iterative

Pipelines

Automation and Configuration

Lesson 3

DVC Tools for Data Scientists & Analysts

2021

Course lessons

Lesson 1. Course Introduction

Lesson 2. Practices and Tools for Efficient Collaboration in ML projects

Lesson 3. Pipelines Automation and Configuration Management

Lesson 4. Versioning Data and Models

Lesson 5. Visualize Metrics & Compare Experiments with DVC and Studio

Lesson 6. Experiments Management and Collaboration

Lesson 7. Tools for Deep Learning Scenarios

Lesson 8. Review Advanced Topics and Use Cases

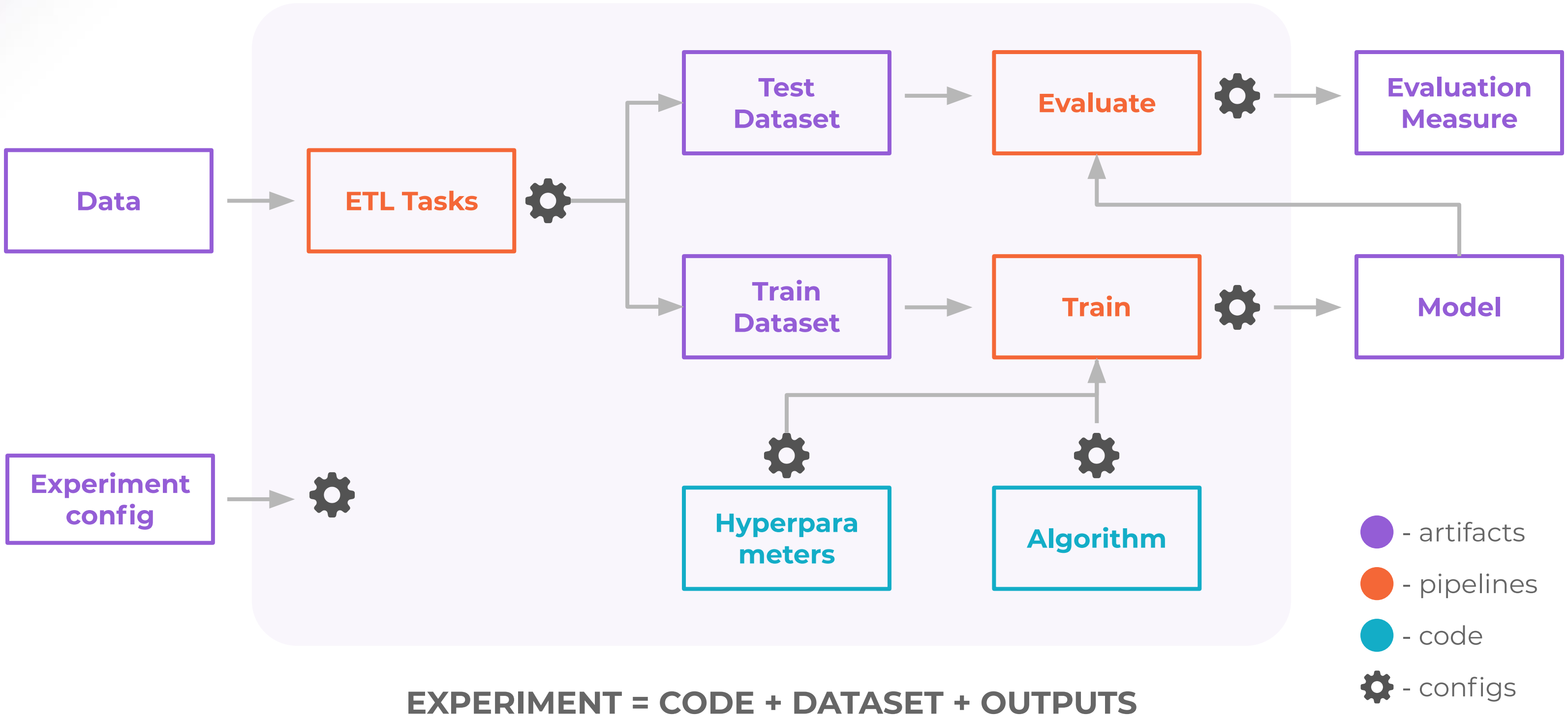
Lesson Outline

- Why automate ML pipelines?
- Requirements for pipeline automation
- Build automated pipelines: step by step guide
- Reproduce end-to-end ML pipelines

Why automate ML pipelines?

