Code organization and refactoring

INTRODUCTION TO DATA VERSIONING WITH DVC



Ravi Bhadauria Machine Learning Engineer

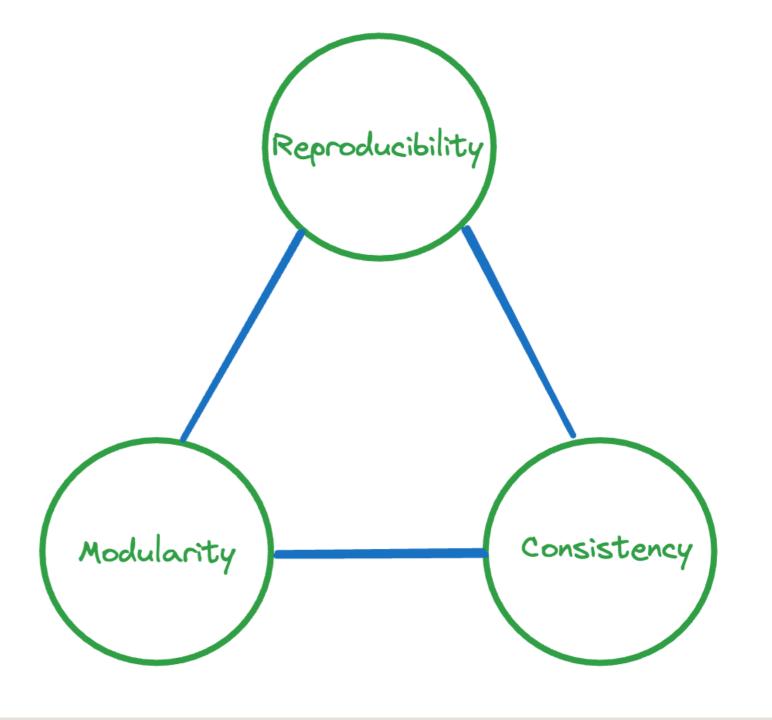


Prototyping vs production code

- Prototyping code allows rapid iteration
- But not suitable for production
 - Untested and prone to errors
 - Not modular with many repeated code blocks
 - Likely not reproducible

Features of good production code

- Reproducible: recreate same outputs in different environments and time
- Modular: written as distinct, independent, and testable modules
- Consistent: Single source of truth for all parameters
 - A configuration/parameter file



Configuration files and YAML

- Files should be in supported format
 - YAML, JSON, TOML, Python
 - Default is params.yaml
- We'll work with YAML
 - YAML Ain't Markup Language
 - Allows a standard format to transfer data between languages or applications
 - Simple and clean format
 - Valid file extensions: .yaml or .yml

¹ https://dvc.org/doc/command-reference/params#description



YAML Syntax

- Specify parameters as dictionaries
 - Keys and values separated by :
- Comments start with #
- Data types:
 - Integer, Floats, Strings
- Data structures:
 - Arrays
 - Nested Dictionaries
- Indentation is important

```
# Key-value pairs
a: 1
b: 1.2
c: "String value"
```

```
# Arrays
a: [1, 2.2, 3, 4.8]
b:
    - 5
    - "String value"
```

```
# Nested dictionaries
a:
   b: "Some value"
   c: "Some other value"
```

Example configuration file

```
# Data preprocessing paramters
preprocess:
  • • •
  target_column: RainTomorrow
  categorical_features:
    - Location
    - WindGustDir
# Model training/evaluation paramters
train_and_evaluate:
  rfc_params:
    n_estimators: 2
```

Example modular function

```
# In entry-point code (train_and_evaluate.py)
from model import evaluate_model
metrics = evaluate_model(model, X_test, y_test)
```

Sample project code layout

```
-> tree .
   params.yaml # Configuration file
   metrics_and_plots.py # Helper functions
   model.py # Model definition
   preprocess_dataset.py # Driver code to preprocess
   train_and_evaluate.py # Driver code to train
   utils and constants.py # More helper functions
```

Let's practice!

