Comparing metrics and plots in DVC

CI/CD FOR MACHINE LEARNING

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Configuring DVC YAML file

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

```
stages:
  preprocess:
    ...
  train:
    ...
    outs:
    - metrics.json
    - confusion_matrix.png
```

- To `metrics`

```
stages:
  preprocess:
    ...
  train:
    ...
    outs:
    - confusion_matrix.png
    metrics:
      - metrics.json:
          cache: false
```

Querying and comparing DVC metrics

```
-> dvc metrics show
Path           accuracy    f1_score    precision    recall
metrics.json   0.947       0.8656      0.988        0.7702
```

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
```

[1] https://dvc.org/doc/command-reference/metrics

Setting up DVC Github Action

- Add `setup-dvc` GitHub Action
- Replace running Python scripts with DVC pipeline

```
steps:
  ...
  - name: Setup DVC
    uses: iterative/setup-dvc@v1
  - name: Run DVC pipeline
    run: dvc repro
```

Setting up DVC Github Action

```
- name: Write CML report
  env:
    REPO_TOKEN: ${{ secrets.GITHUB_TOKEN }}
  run: |
    # Print metrics of current branch
    dvc metrics show --md >> report.md
    # Compare metrics with main branch
    git fetch --prune
    dvc metrics diff --md main >> report.md
    # Create CML report
    cml comment create report.md
```

Pipeline in action

github-actions bot commented 1 minute ago

Metrics

Path	accuracy	f1_score	precision	recall
metrics.json	0.956	0.95359	0.98261	0.92623

Metrics comparison

Path	Metric	main	workspace	Change
metrics.json	accuracy	0.916	0.956	0.04
metrics.json	f1_score	0.91286	0.95359	0.04072
metrics.json	precision	0.92437	0.98261	0.05824
metrics.json	recall	0.90164	0.92623	0.02459

Plot types in DVC

- `scatter` - scatter plot
- `linear` - interactive linear plot
- `simple` - non-interactive customizable linear plot
- `smooth` - linear plot with smoothing
- `confusion` - confusion matrix
- `confusion_normalized` - confusion matrix with values normalized to <0, 1> range
- `bar_horizontal` - horizontal bar plot
- `bar_horizontal_sorted` - horizontal bar plot sorted by bar size

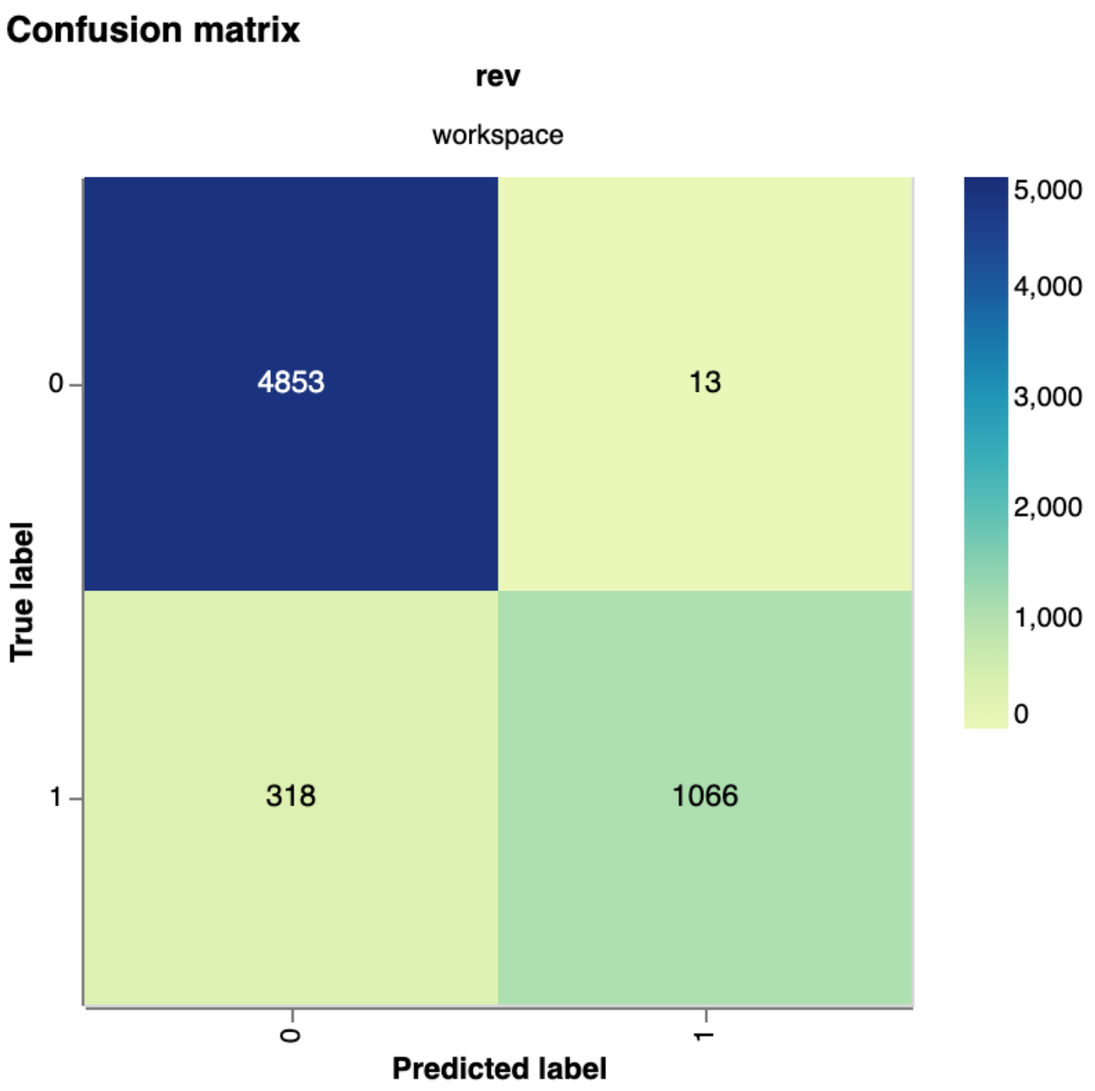
[1] https://dvc.org/doc/user-guide/experiment-management/visualizing-plots#plot-templates-data-series-only

Configuring DVC YAML for plots