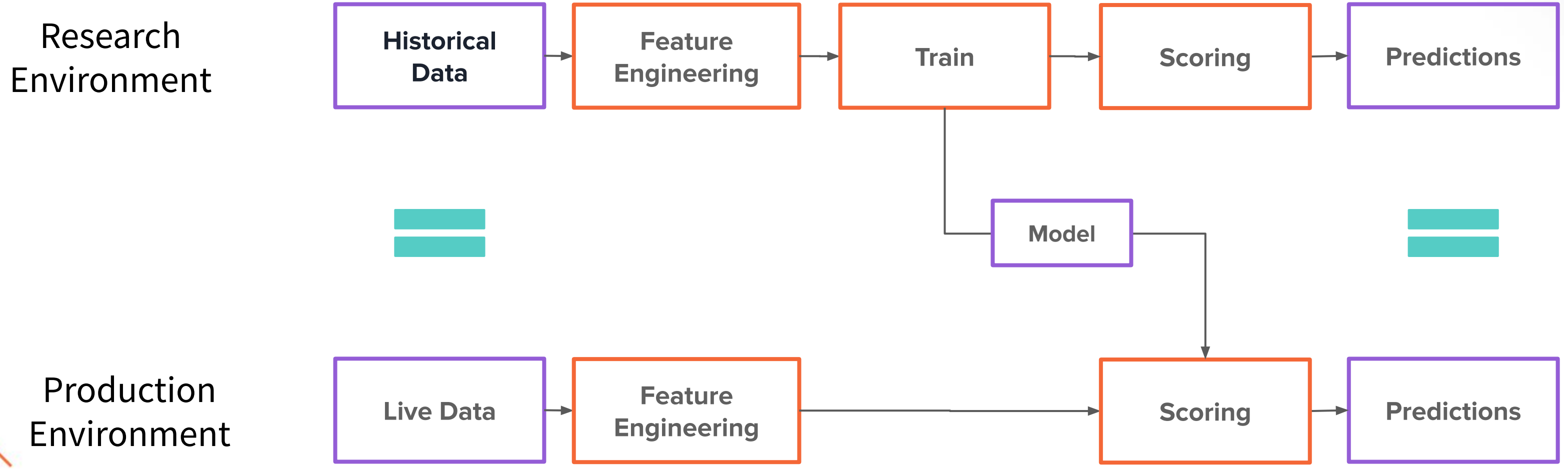
ML Experiments

take long time and produce mess of metrics and artifacts

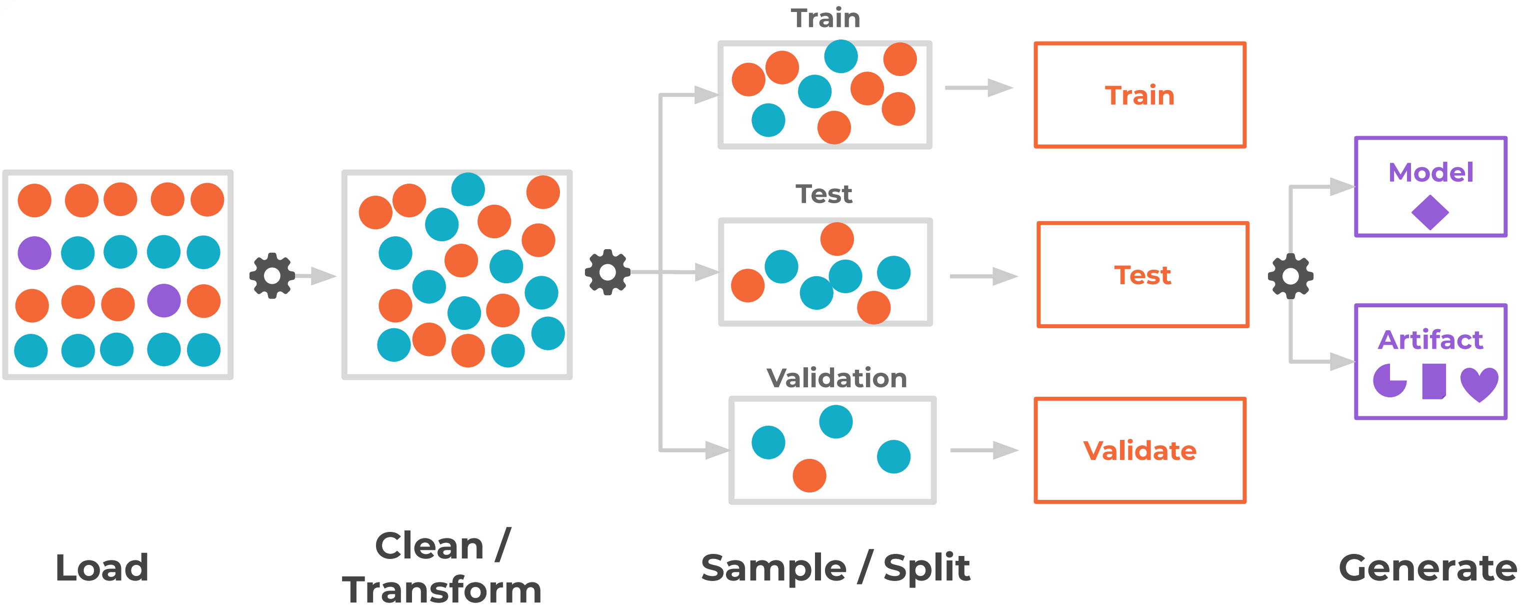


EXPERIMENT = CODE + DATASET + OUTPUTS

Priority 1: Reproducibility

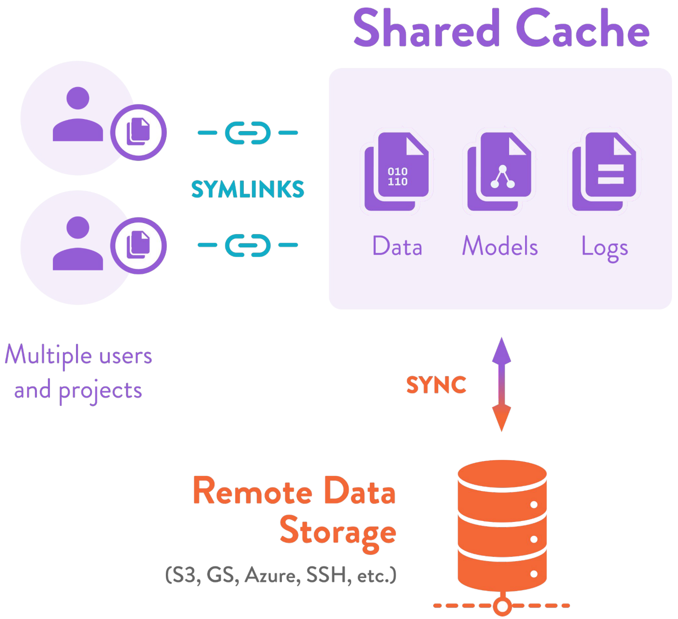


Optimized & deterministic ETL



Improve team collaboration

- Code versioning
- Experiment params control
- Data & artifacts control



Requirements for pipeline automation

From Jupyter Notebooks To .py

Jupyter Notebook

- interactive environment
- can run .py / bash scripts
- great for visualization

.py scripts

- versioning
- reproducible pipelines
- easy to automate

Manage configs

- no `hardcoded` paths & params
- move params to config file
  - ~ **params.yaml**

Reusable code

- clear pipeline workflow and stages
    - inputs
    - jobs
    - outputs
- organize code
- clean code
- reusable code

Build automated pipelines: step by step guide

Step 1: Organize repo & build a prototype

Guide

- Organize your project folder structure
- Use virtual environment or Docker
- Use tools and libraries you are comfortable with
- Keep a linear workflow to run cells in Jupyter Notebook
- Use table of content (TOC) widget and group cells

Tools

- Jupyter Notebooks

Live code example

Step 1:

Build a Prototype with Jupyter Notebook

Step 2: Create a single configuration file

Guide

- Avoid hardcoded paths & params from code
- Move all params to a single config file: params.yaml
- Group parameters (e.g. data, train, test...)

Tools

- Jupyter Notebooks
- YAML

params.yaml: structure example

```
# params.yaml
data_load:
  dataset_csv: 'data/raw/iris.csv'

data_split:
  test_size: 0.2
  trainset_path: 'data/processed/train_iris.csv'
  testset_path: 'data/processed/test_iris.csv'

train:
 cv: 3
 estimator_name: logreg        # sklearn.linear_model.LogisticRegression
 C: 0.001
 max_iter: 100
 solver: 'lbfgs'
 multi_class: 'multinomial'
 model_path: models/model.joblib
```

Set and save configuration

params.yaml: usage example

data_load.py

```python
import yaml

def data_load(config_path: Text) -> None:

    config = yaml.safe_load(open(config_path))
    raw_data_path = config['data_load']['raw_data_path']

    ...
```

Load and use configuration

Live code example

Step 2:

Create a single configuration file

Step 3: Move reusable code to .py modules

Guide

- Move functions and classes into .py modules
  - import in Jupyter Notebooks
- Add .py modules to Git version control
- Organize code repo

Tools

- Jupyter Notebooks
- YAML
- Python scripts (.py)
- Git

Organize code repo (example)

```
├── README.md
├── config/
├── data/
├── models/
├── notebooks/
├── reports/
└── src/
    ├── data/          <- data prepare and/or preprocess
    ├── evaluate/  <- code for model quality evaluation and metrics
    ├── features/   <- code to compute features
    ├── report/        <- code for visualization and plots
    └── train/         <- code for training and hyper-parameters tuning
```

