ML Pipelines, Reproducibility and Experimentation

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We have a Jupyter notebook...

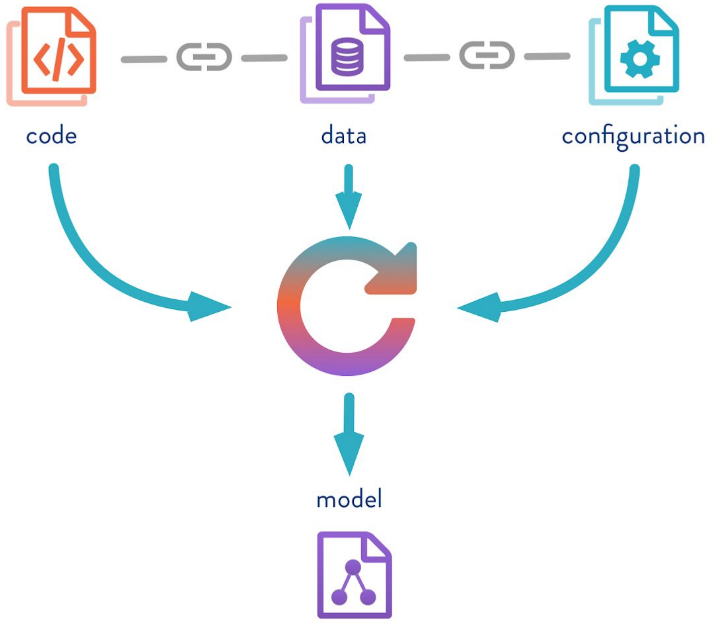
- ◇ Data loading
- ◇ Feature Engineering
- ◇ Model Training
- ◇ Model Evaluation

Can you easily answer these questions?

- What exactly was used to produce a particular model?
- Can you easily compare many ML experiments?
- Will you be able to reproduce them later?

Goal #1: Achieve best performance

- Running many experiments
- **Experiment** = a particular combination of
  Code & **Data** & **Config**



Goal #2: Ensure reproducibility

- **Improving model performance**: you can't improve what you can't reproduce
- **Transparency and team collaboration**: know everything your team members did to achieve certain performance
- **Auditability (laws and regulations)**: e.g. what *exactly* went into the models that prescribes treatment to patients or determines creditworthiness of bank customers

Goal #3: Minimal setup and dependency of 3rd party services

Problems:

1. **Vendor lock-in**: instrument code with framework-specific code
2. **Maintenance & cost**: maintain your own ML tracking server (or pay them to take care of it)
3. **Security concerns**: send data to an external service or database

Most ML tracking solutions (MLflow, W&B, comet.ml, etc) have at least 2 of these problems

