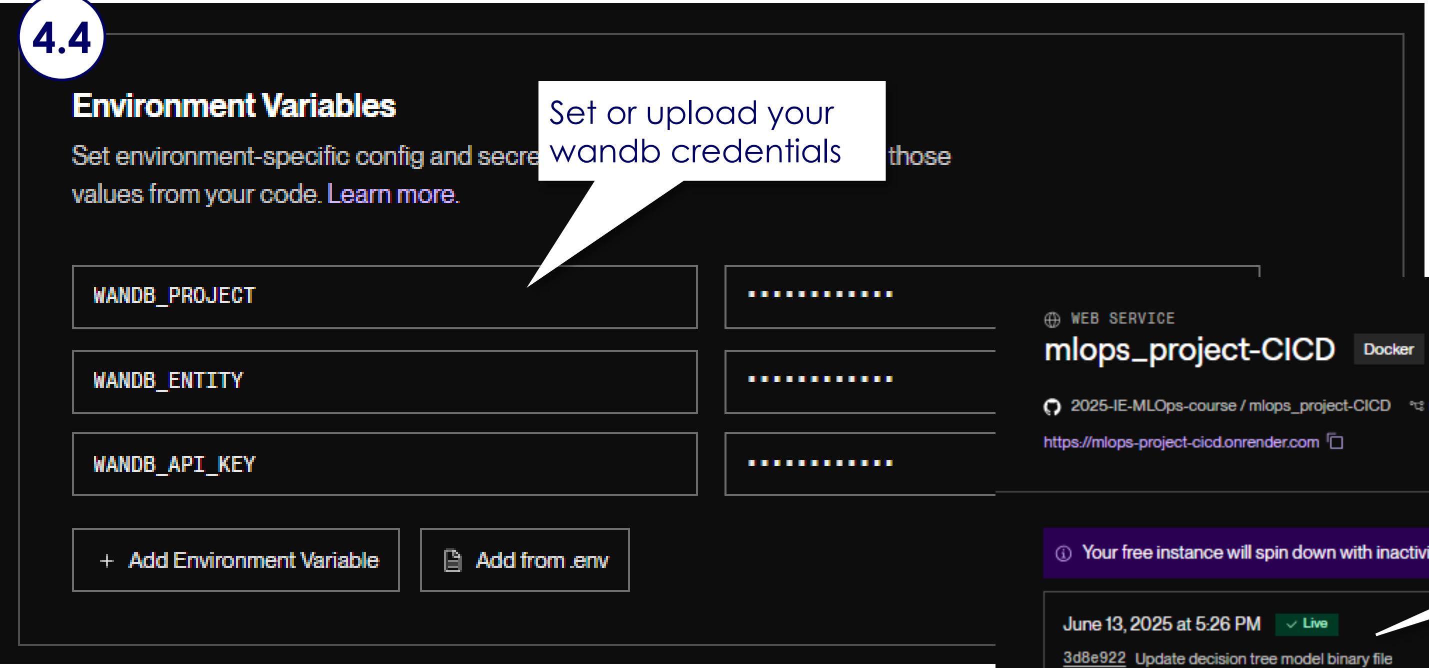
4.2

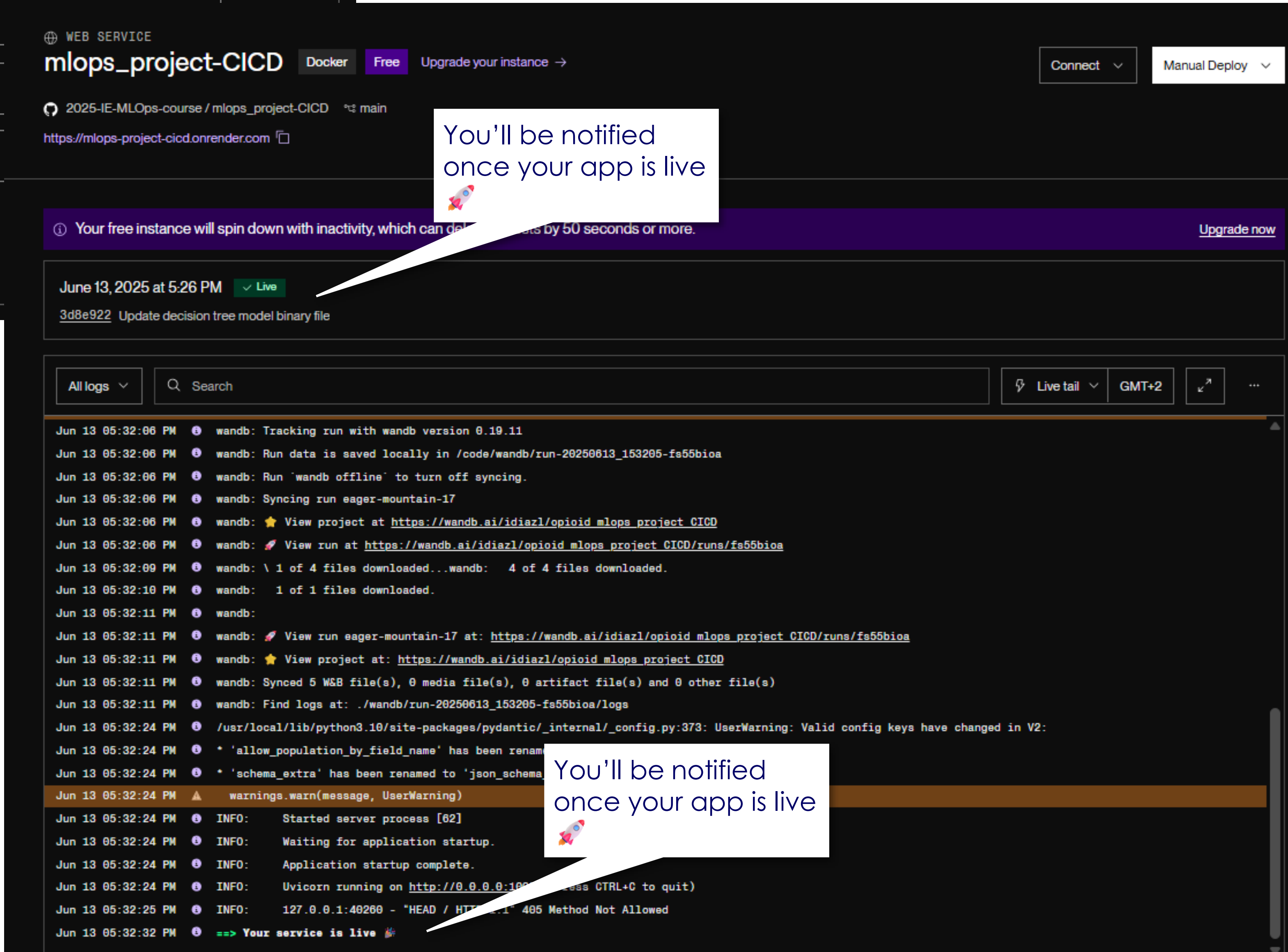


4.3



4.4





Testing the remote app programmatically

```
python scripts/call_api.py --url https://mlops-project-cicd.onrender.com/predict_batch --input data/inference/new_data.csv
```