Move .py code into src/ directory

Organize code repo (example)

```
├── README.md
├── config/
├── data/
├── models/
├── notebooks/
├── reports/
└── src/
    ├── data/
    ├── evaluate/
    ├── features/
    ├── report/
    └── train/
```

Add all Jupyter Notebooks to a separate folder

Live code example

Step 3:

Move reusable code to .py

Step 4: Build ML experiment pipeline

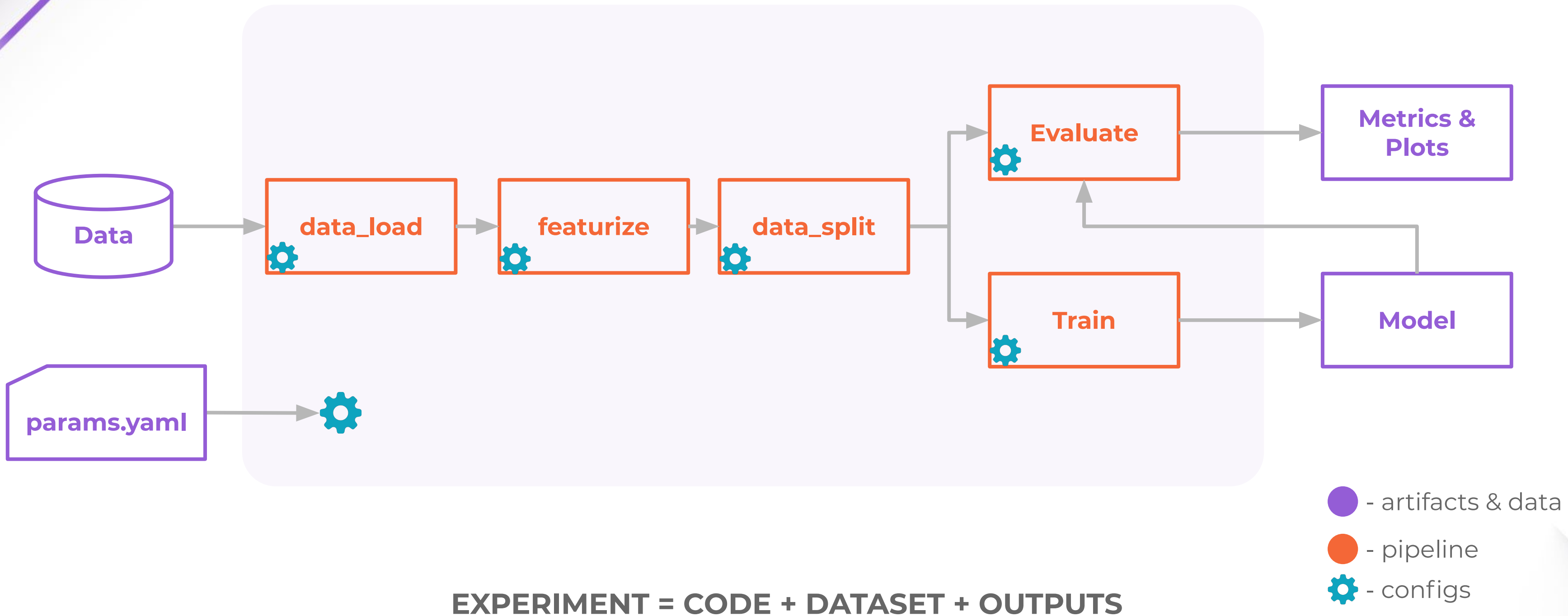
Guide

- Create .py module for each computation task (stage)
- Use **params.yaml** to manage configuration
- Structure **.py** modules to run in both mode
  - by importing in Jupyter Notebook
  - by running in terminal

Tools

- Jupyter Notebooks
- YAML
- Python scripts (.py)
- Git
- CLI

Example: Simple ML pipeline



EXPERIMENT = CODE + DATASET + OUTPUTS

Organize code repo (example)

```
├── README.md
├── config/
├── data/
├── models/
├── notebooks/
├── reports/
└── src/
    ├── data/
    ├── evaluate/
    ├── features/
    ├── stages/
    ├── report/
    └── train/
```

Add code for stages got stages/ folder

Make it simple to run & test with

data_load.py

```
import yaml

def data_load(config_path: Text) -> None:

  config = yaml.safe_load(open(config_path))
  raw_data_path = config['data_load']['raw_data_path']
  …
  data.to_csv(config['dataset_processed_path'])


if __name__ == '__main__':

  args_parser = argparse.ArgumentParser()
  args_parser.add_argument('--config', dest='config', required=True)
  args = args_parser.parse_args()

  data_load(config_path=args.config)
```

Import in Jupyter Notebook or run via CLI

Run data_load stage in CLI

run from the project root folder

```
python src/stages/data_load.py --config=params.yaml
```

Live code example

Step 4:

Build ML experiment pipeline

Step 5: Automate pipelines with DVC

Guide

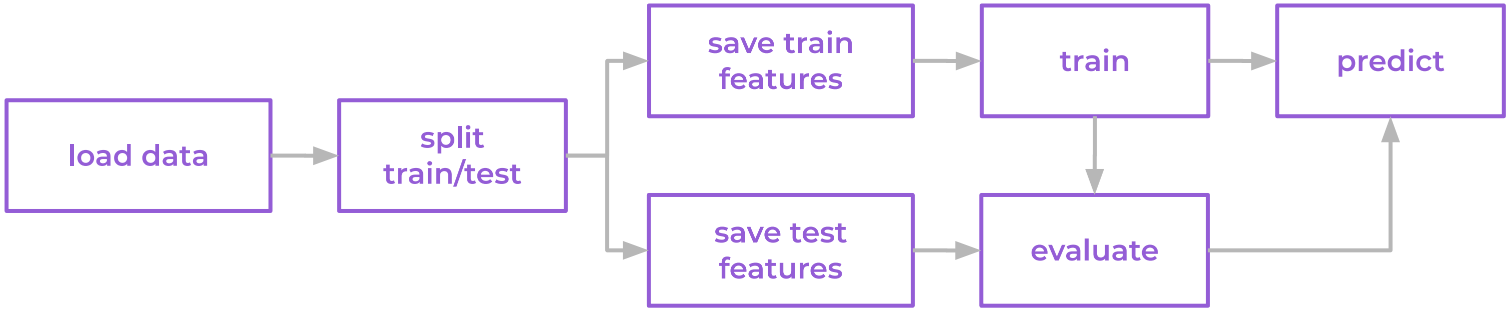
- Install DVC
- Organize stages into a DVC pipeline
- Setup dependencies and outputs
- Setup parameters

Tools

- YAML
- Python scripts (.py)
- Git
- DVC

Pipeline is a sequence of stages

- Each stage is a computation task that may produce data for a next stages
- DVC builds a dependency graph (DAG) of stages (pipeline)
- You decide what dependencies and outputs to control with DVC
- Reproduce stage or pipelines with **dvc repro**



Install DVC

\# Install with pip

```
$ pip install dvc
```

\# Install with support for Amazon S3 storage

```
$ pip install "dvc[s3]"   # [all]  to support all remote storages
```

