Applied Machine Learning for Business Analytics

Lecture 9: Model Evaluation in Machine Learning

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To change your team name on Kaggle, simply **navigate to the "Team" tab within the competition you're participating in and update it there**.

Here's a more detailed breakdown:

- **Access the Competition:** Go to the specific Kaggle competition where you want to change your team name.
- **Navigate to the "Team" Tab:** Locate the "Team" tab within the competition page.
- **Update the Team Name:** You should find an option to edit or change the team name within this tab.
- **Save the Changes:** Once you've made the desired changes, save them, and the new team name will be reflected on the leaderboard.

Agenda

1. Baseline First
2. Model Evaluation
3. Experiment Tracking

1. Baseline First

Neural networks

Bayesian learning	Deep learning
Bayesian models (GPs, BayesNets, PGMs,)	Deep models (MLP, CNN, RNN etc.)
Bayesian inference (Bayes rule)	Stochastic training (SGD, RMSprop, Adam)

	Bayes	DL
Can handle large data and complex models?	✗	✓
Scalable training?	✗	✓
Can estimate uncertainty?	✓	✗
Can perform sequential / active /online / incremental learning?	✓	✗

Source: Deep Learning with Bayesian Principles (Emtiyaz Khan, NeurIPS 2019)

Architecture evolution

- Fancy models come and go
  - LSTM-RNNs: still used for time series (trading) but for text data, transformers is the first-choice

The fall of RNN and LSTM https://towardsdatascience.com/the-fall-of-rnn-lstm-2d1594c74ce0

- Be solution-focused, not architecture/buzzword-focused

Model selection: baselines first

- **Random baseline**
  - Predict at random:
    - uniform
- **Zero rule baseline**
  - Predict the most common class always
- **Human baseline**
  - Human expert?
- **Simple heuristic**:
  - For example, if your device is linked to multiple accounts (10+), your account will have a high fraud risk.
- **Existing solutions**:
  - Existing APIs

Baselines

- Pave the way for iterative development
- Due to low model complexity
  - Rapid experimentation via hyperparameter tuning
  - Discover of data issues, false assumptions, bugs in ETL or code
- Build the benchmark performances
  - Slowly add complexity by addressing limitations and motivating representations and model architectures.

Case study: stackoverflow classification

- Random
  - What is the random performance looks like
    - Binary Classification: np.random.randint(low=0, high=2)
  - All of our following trials should perform better than this
  - **Limitations**: no inputs information is used. No learning happened

Case study: stackoverflow classification

- Random
  - No input information is used
- Rule-based
  - We would like to use signals from input data to make predictions
  - Domain knowledge and auxiliary data can be used here.
  - For example, if len(text) > 200 or code in text, the label will be positive
  - Let us guess how will the rule-based system perform?
    - High Precision low recall
    - Low Precision high recall
  - **Limitations**: Unable to generalize or capture patterns to make predictions

Case study: stackoverflow classification

- Random
  - No input information is used
- Rule-based
  - Unable to generalize or capture patterns to make predictions
- Simple ML Systems
  - Representations: using TF-IDF (capture the importances of a token to the labels)
  - Architecture: can use various classifiers to predict labels based on signals
  - **Limitations**:
    - TF-IDF is only counting tokens' frequency. We need to capture high-level semantic meaning
    - Models need to capture the meaning in a more contextual manner


```
{
  "logistic-regression": {
    "precision": 0.633369022127052,
    "recall": 0.21841541755888652,
    "f1": 0.3064204603390899
  },
  "k-nearest-neighbors": {
    "precision": 0.7410281119097024,
    "recall": 0.47109207708779444,
    "f1": 0.5559182508714337
  },
  "random-forest": {
    "precision": 0.7722866712160075,
    "recall": 0.38329764453961457,
    "f1": 0.4852512297132596
  },
  "gradient-boosting-machine": {
    "precision": 0.8503271303309295,
    "recall": 0.6167023554603854,
    "f1": 0.7045318461336975
  },
  "support-vector-machine": {
    "precision": 0.8938397993500261,
    "recall": 0.5460385438972163,
    "f1": 0.6527334570244009
  }
}
```

Case study: stackoverflow classification

- Random
- Rule-based
- Simple ML Systems
- CNN with word embeddings

In this process, we kind of motivate the need for slowly adding complexity from both the **representation** and **architecture**, as well as address the limitation at each step of the way.