INTRODUCTION TO DATA VERSIONING WITH DVC



Writing and visualizing DVC pipelines

INTRODUCTION TO DATA VERSIONING WITH DVC



Ravi Bhadauria Machine Learning Engineer



DVC Pipelines

- Sequence of stages defining Machine Learning workflow and dependencies
 - Versioned and tracked with Git
- Defined in dvc.yaml file
 - Input data and scripts (deps)
 - Parameters (params)
 - Stage execution commands (cmd)
 - Output artifacts (outs)
 - Special data e.g. metrics and plots

Adding preprocessing stage

Create stages using dvc stage add

```
dvc stage add \
-n preprocess \
-p params.yaml:preprocess \
-d raw_data.csv \
-d preprocess.py \
-o processed_data.csv \
python3 preprocess.py
```

```
stages:
  preprocess:
    cmd: python3 preprocess.py
    params:
      # Keys from params.yaml
      params.yaml
        - preprocess
    deps:
    - preprocess.py
    - raw_data.csv
    outs:
    - processed_data.csv
```

Adding training and evaluation stage

 Add a training step using output from previous step

```
dvc stage add \
-n train_and_evaluate \
-p train_and_evaluate \
-d train_and_evaluate.py \
-d processed_data.csv \
-o plots.png \
-o metrics.json \
python3 train_and_evaluate.py
```

Directed Acyclic Graph (DAG)

```
stages:
  train_and_evaluate:
    cmd: python3 train_and_evaluate.py
    params:
      # Skip specifying parameter file
      # Defaulted to params.yaml
      - train_and_evaluate
    deps:
    - processed_data.csv
    - train_and_evaluate.py
    outs:
    - plots.png
    - metrics.json
```

Updating stages

Running dvc stage add multiple times

```
ERROR: Stage 'train_and_evaluate'
already exists in 'dvc.yaml'.
Use '--force' to overwrite.
```

Use dvc stage add --force

```
dvc stage add --force \
-n train_and_evaluate \
-p train_and_evaluate \
-d train_and_evaluate.py \
-d processed_data.csv \
-o plots.png \
-o metrics.json \
python3 train_and_evaluate.py
```

Visualizing DVC pipelines

```
# Print DAG on terminal
dvc dag
```

```
# Display DAG up to a certain step
dvc dag <target>
```

```
| preprocess |
| train_and_evaluate |
```

Visualizing DVC pipelines

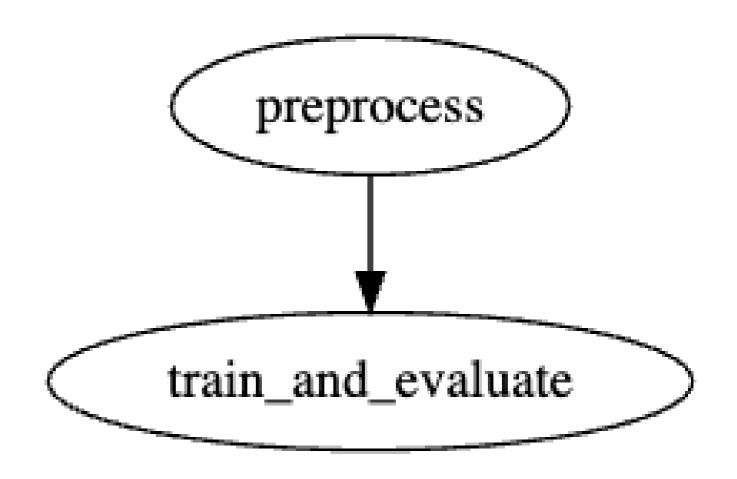
```
# Display step outputs as nodes
dvc dag --outs
```

```
processed_dataset/weather.csv |
                                 ***
                                    ***
            ***
          **
                                       **
metrics.json
                                   | plots.png |
```

Visualizing DVC pipelines

```
dvc dag --dot
```

```
strict digraph {
"preprocess";
"train_and_evaluate";
"preprocess" -> "train_and_evaluate";
}
```



¹ https://dreampuf.github.io/GraphvizOnline/



Let's practice!