```
stages:
  train:
    ...
    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
```

Plotting Confusion Matrix

```
-> dvc plots show predictions.csv
file:///path/to/index.html
```



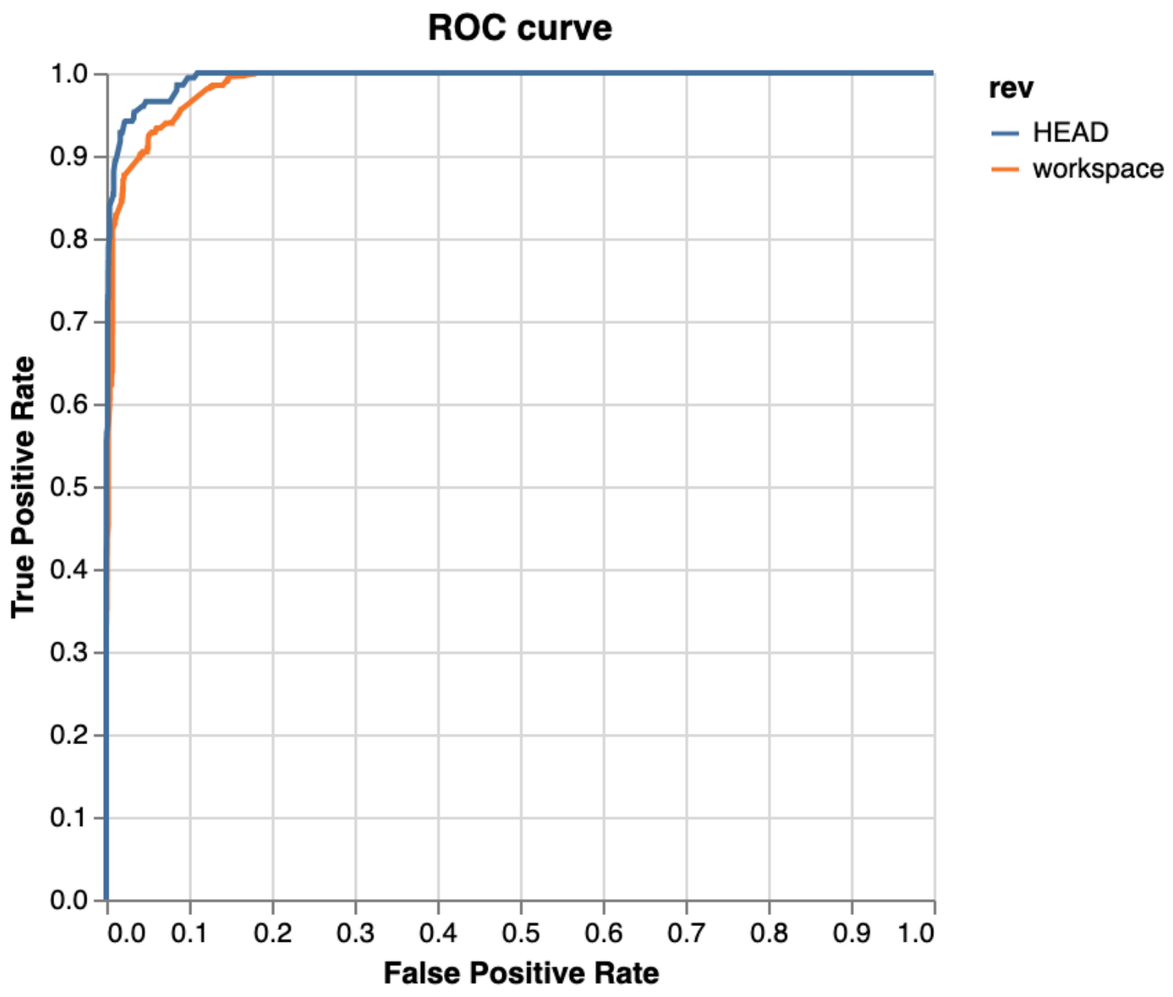
Comparing Confusion Matrix

