Model Development

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We’ll Start with Model Development and Talk About the Data Later

- Goal: to learn how to approach the development of a machine learning model like a scientist.

- How: in the lab we will grab some freely available ML datasets and use a popular tool called MLFlow to conduct “experiments”.

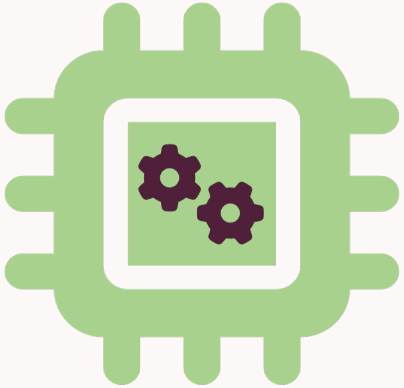
- Note: we are ***not*** going to be all that concerned with the actual model that we build. That is not the point here.

Experiment Tracking

Doing Experiments

- Not talking about Experimentation (A/B testing, Multi-armed Bandit)
- Main idea:
  - Each model you train is a **run** of an **experiment**, with a specific treatment (parameter values, dataset, etc.).

$\lambda = 0.1 \longrightarrow$



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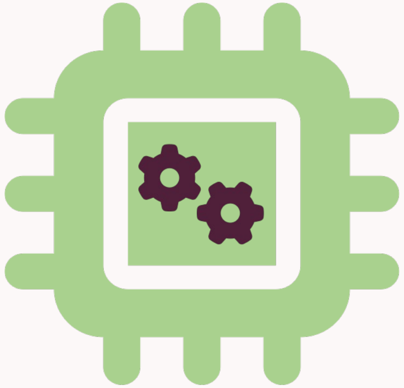

$\longrightarrow \hat{y}$

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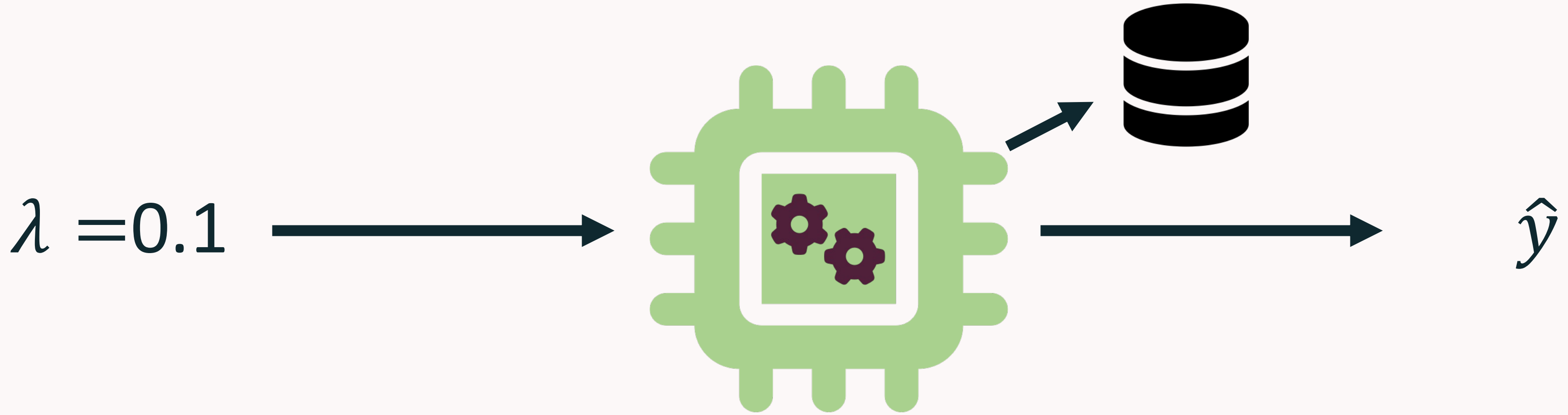
  - Each run has **artifacts** and **metadata**.