\# Install with conda

```
$ conda install -c conda-forge dvc
```

Installation docs link: https://dvc.org/doc/install

Initialize DVC

run command

```
$ dvc init
```

output

```
Adding '.dvc/state' to '.dvc/.gitignore'.
Adding '.dvc/lock' to '.dvc/.gitignore'.
Adding '.dvc/config.local' to '.dvc/.gitignore'.
Adding '.dvc/updater' to '.dvc/.gitignore'.
Adding '.dvc/updater.lock' to '.dvc/.gitignore'.
Adding '.dvc/state-journal' to '.dvc/.gitignore'.
Adding '.dvc/state-wal' to '.dvc/.gitignore'.
Adding '.dvc/cache' to '.dvc/.gitignore'.

You can now commit the changes to Git.
```

We will learn more about Internal files and directories in during the Course

Commit changes

run command

```
$ git add .
$ git commit -m "Initialize DVC"
```

output

```
Initialize DVC
 2 files changed, 8 insertions(+)
 create mode 100644 .dvc/.gitignore
 create mode 100644 .dvc/config
```

Add pipeline stages with dvc run

-n specifies name
for DVC stage

```
dvc run -n data_load \
python src/data_load.py --config=params.yaml
```

command to run
for the stage

Notes

- \ symbol at the end of each line helps to continue command at the next line

Add pipeline stages with dvc run

Specify
-d dependencies
-o outputs

```
dvc run -n data_load \
  -d src/data_load.py \
  -o data/iris.csv \
  -p data_load \
  python src/data_load.py --config=params.yaml
```

-p specifies stage parameters

Add pipeline stages with dvc run

Specify
-d dependencies
-o outputs

-n specifies name
for DVC stage

```
dvc run -n data_load \
    -d src/data_load.py \
    -o data/iris.csv  \
    -p data_load \
    python src/data_load.py --config=params.yaml
```

command to run
for the stage

-p specifies stage
parameters

Add pipeline stages with dvc run

run command

```
$ dvc run -n data_load \
    -d src/data_load.py \
    -o data/iris.csv \
    -p base,data_load \
    python src/data_load.py  --config=params.yaml
```

output

```
Running stage 'data_load' with command:
        python src/data_load.py --config=params.yaml
Creating 'dvc.yaml'
Adding stage 'data_load' in 'dvc.yaml'
Generating lock file 'dvc.lock'
To track the changes with git, run:
        git add dvc.yaml dvc.lock
```

Create dvc.yaml file

dvc.yaml file content

```yaml
stages:
  data_load:
    cmd: python src/stages/data_load.py --config=params.yaml
    deps:
    - src/stages/data_load.py
    params:
    - base
    - data_load
    outs:
    - data/raw/iris.csv
```

Stage name

dvc.yaml file content

```yaml
stages:
 data_load:
   cmd: python src/stages/data_load.py --config=params.yaml
   deps:
   - src/stages/data_load.py
   params:
   - base
   - data_load
   outs:
   - data/raw/iris.csv
```

A command to run this stage

dvc.yaml file content

```
stages:
 data_load:
   cmd: python src/stages/data_load.py --config=params.yaml
   deps:
   - src/stages/data_load.py
   params:
   - base
   - data_load
   outs:
   - data/raw/iris.csv
```

List of dependencies

dvc.yaml file content

```yaml
stages:
 data_load:
  cmd: python src/stages/data_load.py --config=params.yaml
  deps:
  - src/stages/data_load.py
  params:
  - base
  - data_load
  outs:
  - data/raw/iris.csv
```

Parameters from params.yaml (by default)

dvc.yaml file content

```yaml
stages:
 data_load:
   cmd: python src/stages/data_load.py --config=params.yaml
   deps:
   - src/stages/data_load.py
   params:
   - base
   - data_load
   outs:
   - data/raw/iris.csv
```

Stage outputs

Manual update dvc.yaml

```yaml
stages:
 data_load:
  cmd: python src/stages/data_load.py --config=params.yaml
  deps:
  - src/stages/data_load.py
  params:
  - base
  - data_load
  outs:
  - data/raw/iris.csv

 featurize:
  cmd: python src/stages/featurize.py --config=params.yaml
  deps:
  - data/raw/iris.csv
  - src/stages/featurize.py
  params:
  - base
  - data_load
  - featurize
  outs:
  - data/processed/featured_iris.csv
```

Add a stage configuration manually

Live code example

Step 5:

Automate pipelines with DVC

Build end-to-end pipeline

Reproduce end-to-end ML pipelines

Reproduce **end-to-end** ML pipelines

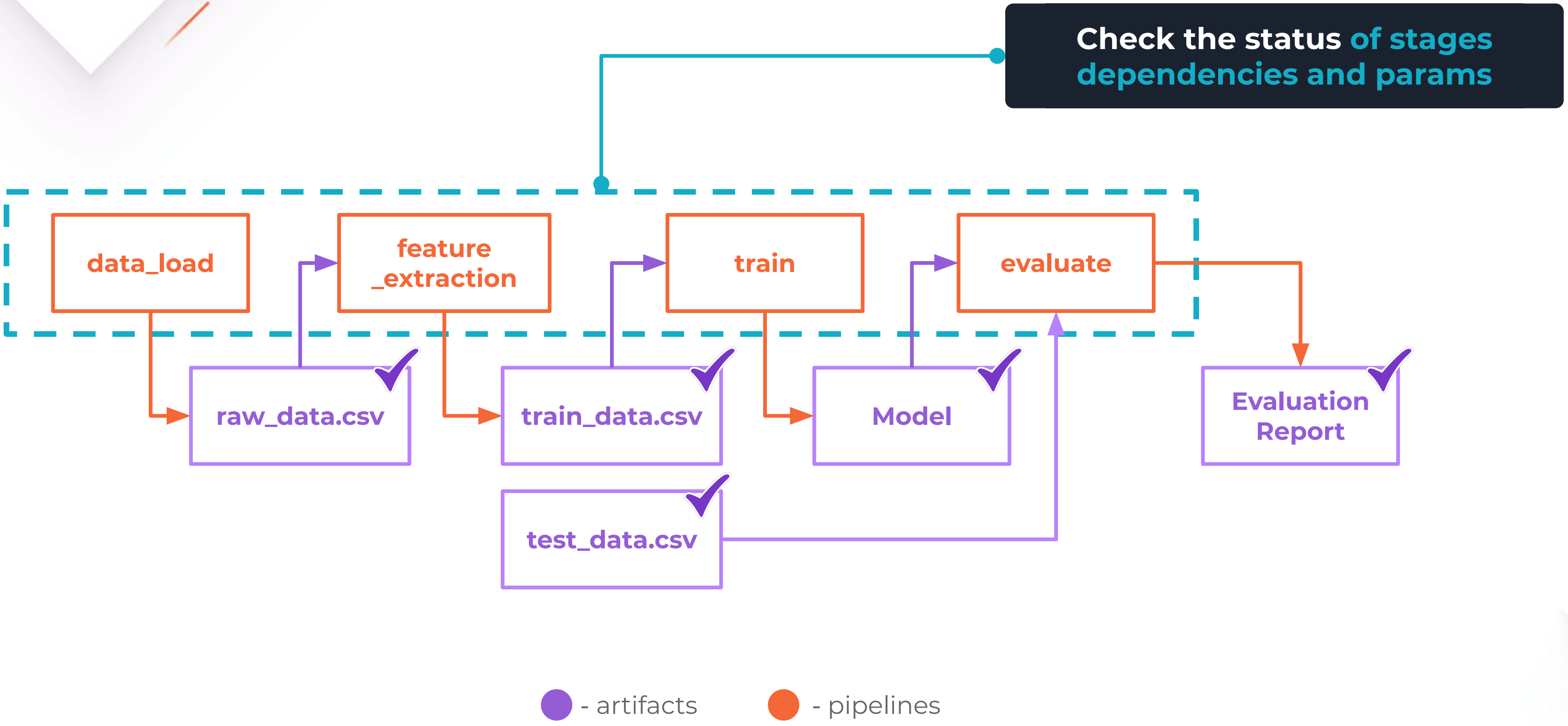
Guide

- Update code & params.yaml
- Run **dvc repro** / **dvc exp run**
- Commit changes to Git
- Store artifacts with DVC

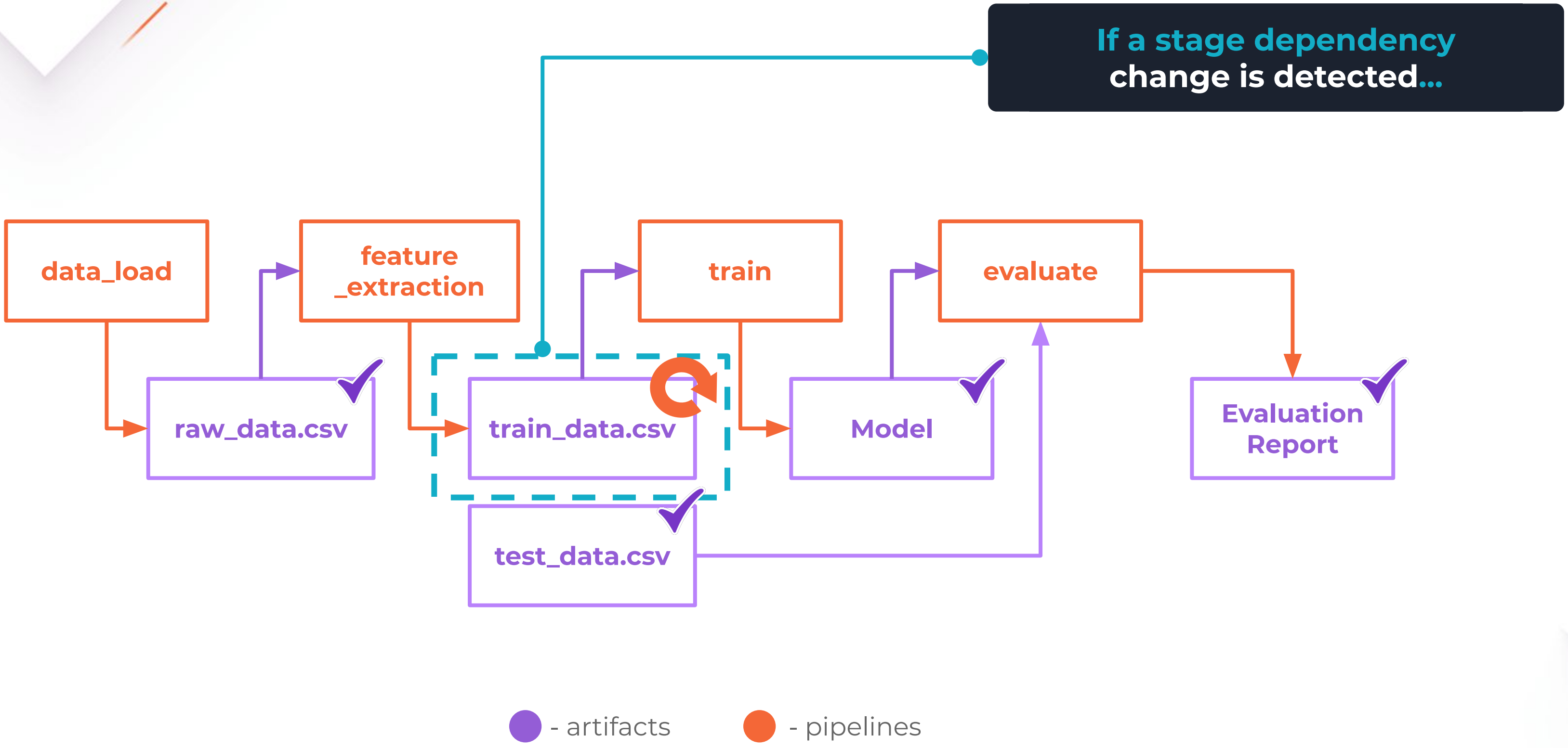
Tools

- DVC
- Git

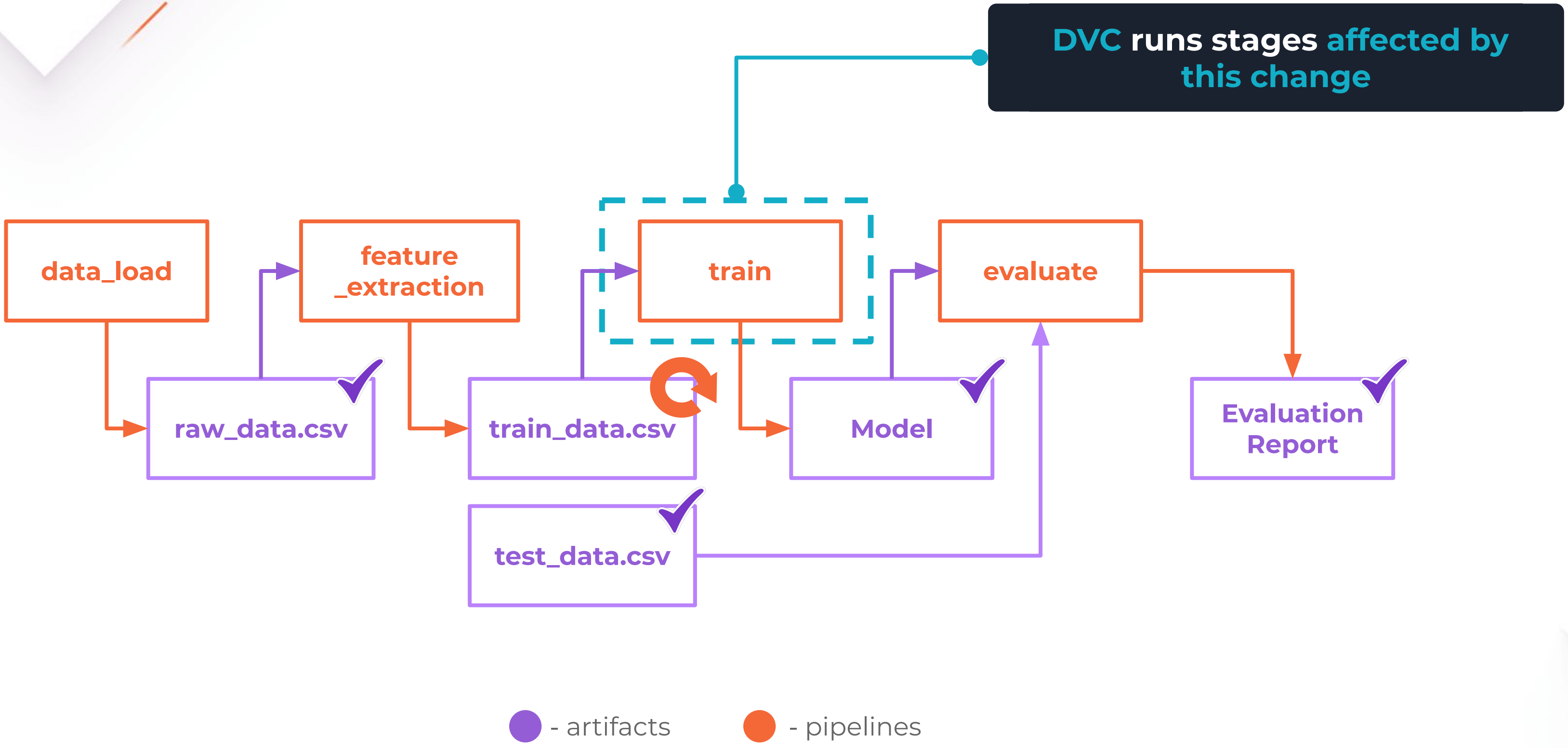
How dvc repro works?