```
-> dvc plots diff --target predictions.csv main
file:///path/to/index.html
```

Comparing ROC Curves

```
# Changes in Python
y_proba = model.predict_proba(X_test)
fpr, tpr, _ = roc_curve(y_test,
                        y_proba[:, 1])
```

```
# Changes in dvc.yaml
plots:
- roc_curve.csv:
    template: simple
    x: fpr
    y: tpr
    x_label: 'False Positive Rate'
    y_label: 'True Positive Rate'
    title: ROC curve
    cache: false
```



Let's practice!

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Hyperparameter Tuning with DVC

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Hyperparameter tuning workflow

- Hyperparameter tuning
  - Input: Parameter sweep ranges
  - Output: Best parameters
- Training
  - Input: Best parameters
  - Output: Metrics and plots (already covered)
- Loose coupling for independent training
  - Hyperparameter tuning sufficient but not necessary
- Both jobs are dataset dependent

```
# Contents of hp configuration
{
    "n_estimators": [2, 4, 5],
    "max_depth": [10, 20, 50],
    "random_state": [1993]
}
```

```
# Contents of best parameters
{
    "n_estimators": 5,
    "max_depth": 20,
    "random_state": 1993
}
```

Training code changes

Changes in Python Hyperparameter tuning script

```
# Load hyperparameters from the JSON file
with open("rfc_best_params.json", "r") as params_file:
  rfc_params = json.load(params_file)

# Define and train model
model = RandomForestClassifier(**rfc_params)
model.fit(X_train, y_train)
```

Hyperparameter Tuning with GridSearch

```
# Define the model and hyperparameter search space
model = RandomForestClassifier()
param_grid = json.load(open("hp_config.json", "r"))

# Perform GridSearch with five fold CV
grid_search = GridSearchCV(model, param_grid, cv=5)
grid_search.fit(X_train, y_train)

# Get the best hyperparameters
best_params = grid_search.best_params_
with open("rfc_best_params.json", "w") as outfile:
        json.dump(best_params, outfile)
```

DVC YAML changes

Hyperparameter Tuning

```
stages:
  preprocess: ...
  train: ...
  hp_tune:
    cmd: python hp_tuning.py
    deps:
    - processed_dataset/weather.csv
    - hp_config.json
    - hp_tuning.py
    outs: # Not tracking best parameters
      - hp_tuning_results.md:
          cache: false
```

Training

