

Model Development

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

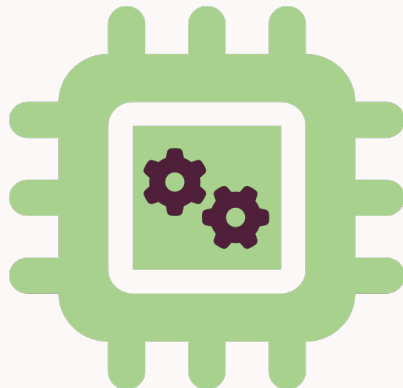
- Goal: to learn how to approach the development of a machine learning model like a scientist.
- How: in the lab we will grab some freely available ML datasets and use a popular tool called MLFlow to conduct “experiments”.
- Note: we are ***not*** going to be all that concerned with the actual model that we build. That is not the point here.

Experiment Tracking

Doing Experiments

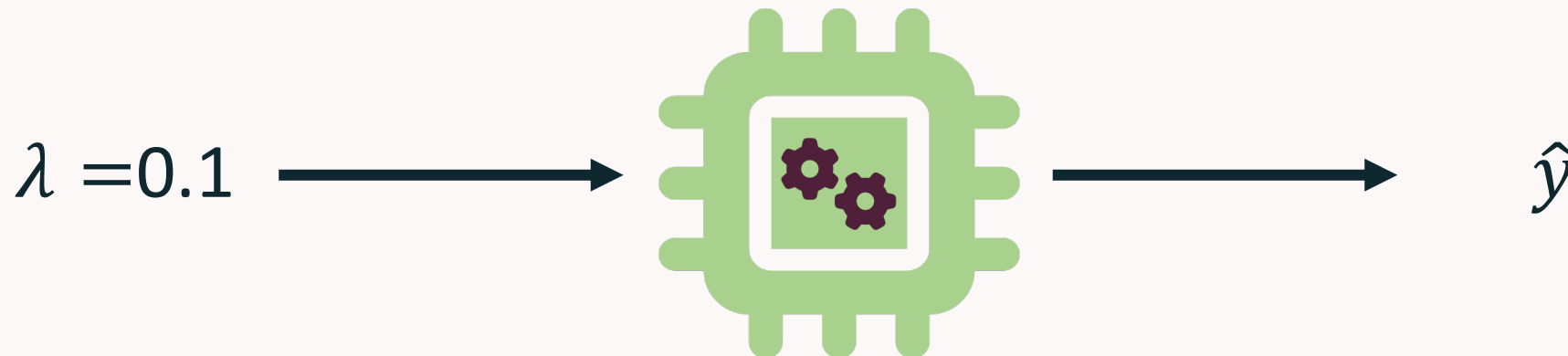
- Not talking about Experimentation (A/B testing, Multi-armed Bandit)
- Main idea:
 - Each model you train is a **run** of an **experiment**, with a specific treatment (parameter values, dataset, etc.).