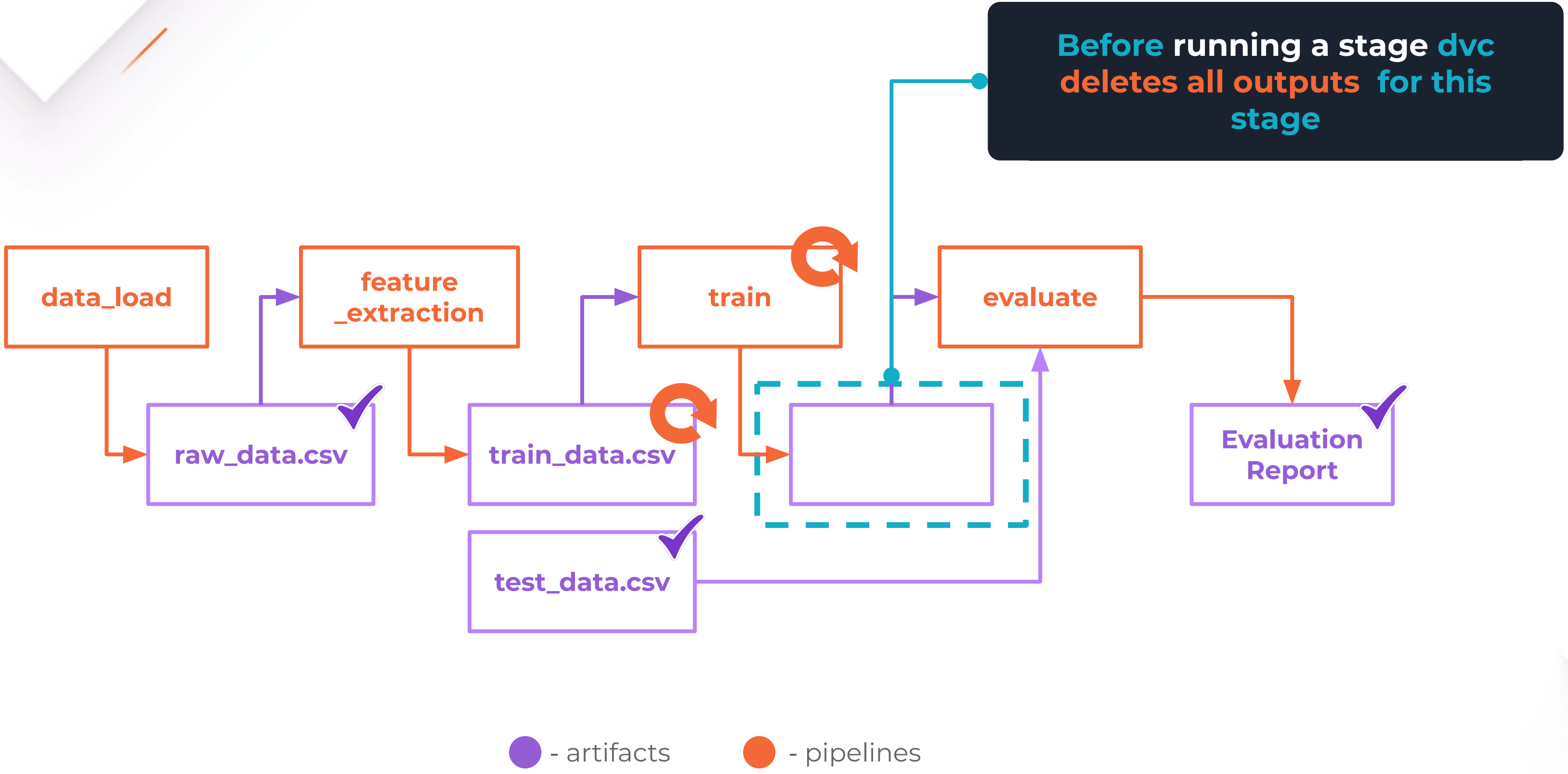
How dvc repro works?