```
stages:
  preprocess: ...
  hp_tune: ...
  train:
    cmd: python train.py
    deps:
    - processed_dataset/weather.csv
    - rfc_best_params.json # Best parameters
    - train.py
    metrics:
      - metrics.json:
          cache: false
```

Triggering individual stages

- Stages can be triggered independently `dvc repro <stage_name>`
- Force run hyperparameter tuning stage `dvc repro -f hp_tune`
  - Ensures best parameter file will update
- Training can be run with `dvc repro train`
- Both stages trigger preprocessing step as dependency

Hyperparameter Run Output

mean_test_score	std_test_score	max_depth	n_estimators	random_state
0.999733	0.000413118	20	5	1993
0.999307	0.000574418	50	5	1993
0.99888	0.000617378	10	5	1993
0.997813	0.00117333	10	4	1993

Changes in Python hyperparameter tuning script

```python
# Save the results of hyperparameter tuning
cv_results = pd.DataFrame(grid_search.cv_results_)
markdown_table = cv_results.to_markdown(index=False)
with open("hp_tuning_results.md", "w") as markdown_file:
  markdown_file.write(markdown_table)
```

Summary

- Hyperparameter tuning route
  - Branch name `hp_tune/<some-string>`
  - Make changes to search configuration
  - Manually open a PR
    - Force runs DVC pipeline `dvc repro -f hp_tune`
    - Uses `cml pr create` to create a new training PR with best parameters
  - Force push a commit to training PR to kick off model training job
- Manual route
  - Branch name `train/<some-string>`
  - Edit best parameters file and commit changes
  - Manually open a PR to kick off model training job

Let's practice!

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GitHub Actions workflow for Hyperparameter Tuning

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Branching workflow

- Separate feature branches for training and hyperparameter tuning
  - Intended job should trigger
  - Other job should not trigger
  - Implemented using `if` condition
- Hyperparameter tuning
  - Print statistics table for analysis
  - Automatically open a new PR with parameter changes
- Training
  - Read new parameter file in training PR

Setting conditionals

Hyperparameter Tuning

```
jobs:
  hp_tune_and_publish_report:
    # Run when branch name starts with hp_tune/
    if: startsWith(github.head_ref, 'hp_tune/')
    steps:
      ...
      - name: |
          DVC pipeline for hyperparameter tuning
        run: dvc repro -f hp_tune
```

Training