Fact:
It’s difficult to achieve all three goals

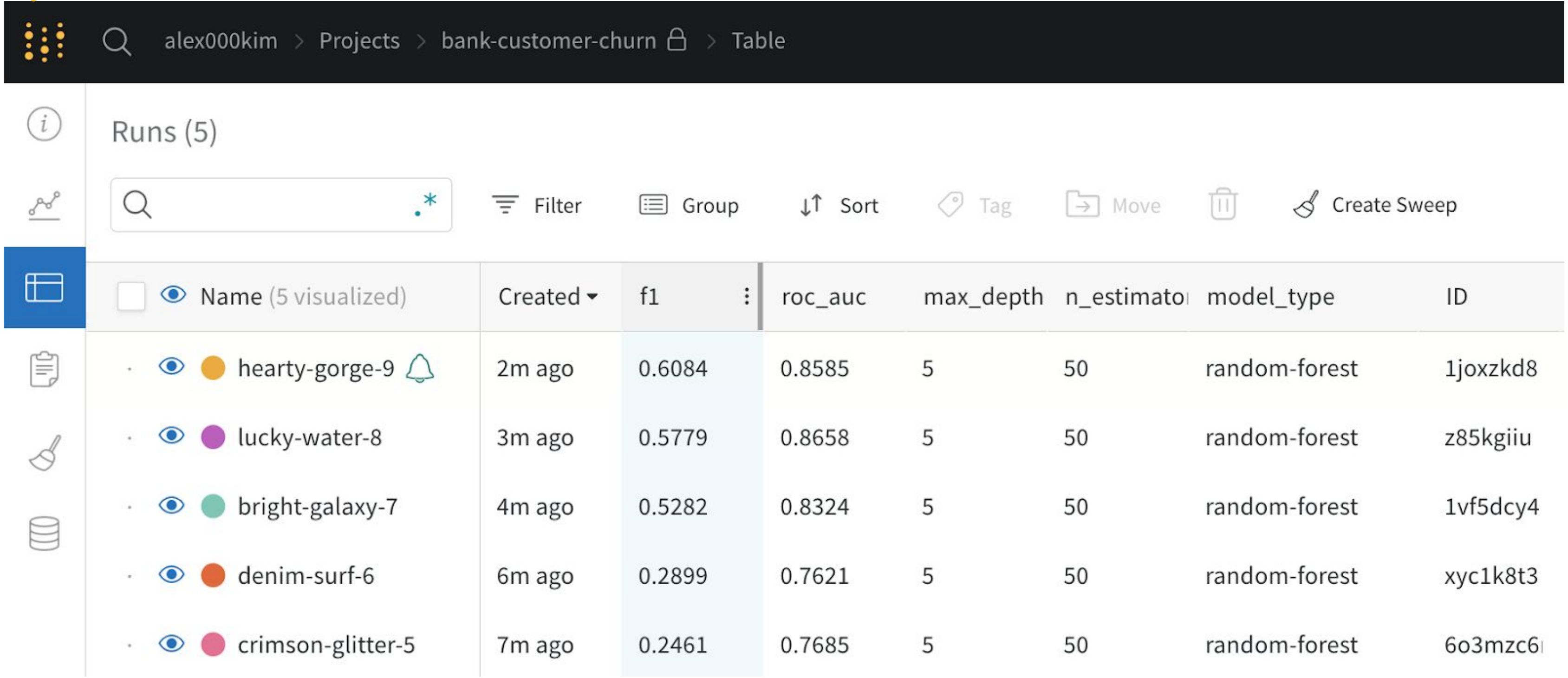
Can we do all of the following?

1. Iterate quickly i.e. generate many experiments
2. Automatically track **all** changes to code, configs and data
3. Avoid dependency on 3rd party services to store data, metrics and params

Same experiments, but different metrics?

🤔🤔🤔

W&B



Runs (5)