$\lambda = 0.1$



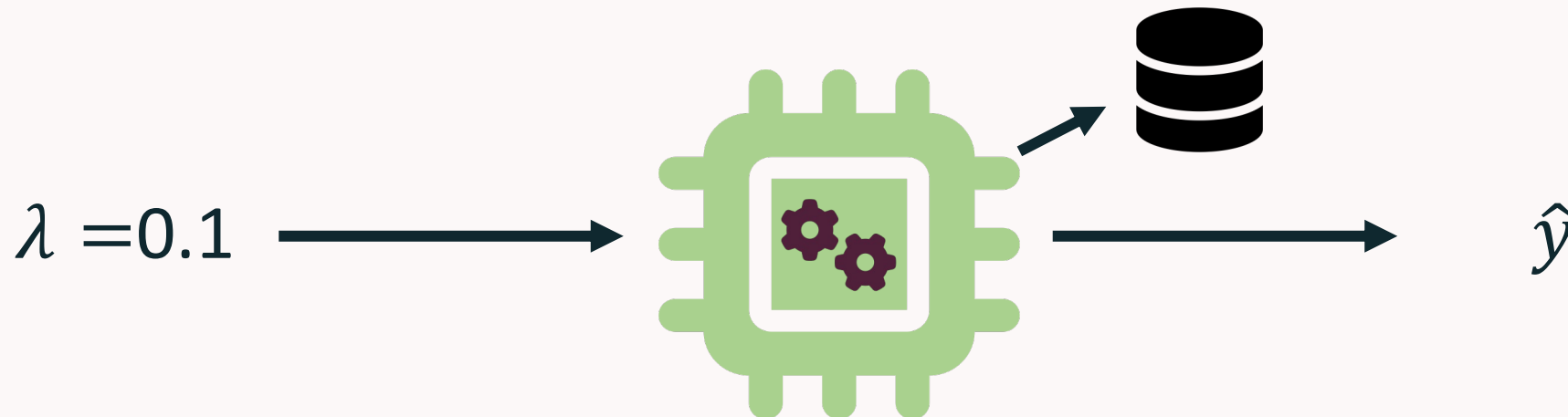
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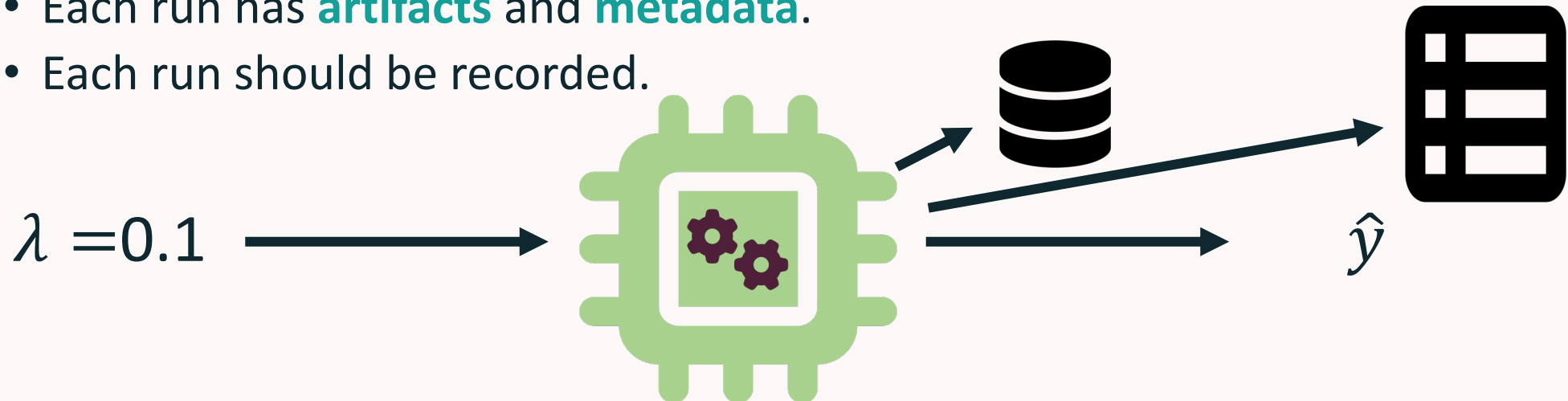
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 - Each run has **artifacts** and **metadata**.
 - Each run should be recorded.



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.

[illegible]

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

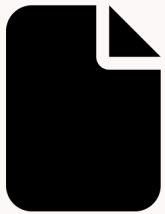
- Where should everything be recorded?
- Options:
 - Local file system on your laptop.
 - Local file system (artifacts) + local sqlite (entities).
 - Remote tracking server (in GCP for instance):
 - Storage for artifacts and entities can be local or remote
 - If remote, maybe S3 for artifacts and postgres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

MLFlow Experiment Tracking Demo

Artifact Tracking and Model Registry

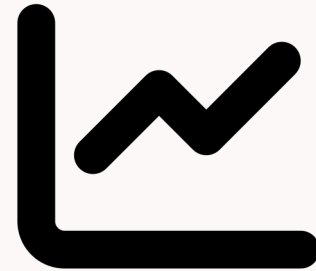
What are artifacts?

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



Model File

Data



Plots/images

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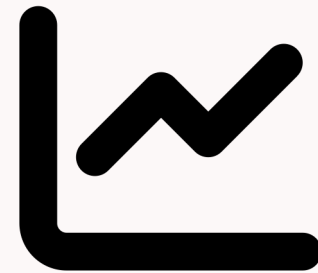
- An artifact is any output file that you'd like to store from the runs of your experiments:

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

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

Model File

Data

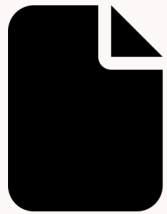


Plots/images

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

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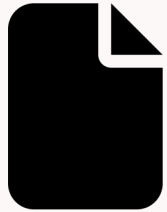
Model files can be serialized and stored, typically as pickle files when using python.

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

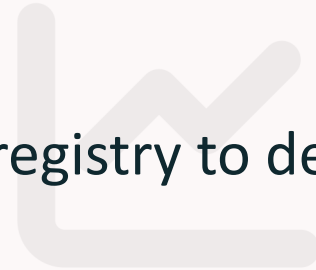
Models are versioned.

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

Data



Plots/images



MLFlow Artifact Tracking and Model Registry Demo

Experiment Tracking Lab