INTRODUCTION TO DATA VERSIONING WITH DVC



Executing DVC pipelines

INTRODUCTION TO DATA VERSIONING WITH DVC



Ravi Bhadauria Machine Learning Engineer



Recap

Preprocessing stage

```
stages:
 preprocess:
    cmd: python3 preprocess.py
    params:
      - preprocess
    deps:
    - preprocess.py
    - raw_data.csv
    outs:
    - processed_data.csv
```

Training and evaluation

```
stages:
  train_and_evaluate:
    cmd: python3 train_and_evaluate.py
    params:
      train_and_evaluate
    deps:
    - processed_data.csv
    - train_and_evaluate.py
    outs:
    - plots.png
    - metrics.json
```

Reproducing a pipeline

Reproduce the pipeline using dvc repro

```
$ dvc repro
```

```
Running stage 'preprocess':

> python preprocess.py
Running stage 'train_and_evaluate':

> python train_and_evaluate.py
Updating lock file 'dvc.lock'
```

- A state file dvc.lock is generated
 - Similar to .dvc file, captures MD5 hashes

```
$ git add dvc.lock && git commit -m "first pipeline run"
```

Using cached results

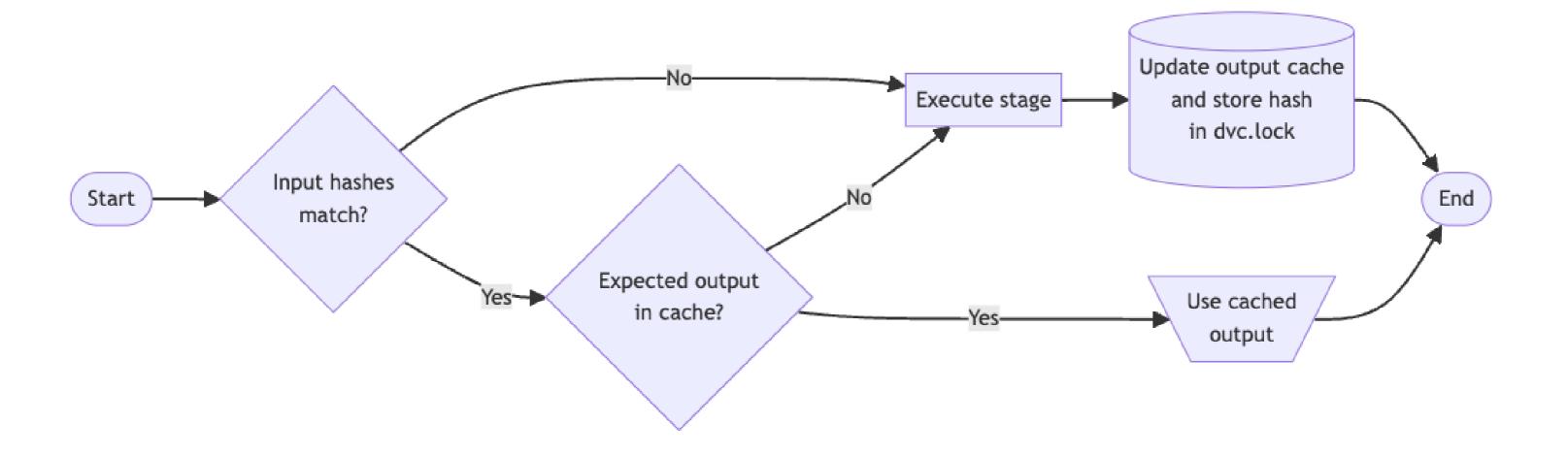
• Using cached results to speed up iteration

```
$ dvc repro
```

```
Stage 'preprocess' didn't change, skipping
Running stage 'train_and_evaluate' with command: ...
```



Stage caching in DVC



Dry running a pipeline

• Use --dry flag to only print commands without running the pipeline

```
$ dvc repro --dry
```

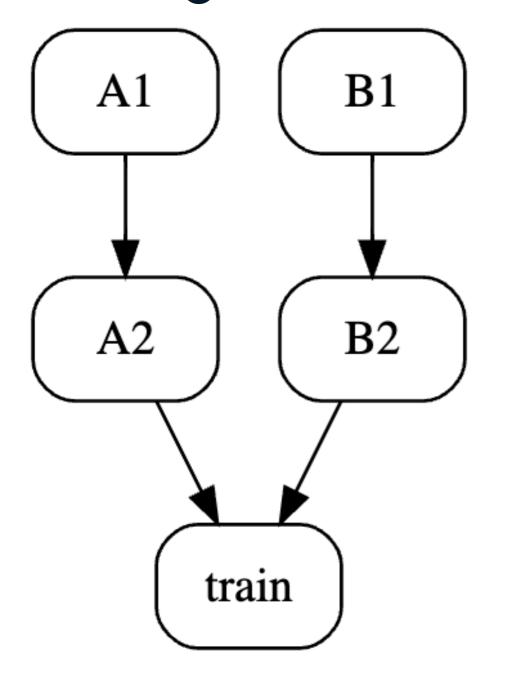
```
Running stage 'preprocess':
> python3 preprocess_dataset.py

Running stage 'train_and_evaluate':
> python3 train_and_evaluate.py
```