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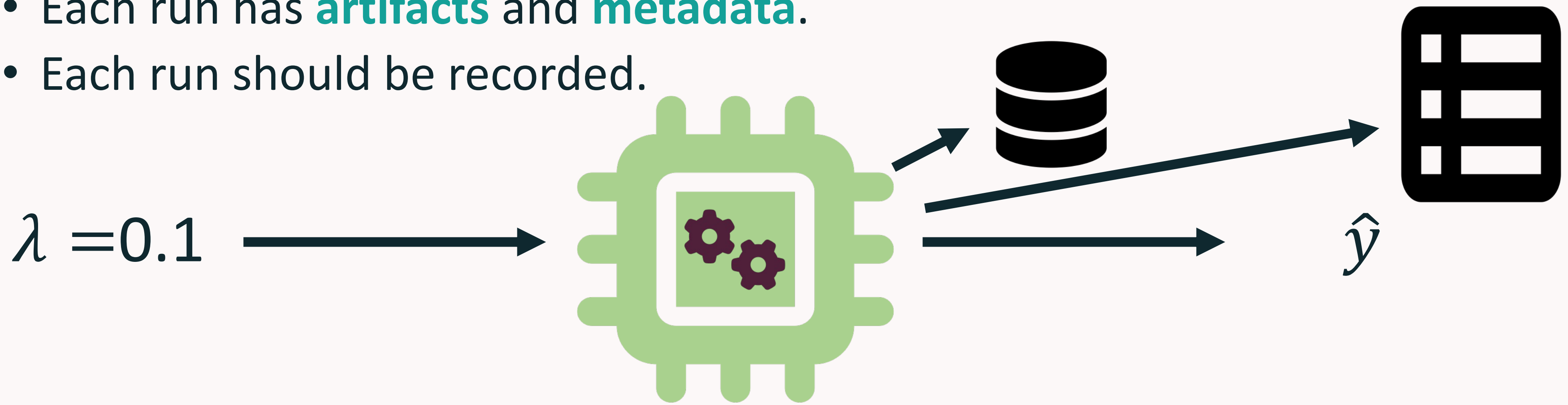
  - Each run has **artifacts** and **metadata**.
  - Each run should be recorded.



What Should We Track in our Experiments?

- Training, validation, and testing dataset versions
- Feature subsets
- Model hyperparameters
- Code changes
- Model evaluation metrics
- Model parameters/weights
- Score distributions
- Environment config files
- Feature importances
- Prediction explanations
- If doing deep learning: resource usage, gradient norms, predictions after each epoch (CV)

Examples

- You randomly split your data into a training and testing set using a random seed:
  - You should log the seed and version your training, validation and testing sets.
- You decide to build a model using a subset of all of your features:
  - You should log this as a new version of your data.
- You do hyperparameter tuning to find the optimal model:
  - You should log all results from each model (metric, performance charts, model weights, hyperparameter values) for each combination of hyperparameter values.
- You decide to try a different algorithm:
  - You should log all results of this model (metric, performance charts, model weights, hyperparameter values) to compare with your other models.
- You make one small change to your code to test something out really quickly:
  - You should log this code change.

Why do we need a new tool to do this for us?

- It is difficult, and prone to error, to track results by porting them over to a spreadsheet.

Iteration	Training	Validation	Testing	Model-ID	algorithm	mtry	ntree	AUC
1	dataA	valA	testA	rf1.1	rf	3	50	0.65
2	dataA	ValA	testA	rf1.2	rf	4	50	0.652
3	dataA	valA	testA	rf1.3	rf	5	50	0.652
4	dataA	ValA	testA	rf2.1	rf	3	70	0.651
5	dataA	valA	testA	rf2.2	rf	4	70	0.652
6	dataA	ValA	testA	rf2.3	rf	5	70	0.65
7	dataA	valA	testA	rf3.1	rf	3	90	0.651
8	dataA	ValA	testA	rf3.2	rf	4	90	0.653
9	dataA	valA	testA	rf3.3	rf	5	90	0.654
10	dataA	ValA	testA	rf4.1	rf	3	100	0.654
11	dataA	valA	testA	rf5.1	rf	3	120	0.655
12	dataA	ValA	testA	rf5.2	rf	4	120	0.6551
13	dataA	valA	testA	rf5.3	rf	5	120	0.6551
14	dataA	ValA	testA	rf5.4	rf	5	150	0.655
15	dataA	valA	testA	rf5.5	rf	5	200	0.65

Why do we need a new tool to do this for us?