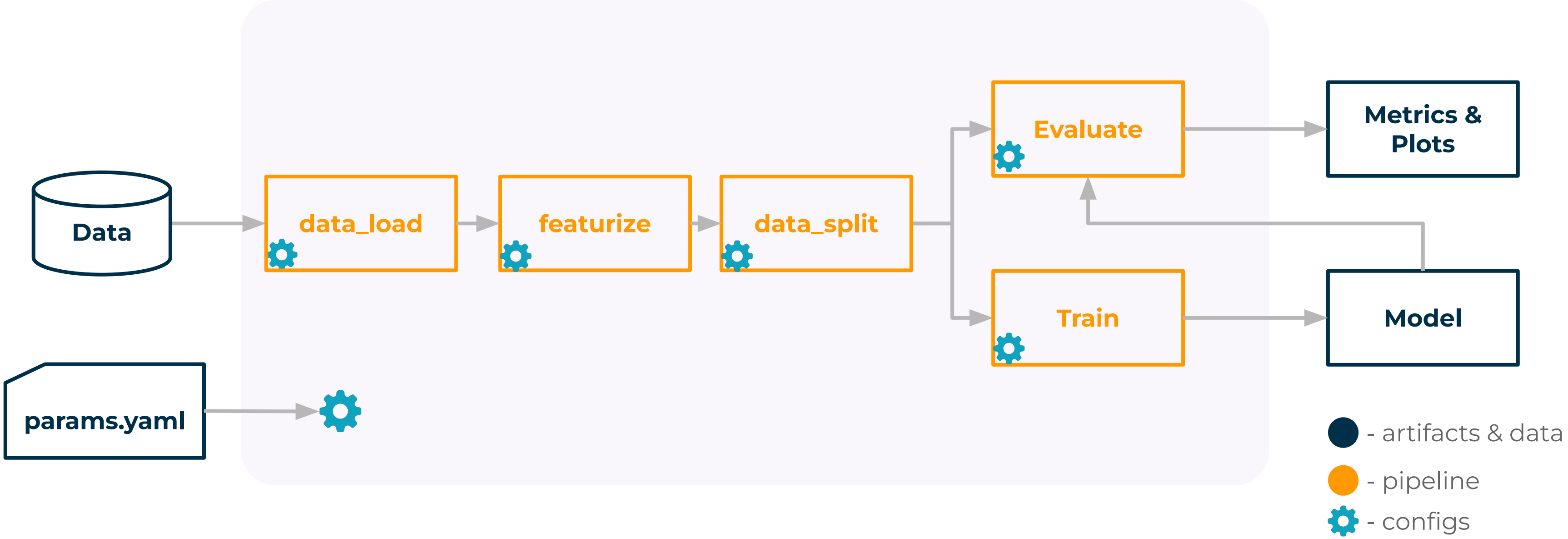
Name (5 visualized)	Created	f1	roc_auc	max_depth	n_estimato	model_type	ID
hearty-gorge-9	2m ago	0.6084	0.8585	5	50	random-forest	1joxzkd8
lucky-water-8	3m ago	0.5779	0.8658	5	50	random-forest	z85kgiiu
bright-galaxy-7	4m ago	0.5282	0.8324	5	50	random-forest	1vf5dcy4
denim-surf-6	6m ago	0.2899	0.7621	5	50	random-forest	xyc1k8t3
crimson-glitter-5	7m ago	0.2461	0.7685	5	50	random-forest	6o3mzc6

Reproducibility VS. Experimentation?