```
jobs:
  train_and_publish_report:
    # Run when branch name starts with train/
    if: startsWith(github.head_ref, 'train/')
    steps:
      ...
      - name: Run DVC pipeline for training
        run: dvc repro train
```

Setup workflow permissions

Repository Settings > Actions > General

Workflow permissions

Choose the default permissions granted to the GITHUB_TOKEN when running workflows in this repository. You can specify more granular permissions in the workflow using YAML. Learn more about managing permissions.

- ○ **Read and write permissions**
  Workflows have read and write permissions in the repository for all scopes.
- ◉ **Read repository contents and packages permissions**
  Workflows have read permissions in the repository for the contents and packages scopes only.

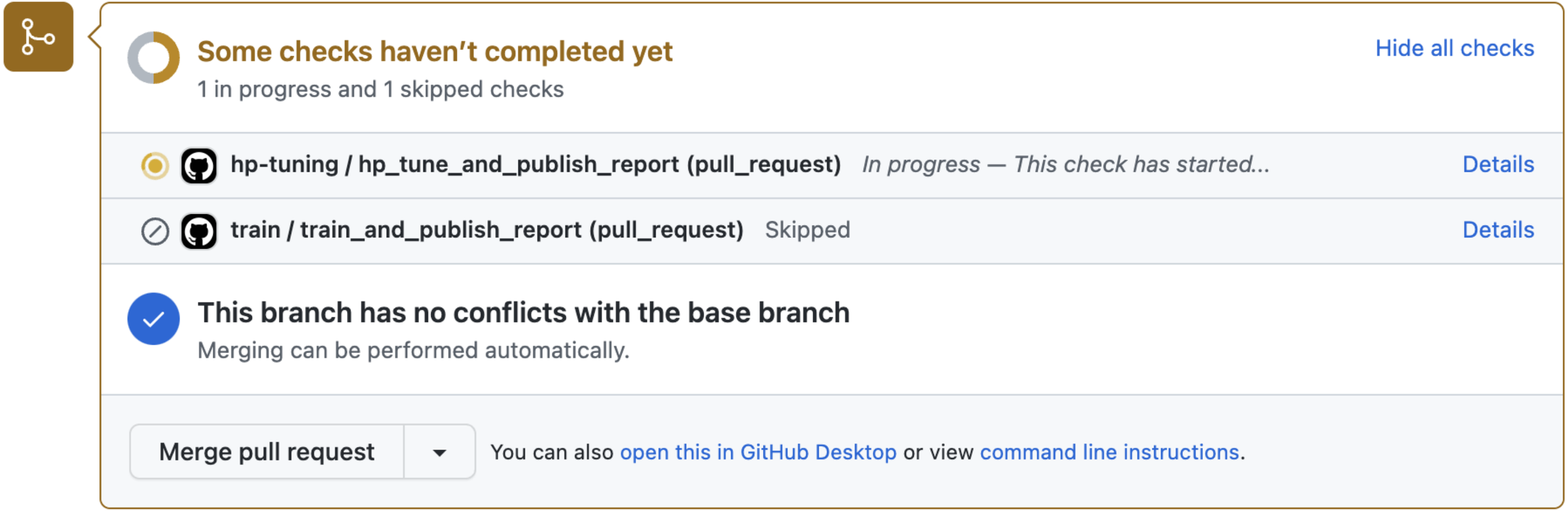
Choose whether GitHub Actions can create pull requests or submit approving pull request reviews.

- ☑ **Allow GitHub Actions to create and approve pull requests**

Save

Hyperparameter tuning job kickoff

- Make sure to prefix branch name with `hp_tune/`



Hyperparameter tuning job metrics

github-actions bot commented now

rank_test_score	mean_test_score	std_test_score	max_depth	n_estimators	random_state
1	0.999733	0.000413118	20	5	1993
2	0.999307	0.000574418	50	5	1993
3	0.99888	0.000617378	10	5	1993
4	0.997813	0.00117333	10	4	1993
5	0.997173	0.0011997	20	4	1993
6	0.996107	0.00184444	50	4	1993
7	0.982613	0.00441863	10	2	1993
8	0.974187	0.00522122	20	2	1993
9	0.972907	0.00835412	50	2	1993

Creating a training PR from hyperparameter run

```
steps:
  - name: Create training branch
    env:
      REPO_TOKEN: ${{ secrets.GITHUB_TOKEN }}
    run: |
      # Branch name begins with train/
      export BRANCH_NAME=train/$(git rev-parse --short "${{ github.sha }}")
      # Create PR for training
      cml pr create \
        --user-email hp-bot@cicd.ai \
        --user-name HPBot \
        --message "Hyperparameter tuning" \
        --branch $BRANCH_NAME \
        --target-branch main \
          rfc_best_params.json
```

New training branch PR

CML PR for main 918351a5 #12

Open **github-actions** wants to merge 14 commits into `main` from `train/5ec553d`

Conversation 0 | Commits 14 | Checks 0 | Files changed 28

github-actions bot commented 1 minute ago

Automated commits for `918351a` created by CML.

HP tuning e4707d4

Add more commits by pushing to the **`train/5ec553d`** branch on **rbhadauria29/ci-cd-for-ml-demo**.

Require approval from specific reviewers before merging
Branch protection rules ensure specific people approve pull requests before they're merged.

Add rule

This branch has no conflicts with the base branch
Merging can be performed automatically.

Merge pull request

You can also open this in GitHub Desktop or view command line instructions.

New training branch PR

HP tuning

train/5ec553d (#12)

HPBot committed 13 minutes ago

2 rfc_best_params.json