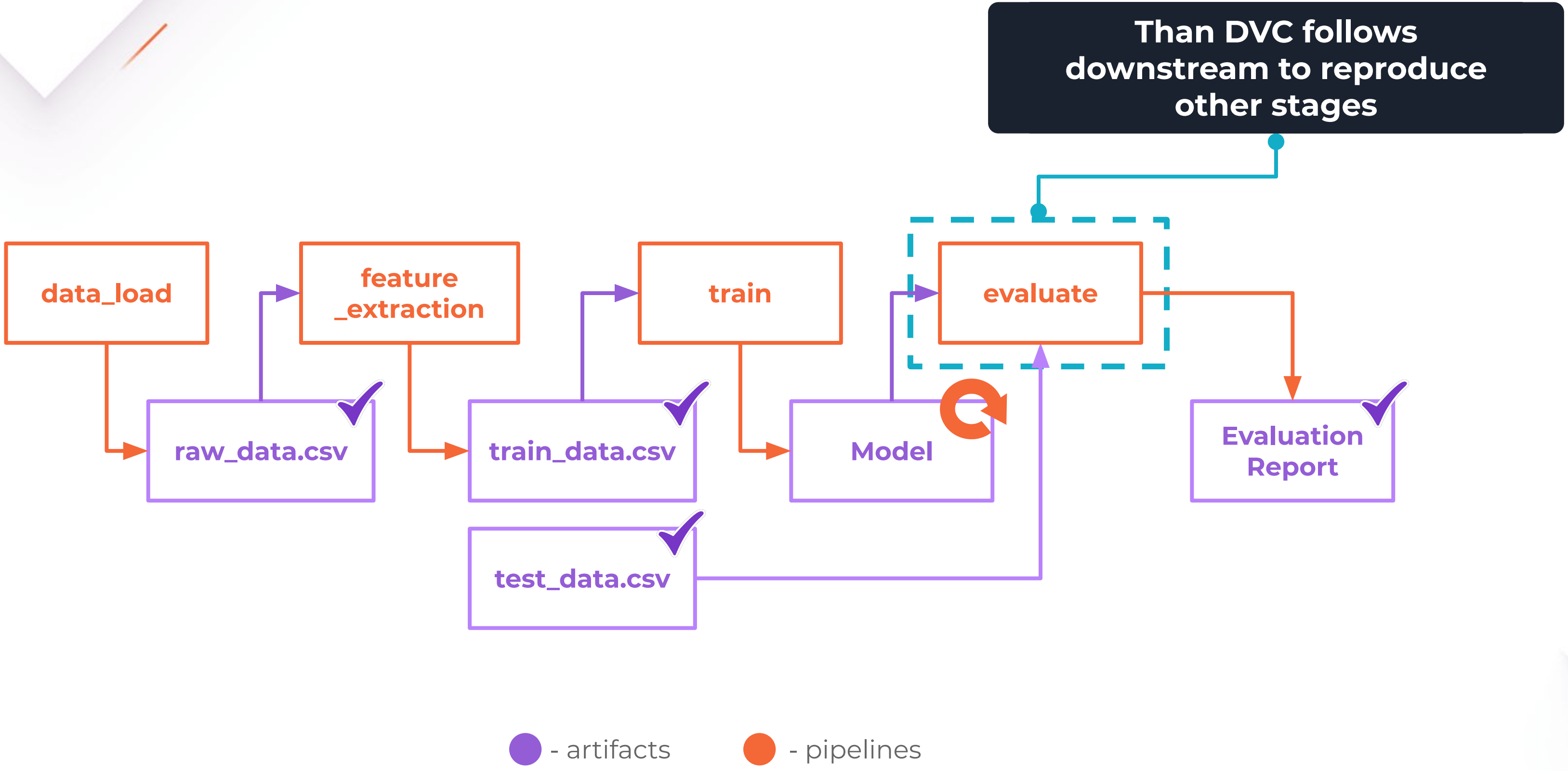
How dvc repro works?



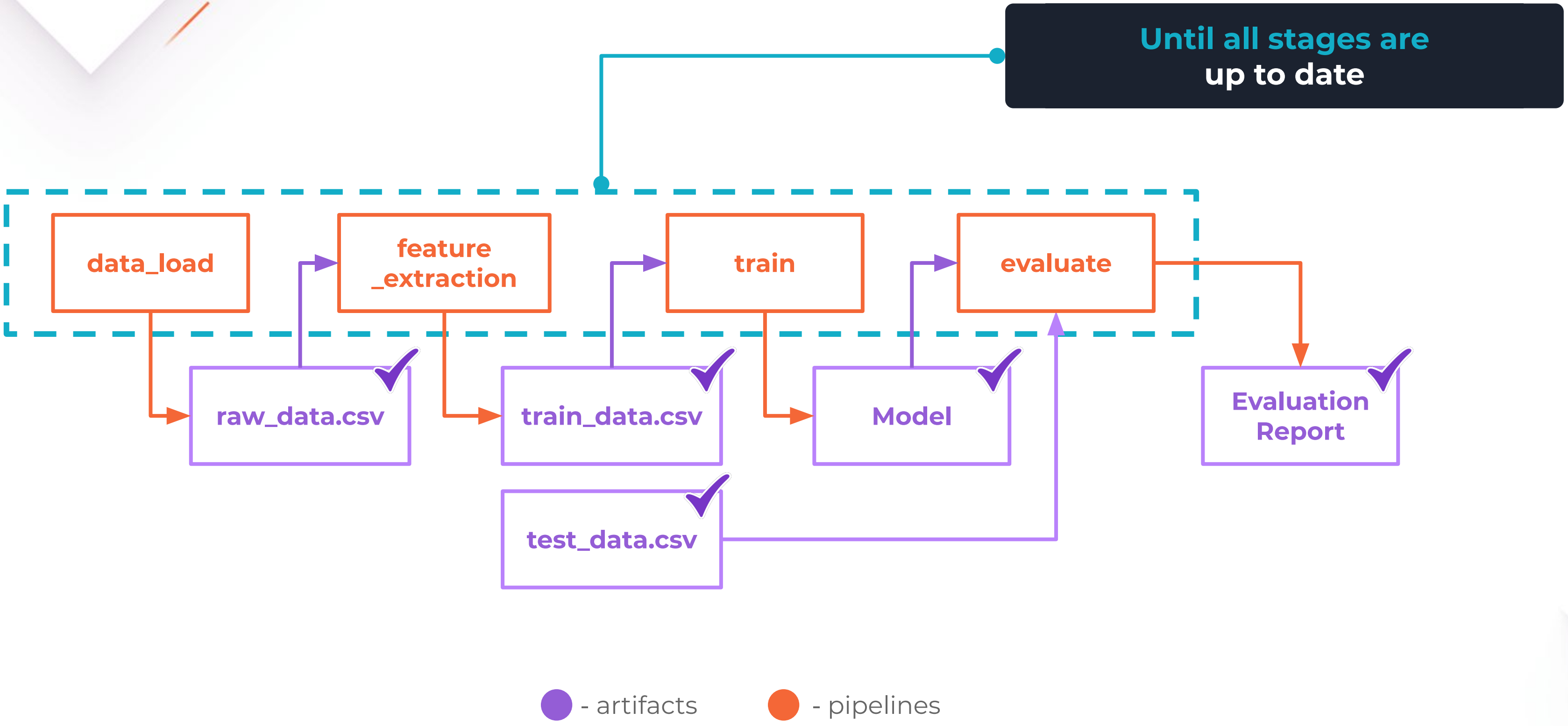
How dvc repro works?