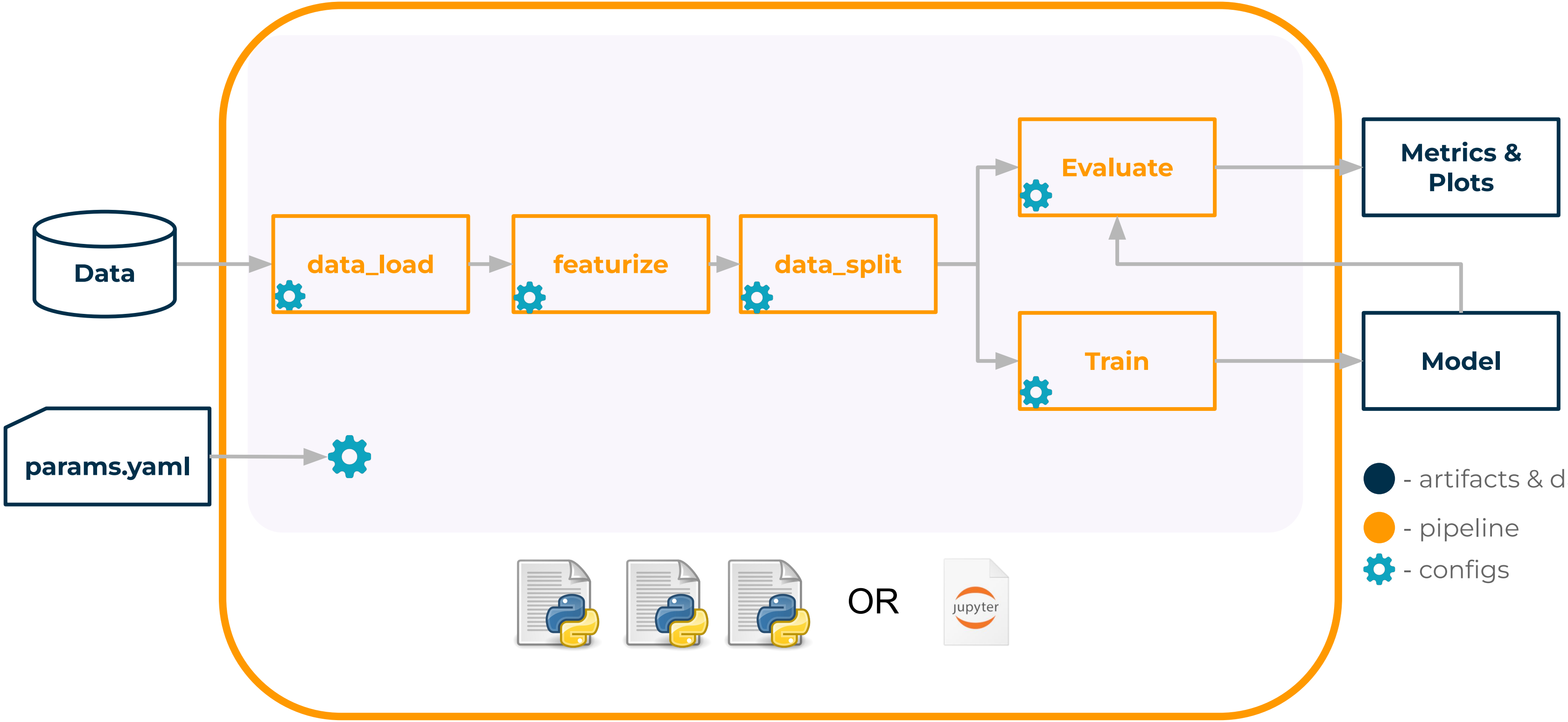
- DVC pipelines for generating many experiments
- Achieve complete reproducibility by versioning **everything**!
  - code and configs --> Git
  - dataset, models, other artifacts --> DVC remote storage (cloud buckets, NAS, SFTP, etc)
- VS Code as a convenient UI for experiment management
- No need to maintain (or pay for) additional services

Visual Studio Code git DVC

What are DVC pipelines?



What are DVC pipelines?