- It is difficult, and prone to error, to track results by porting them over to a spreadsheet.
- You do not commit all code changes – that is not efficient – and so you are bound to forget.
- Github does not help you compare models, or objects, even though you *can* version the results of your experiments in an automated way using git hooks.
- Reproducing results is hard to do without help. You absolutely will struggle to reproduce a good result you had without proper tracking. **You will forget**.

Experiment Tracking Tools

- MLFlow and Weights & Biases arguably the most popular

- We'll use MLFlow
  - Free to use
  - Large user community
  - Integrated with several other ML platforms such as Databricks and Dagshub

- Neptune and Comet are paid tools with more features
  - Neptune has a comparison of tools here: https://neptune.ai/blog/best-ml-experiment-tracking-tools

MLFlow

- MLFlow is a tool that promises to do four things:
  - Track experiments
  - Package projects
  - Store artifacts
  - Deploy models

- MLFlow is a python library:
  - Needs a backend store
  - Can run locally or on a server

MLFlow Architecture

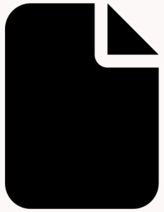
- Where should everything be recorded?
- Options:
  - Local file system on your laptop.
  - Local file system (artifacts) + local sqlite (entities).
  - Remote tracking server (in GCP for instance):
    - Storage for artifacts and entities can be local or remote
    - If remote, maybe S3 for artifacts and postgres for entities
    - Good explanation here

MLFlow Experiment Tracking Demo

Artifact Tracking and Model Registry

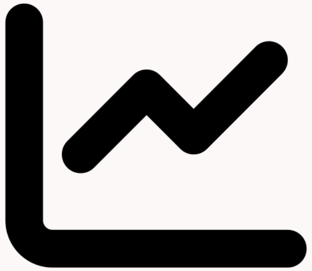
What are artifacts?

- An artifact is any output file that you'd like to store from the runs of your experiments:



Model File

Data



Plots/images

What are artifacts?

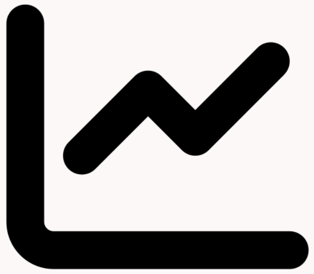
- An artifact is any output file that you'd like to store from the runs of your experiments:

Plots can be stored as image files.

You will create lots of images during model dev:

- EDA visualizations
- Model performance charts (ROC plots, PR curves, etc.)

Not everything needs to be stored, but these images can come in handy for reporting purposes.



Plots/images

What are artifacts?

- An artifact is any output file that you'd like to store from the runs of your experiments:

Datasets can be stored in a compressed format such as parquet, particularly specific training, validation and test sets used.

Model File

Data

Plots/images

The data sets can come in handy later, especially if something goes wrong with your deployed model.

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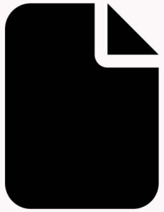


Model File

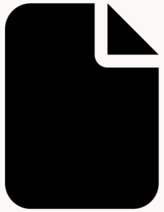
Model files can be serialized and stored, typically as pickle files when using python.

You may end up storing several versions of your model:

- You find one you want to save for later
- You find one you want to deploy
- You create a new version to replace the previously deployed model

What is a model registry?

- A model registry is where you store and register your models.



Model File

Models are versioned.

Model files are retrieved from the registry to deploy in production.

Data

Plots/images

MLFlow Artifact Tracking and Model Registry Demo

Experiment Tracking Lab

Project Check-in

- Groups: choose project dataset.
- Groups: choose group members for experiment tracking POC.
- Group members doing POC: choose tools to compare.
- Designated communicator: let me know in Piazza who is doing the POC and on what tools.
- Group members doing POC: work on POC.
- **ALL group members**: complete the experiment tracking demo and lab.