Additional arguments

- Running specific files dvc repro linear/dvc.yaml
 - Multiple dvc.yaml in one folder are not allowed
- Running specific stages dvc repro <target_stage>
 - This will also run upstream dependencies
- Force run a pipeline/stage dvc repro -f
- Not storing execution outputs in cache dvc repro --no-commit
 - Use dvc commit later

Parallel stage execution



Run independent steps concurrently

```
# Run A2 and its upstream dependencies
$ dvc repro A2

# Run B2 and its upstream dependencies
$ dvc repro B2
```

Use caching to speed up execution

```
$ dvc repro train
```

```
Stage 'A2' didn't change, skipping
Stage 'B2' didn't change, skipping
Running stage 'train' with command: ...
```

Let's practice!

INTRODUCTION TO DATA VERSIONING WITH DVC



Evaluation: Metrics and plots in DVC

INTRODUCTION TO DATA VERSIONING WITH DVC



Ravi Bhadauria Machine Learning Engineer



Metrics: changes in dvc.yaml

- Configure DVC YAML file to track metrics across experiments
- Change from outs

```
stages:
    train_and_evaluate:
    outs:
    - metrics.json
    - plots.png
```

• To metrics

```
stages:
    train_and_evaluate:
    outs:
    - plots.png
    metrics:
    - metrics.json:
        cache: false
```

Printing DVC metrics

```
$ dvc metrics show
```

Path	accuracy	f1_score	precision	recall
metrics.json	0.947	0.8656	0.988	0.7702



Compare metrics across runs

• Change a hyperparameter and rerun dvc repro

```
$ dvc metrics diff
```

Path	Metric	HEAD	workspace	Change
metrics.json	accuracy	0.947	0.9995	0.0525
metrics.json	f1_score	0.8656	0.9989	0.1333
metrics.json	precision	0.988	0.9993	0.0113
metrics.json	recall	0.7702	0.9986	0.2284

Plots: changes in dvc.yaml

```
stages:
 train_and_evaluate:
    plots:
    - predictions.csv: # Name of file containing predictions
        template: confusion # Style of plot
        x: predicted_label # X-axis column name in csv file
        y: true_label # Y-axis column name in csv file
        x_label: 'Predicted label'
        y_label: 'True label'
        title: Confusion matrix
        cache: false # Save in Git
```

¹ https://dvc.org/doc/user-guide/experiment-management/visualizing-plots#plot-templates-data-series-only