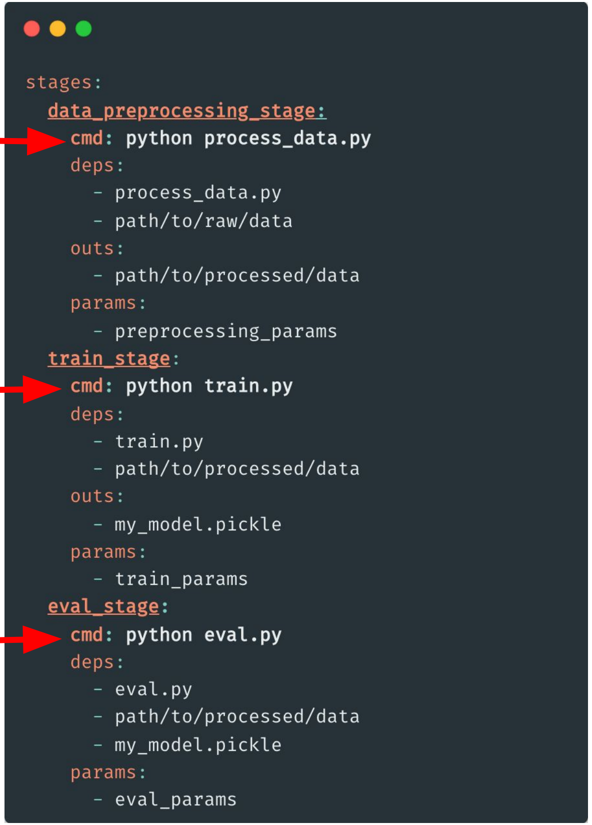
● - artifacts & data

● - pipeline

⚙ - configs

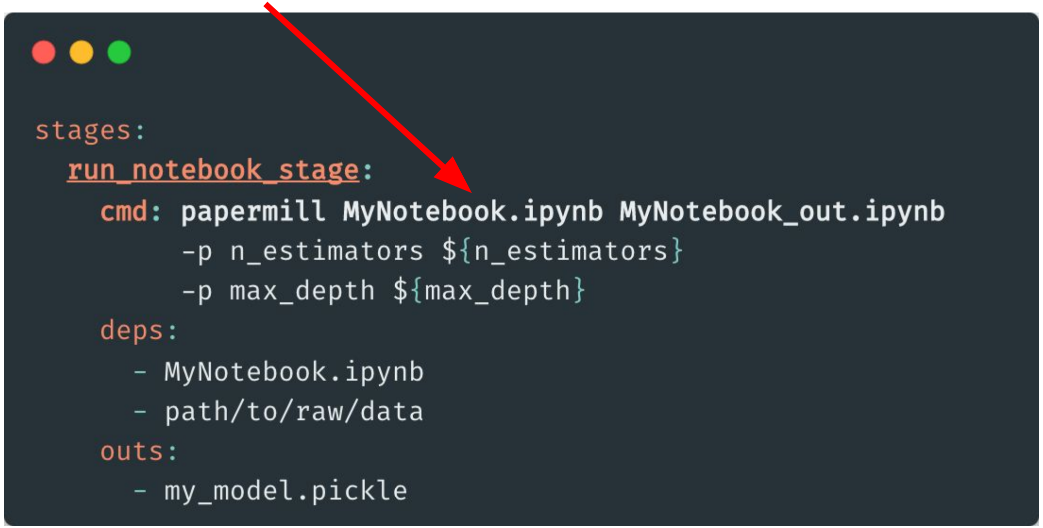
DVC pipeline (defined in dvc.yaml) as:

a sequence of Python modules



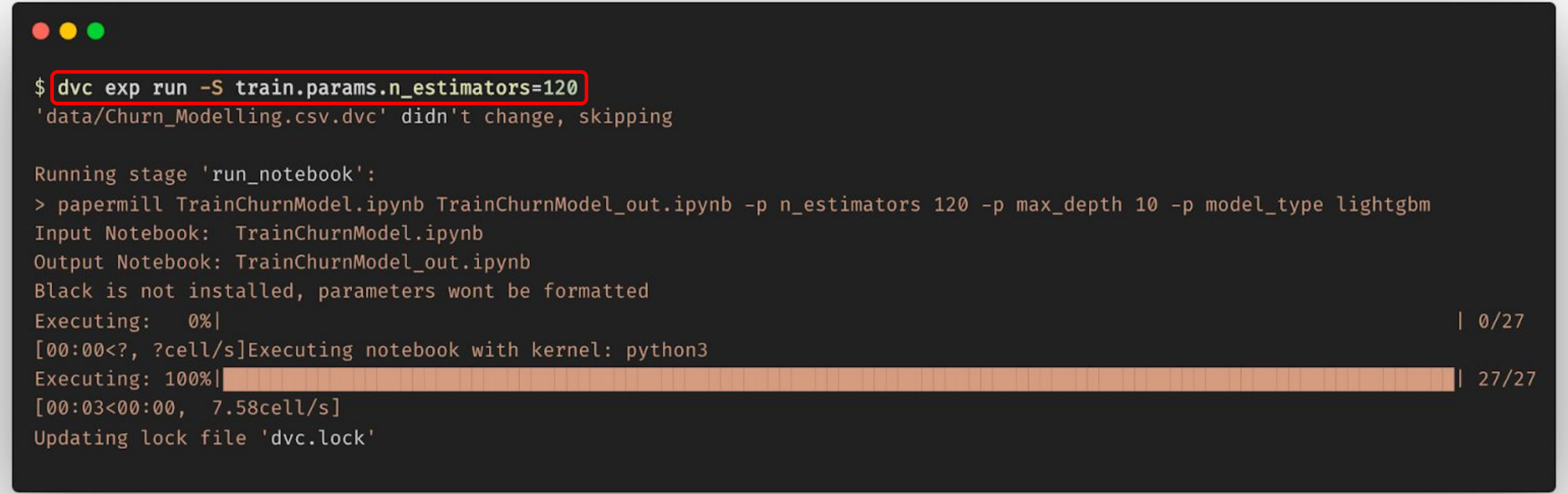
```yaml
stages:
  data_preprocessing_stage:
    cmd: python process_data.py
    deps:
      - process_data.py
      - path/to/raw/data
    outs:
      - path/to/processed/data
    params:
      - preprocessing_params
  train_stage:
    cmd: python train.py
    deps:
      - train.py
      - path/to/processed/data
    outs:
      - my_model.pickle
    params:
      - train_params
  eval_stage:
    cmd: python eval.py
    deps:
      - eval.py
      - path/to/processed/data
      - my_model.pickle
    params:
      - eval_params
```