```
...    ...    @@ -1 +1 @@
  1         - {"max_depth": 15, "n_estimators": 1, "random_state": 1993}
          1 + {"max_depth": 20, "n_estimators": 5, "random_state": 1993}
```

Starting training run manually

- `GITHUB_TOKEN` cannot trigger workflows on self created PRs
  - Prevention from recursive runs
- Workarounds
  - Use a Personal access token with proper permissions

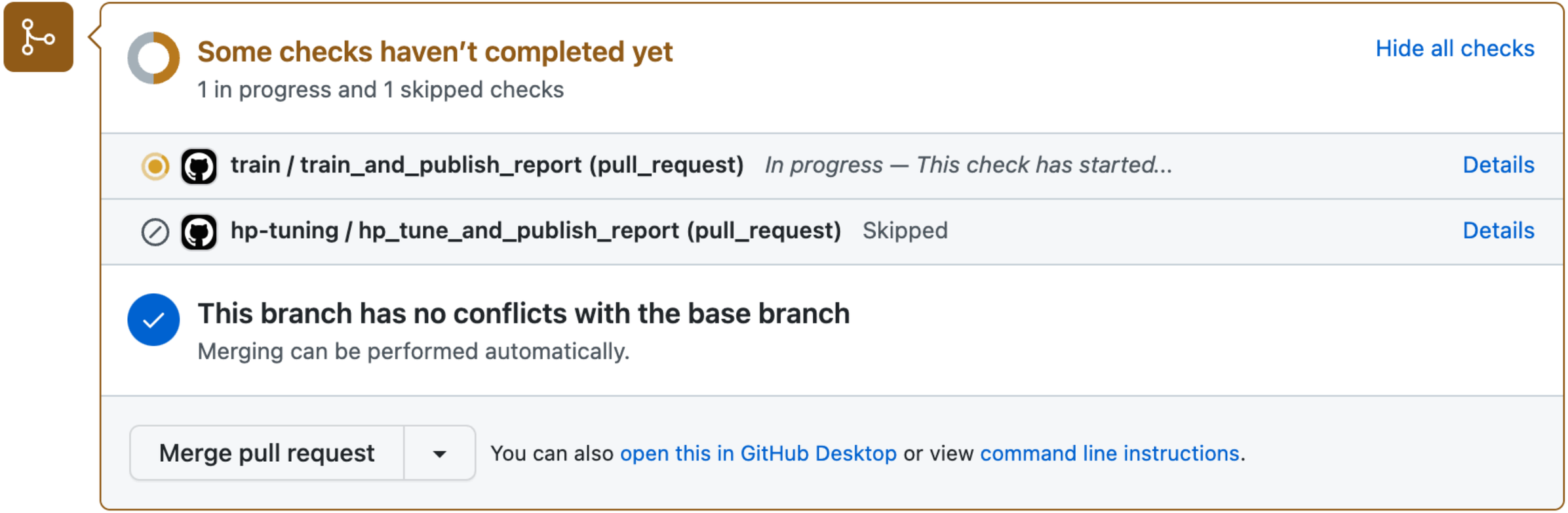
```
steps:
  - env:
      GITHUB_TOKEN: ${{ secrets.MY_TOKEN }}
```

  - Run training job right after hyperparameter tuning in GHA pipeline
  - Force push the code to trigger a run (forces inspection)

```
-> git checkout train/1f34fs
-> git commit --amend --no-edit && git push -f
```

[1] https://docs.github.com/en/actions/using-workflows/triggering-a-workflow#triggering-a-workflow-from-a-workflow

Training job kickoff



Let's practice!

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Congratulations!

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YAML Syntax

- Indentation
- Mappings `a: 1`
- Arrays
  - Flow `[1, 2]`
  - Block

```
- 1
- 2
```

- Multi-line strings
  - Style indicators (`|` , `>`)
  - Chomping indicators (`-` , `+`)

GitHub Actions

- Workflow (pipeline)
- Events (`on`)
- Jobs (`jobs`)
- Runners (`runs-on`)
- Steps (`steps`)
- Contexts
- Secrets and environment variables (`GITHUB_TOKEN`)
- Actions (`checkout` , `setup-python`)
  - CML: `cml comment create` , `cml pr create`

Versioning data and building reproducible pipelines

- `dvc init`
- DVC remotes (including local)
- `dvc push` , `dvc pull`
- `dvc repro <target>`
- `dvc metrics show/diff`
- `dvc plots show/diff`

- DVC YAML (`dvc.yaml`)
  - Steps or targets
  - Commands (`cmd`)
  - Dependencies (`deps`)
  - Outputs (`outs`)
  - Metrics (`metrics`)
  - Plots (`plots`)

Datacamp resources

- Courses
  - Developing Machine Learning Models for Production
  - MLOps Deployment and Life Cycling
  - Fully Automated MLOps
  - Introduction to DevOps
- Blogs
  - Version Control For Data Science

Further reading

CI/CD and branching patterns

DevOps vs MLOps

Data Version Control

Model registry and life cycle management

Thank you!

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