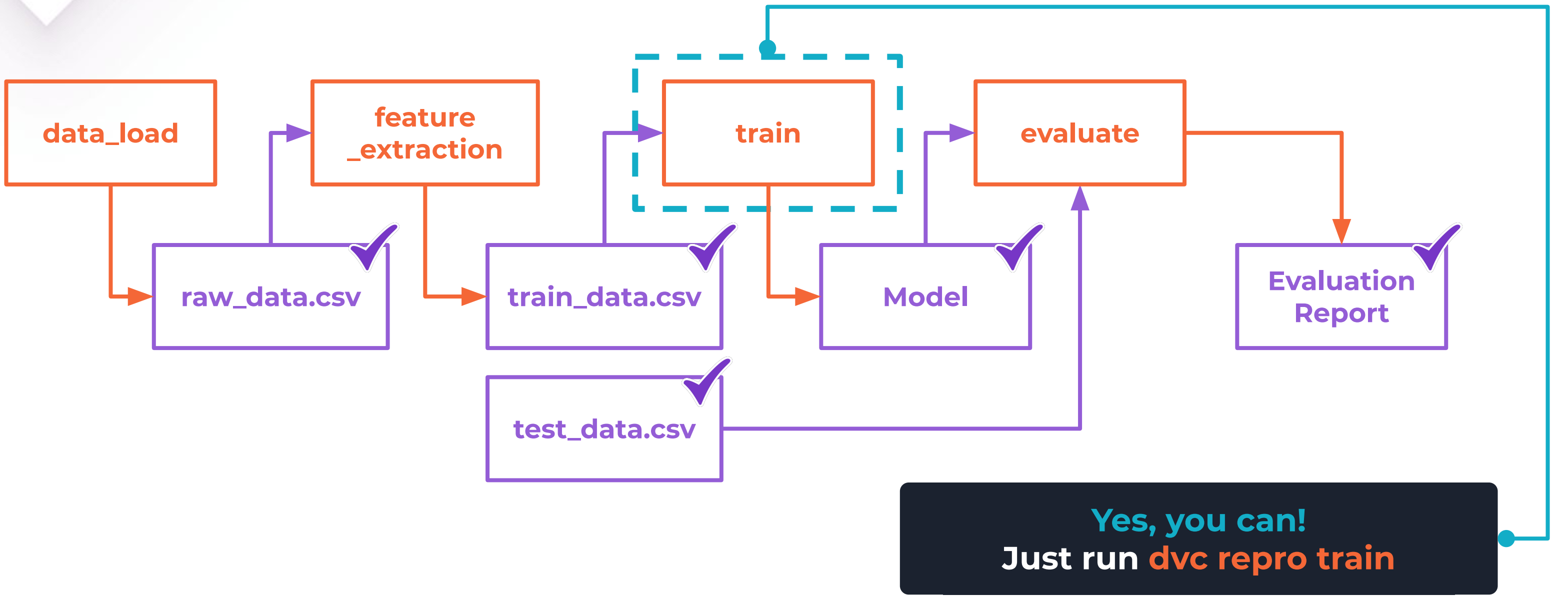
How dvc repro works?



How dvc repro works?



Can I reproduce only ‘train’ stage?



- artifacts
- pipelines

Tips to avoid unexpected behavior

- Read/write only from/to the specified dependencies and outputs (including parameters files, metrics, and plots)
- Completely rewrite outputs. Do not append or edit.
- Stop reading and writing files when the command exits
- Pipeline code should be deterministic (freeze random seeds, software and hardware dependencies, etc.)

References: https://dvc.org/doc/command-reference/run#dependencies-and-outputs

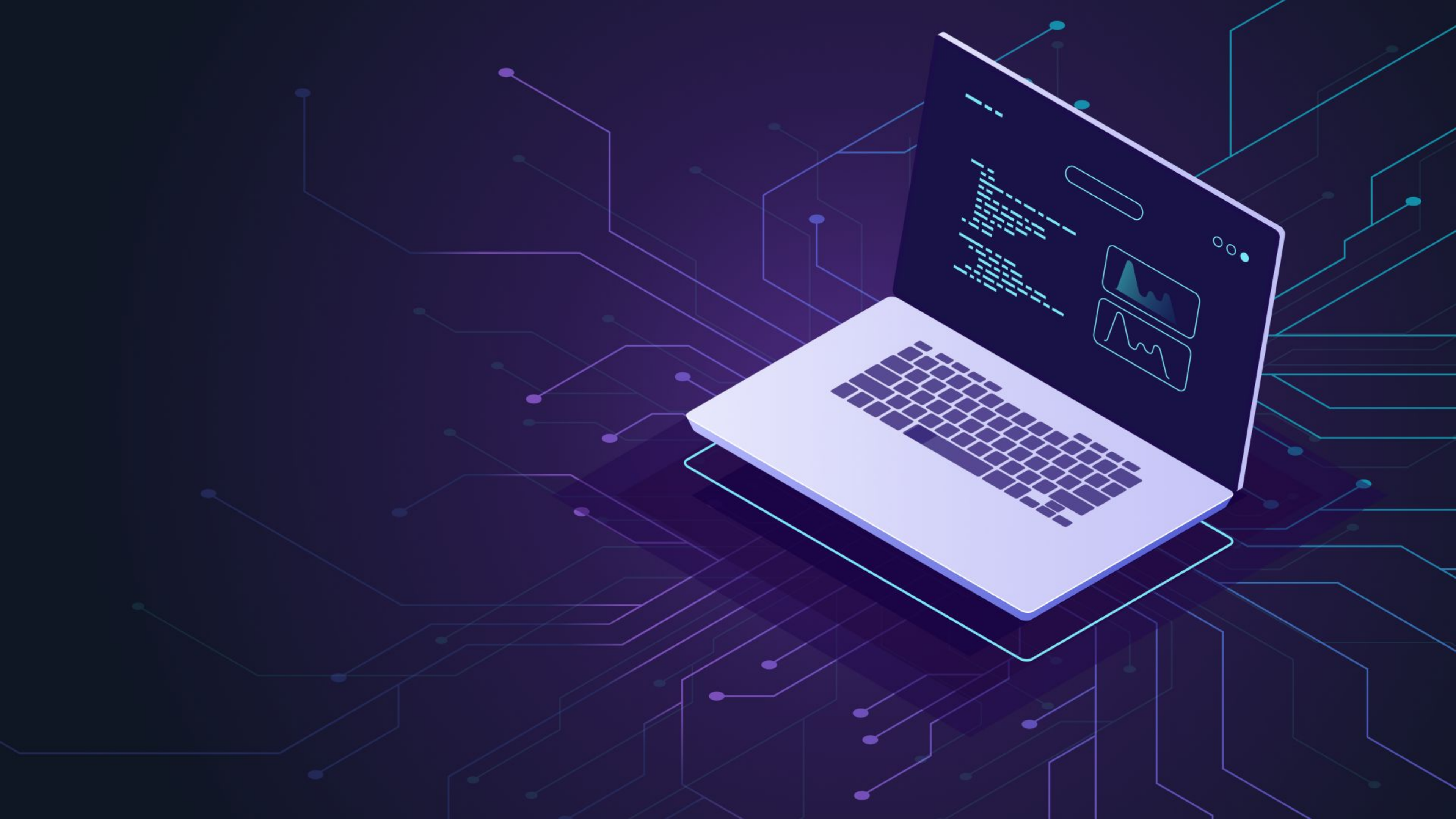
Live code example

Reproduce end-to-end ML pipelines

What have we learned?

What have we learned?

1. Simple way to upgrade code from Jupyter Notebook to automated pipelines
2. How to automated pipelines with DVC
3. How dvc repro works



Links

- DVC docs: **dvc repro** https://dvc.org/doc/command-reference/repro#options
- Deployment of Machine Learning Models (online course on Udemy created by Christopher Samiullah and Soledad Galli) https://www.udemy.com/course/deployment-of-machine-learning-models/