a Jupyter notebook



```yaml
stages:
  run_notebook_stage:
    cmd: papermill MyNotebook.ipynb MyNotebook_out.ipynb
         -p n_estimators ${n_estimators}
         -p max_depth ${max_depth}
    deps:
      - MyNotebook.ipynb
      - path/to/raw/data
    outs:
      - my_model.pickle
```

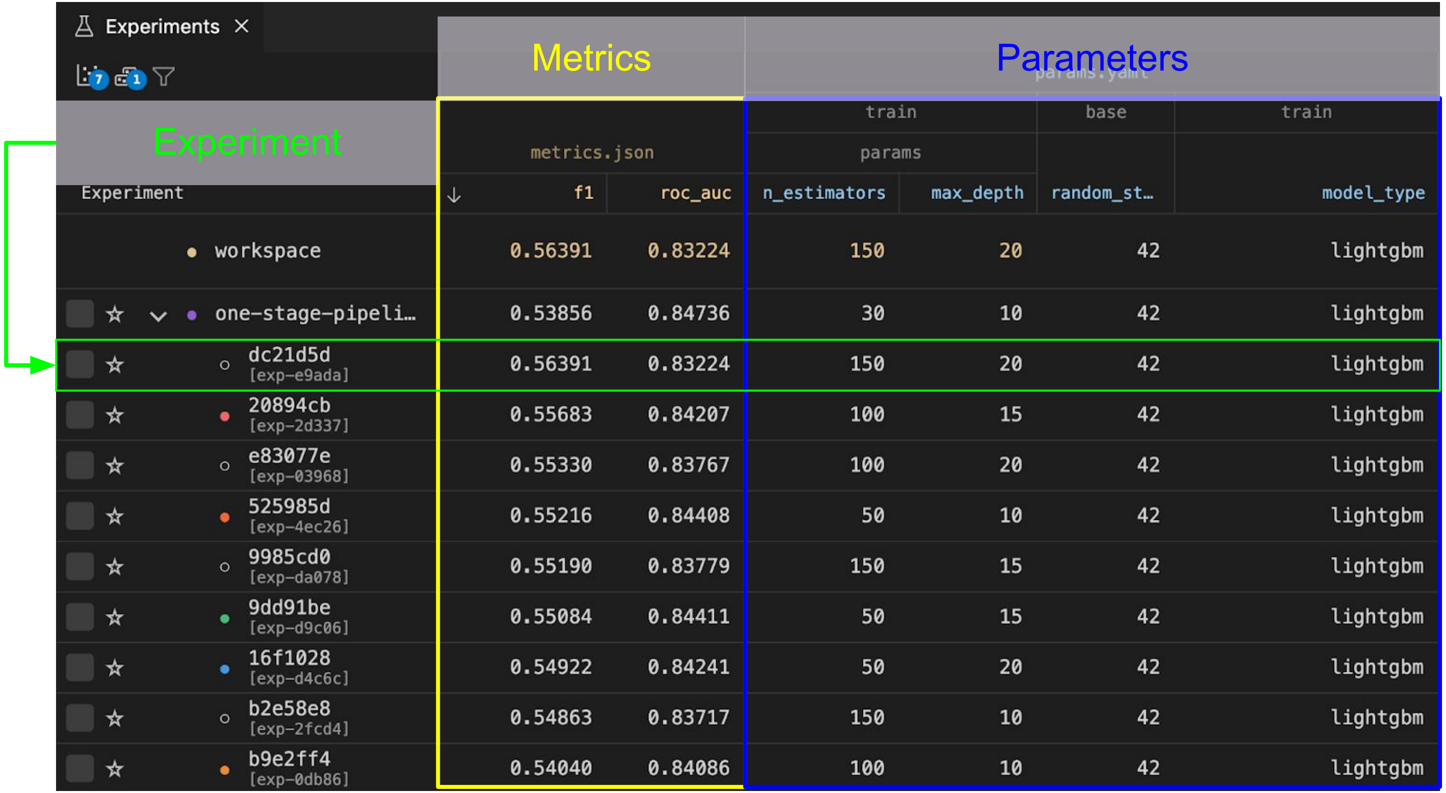
Run an experiment



```
$ dvc exp run -S train.params.n_estimators=120
'data/Churn_Modelling.csv.dvc' didn't change, skipping

Running stage 'run_notebook':
> papermill TrainChurnModel.ipynb TrainChurnModel_out.ipynb -p n_estimators 120 -p max_depth 10 -p model_type lightgbm
Input Notebook:  TrainChurnModel.ipynb
Output Notebook: TrainChurnModel_out.ipynb
Black is not installed, parameters wont be formatted
Executing:   0%|                                                                                                     | 0/27
[00:00<?, ?cell/s]Executing notebook with kernel: python3
Executing: 100%|█████████████████████████████████████████████████████████████████████████████████████████████| 27/27
[00:03<00:00,  7.58cell/s]
Updating lock file 'dvc.lock'
```

Track and manage many experiments



			params.yaml			
			train		base	train
	metrics.json		params			
Experiment	↓ f1	roc_auc	n_estimators	max_depth	random_st…	model_type
● workspace	0.56391	0.83224	150	20	42	lightgbm
□ ☆ ⌄ ● one-stage-pipeli…	0.53856	0.84736	30	10	42	lightgbm
□ ☆ ○ dc21d5d [exp-e9ada]	0.56391	0.83224	150	20	42	lightgbm
□ ☆ ● 20894cb [exp-2d337]	0.55683	0.84207	100	15	42	lightgbm
□ ☆ ○ e83077e [exp-03968]	0.55330	0.83767	100	20	42	lightgbm
□ ☆ ● 525985d [exp-4ec26]	0.55216	0.84408	50	10	42	lightgbm
□ ☆ ○ 9985cd0 [exp-da078]	0.55190	0.83779	150	15	42	lightgbm
□ ☆ ● 9dd91be [exp-d9c06]	0.55084	0.84411	50	15	42	lightgbm
□ ☆ ● 16f1028 [exp-d4c6c]	0.54922	0.84241	50	20	42	lightgbm
□ ☆ ○ b2e58e8 [exp-2fcd4]	0.54863	0.83717	150	10	42	lightgbm
□ ☆ ● b9e2ff4 [exp-0db86]	0.54040	0.84086	100	10	42	lightgbm

Practice time!