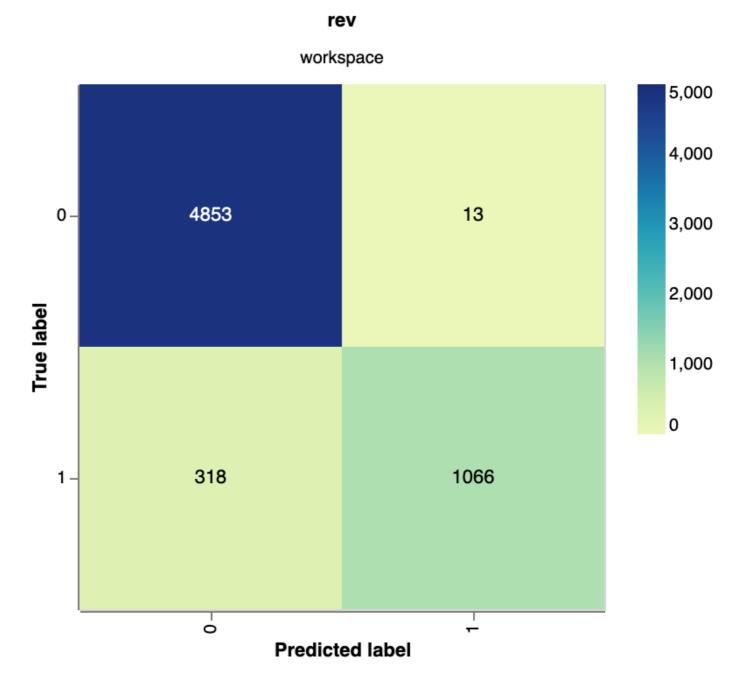


Printing DVC plots to file

\$ dvc plots show predictions.csv

file:///path/to/index.html

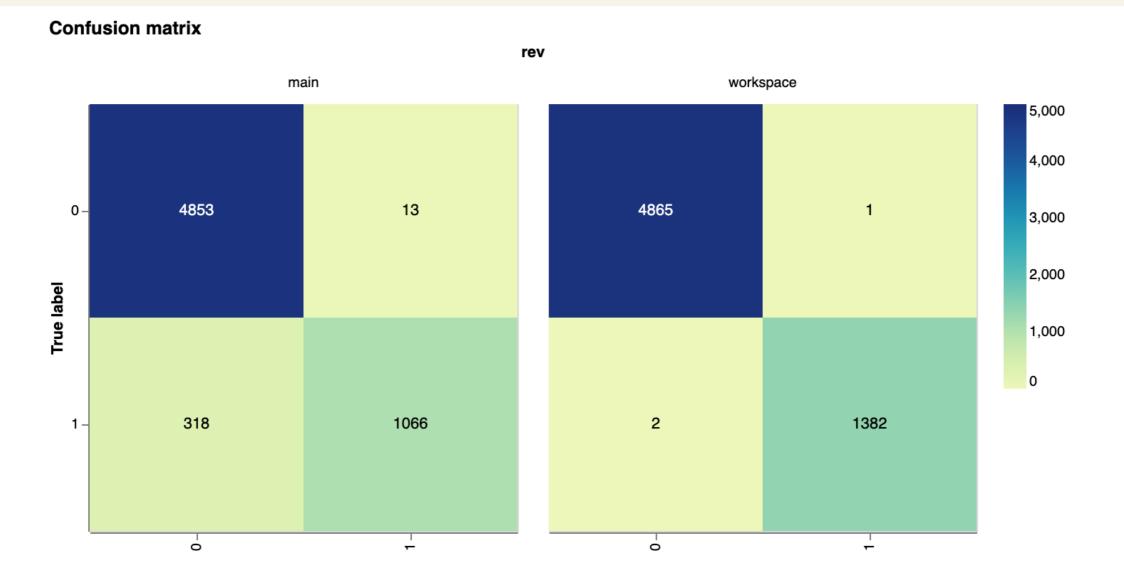
Confusion matrix





Comparing DVC plots

comapre plot in predictions.csv against branch main
\$ dvc plots diff --target predictions.csv <branch name or commit SHA>





Let's practice!

INTRODUCTION TO DATA VERSIONING WITH DVC



Congratulations!

INTRODUCTION TO DATA VERSIONING WITH DVC



Ravi Bhadauria Machine Learning Engineer



Data versioning and DVC

- Anatomy of Machine Learning Model
 - Code, data, and hyper-parameters precisely define a model
 - All three need to be tracked and versioned
- Git and DVC
 - Git helps with tracking code, DVC helps with tracking data
 - Git tracks metadata about the actual data
- DVC enables us
 - To version data and models
 - Run reproducible experiment pipelines
 - Track changes in metrics and plots

DVC setup, cache, and remotes

- Setup
 - Install using pip install dvc
 - Initialize using dvc init
 - Use .dvcignore to control file patterns to track
- Cache
 - Add files using dvc add
 - Track metadata using .dvc files
 - Remove using dvc remove, clean with dvc gc
- Remotes
 - Configure using dvc remote add, list using dvc remote list
 - Upload and download data using dvc push and dvc pull

DVC pipelines

- Anatomy of the dvc.yaml file
 - Use dvc stage add to add stages
 - Components include steps, commands, dependencies, params, and outputs
 - Track metrics and plots using the metrics and plots keys
- Visualize and run DAG
 - Visualize using dvc dag
 - Run with dvc repro
- Show and compare metrics and plots
 - Visualize using dvc plots show and dvc metrics show
 - Compare using dvc plots diff and dvc metrics diff

Thank you!

INTRODUCTION TO DATA VERSIONING WITH DVC