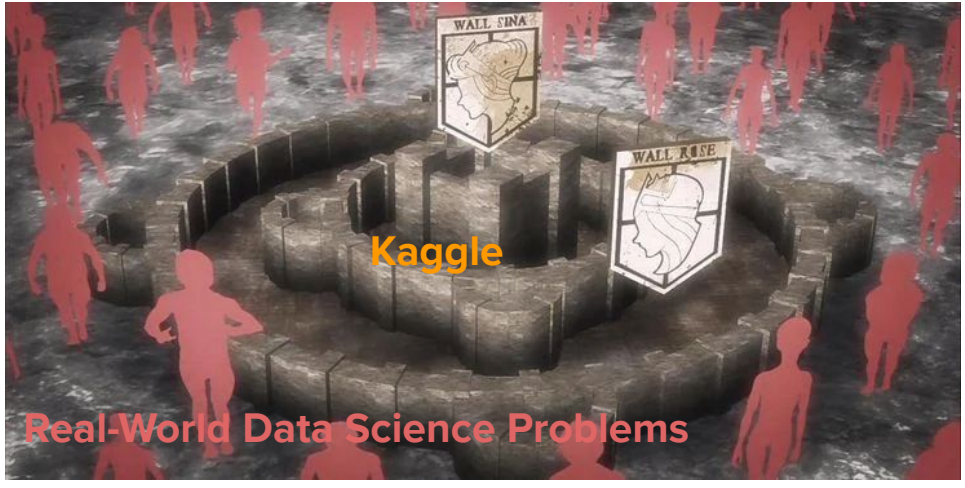
2. Model Evaluation

Model evaluation

- Offline evaluation:
  - Before deployment
  - Our focus today
- Online evaluation:
  - After deployment
  - ML model monitoring
  - https://christophergs.com/machine%20learning/2020/03/14/how-to-monitor-machine-learning-models/

ML offline evaluation

It is not simply computing the accuracy or other global metrics.



Intuition behind model evaluation

- Be clear about what metrics we are prioritizing
- Be careful not to over-optimize on any single metric
    - Trade-off is always there

Evaluation methods

1. Interpretability
2. Samples Inspection
3. Perturbation Tests
4. Directional Expectation Tests
5. Slice-based Evaluation
6. Model Calibration

Interpretability

- Interpretability methods such as LIME or SHAP can enable us to inspect the inputs to our models
- We can check:
  - Global level -> per class
  - Local level -> per single prediction

Samples inspection

- Confusion Matrix:
  - True positives: prediction = ground-truth
    - Learn about where our model performans well
  - False positives: predict wrongly samples belongs to the class
    - Identify potentially mislabeled samples
  - False negatives: predict wrongly samples does not belongs to the class
    - Identify the model's less performant areas to upsample later

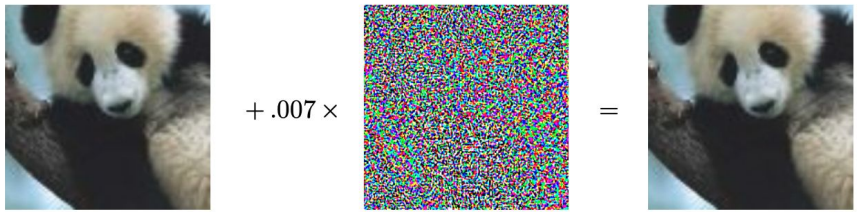
Check those FP/FN samples

Perturbation tests

- Motivation: users input might contain noise, making it different from test data
- Idea: randomly add small noise to test data to see how much outputs change

Perturbation tests

- Motivation: users input might contain noise, making it different from test data
- Idea: randomly add small noise to test data to see how much outputs change
- The more sensitive the model is to noise:
  - The harder it is to maintain
  - The more vulnerable the model is to adversarial attacks



Perturbation tests

- Motivation: users input might contain noise, making it different from test data
- Idea: randomly add small noise to test data to see how much outputs change
- If the model failed the perturbation tests, the solutions could be:
  - Add noise to training data
  - Add more training data
  - Select more robust model (simpler model)

Directional expectation tests

- Motivation: some changes to inputs should cause predictable changes in outputs
  - E.g. when predicting housing prices:
    - Increasing lot size shouldn't decrease the predicted price
    - Decreasing square footage shouldn't increase the predicted price

Directional expectation tests

- Motivation: some changes to inputs should cause predictable changes in outputs
- Idea: keep most features the same, but change certain features to see if outputs change predictably
- For example, if increasing lot size consistently reduces the predicted price, you might want to investigate why!

2.5 Slice-based Evaluation

Why not coarse-grained evaluation

- Overall metrics is a good start. However, it may hide:
  - Model biases
  - Potential for improvement
  - Which model will you select?

	Overall accuracy
Model A	96.2%
Model B	95%

Different performance on different slices

- Classes
  - Might perform worse on minority classes
- Subgroups
  - Gender
  - Location
  - Time of using the app
  - etc.

Fine-grained evaluation

- The date samples have:
  - Majority group: 90%
  - Minority group: 10%
- Then, which model will you chose?

	Majority accuracy	**Minority accuracy**	**Overall accuracy**
Model A	98%	80%	96.2%
Model B	95%	95%	95%

Same performance on different slices with different cost

- User churn prediction
  - Paying users are more critical
- Predicting adverse drug reactions
  - Patients with underlying conditions are more critical

Focusing on improving only overall metrics might hurt performance on subgroups

Slice-based evaluation

- Evaluate your model on different slices
  - E.g. when working with website traffic data, slice data among:
    - gender
    - mobile vs. desktop
    - browser
    - location
- Check for consistency over time
  - E.g. evaluate your model on data slices from each day

Slice-based evaluation

- Improve model's performance both overall and on critical data
- Help avoid biases
- Even when you don't think slices matter, slicing can:
  - give you confidence on your model (to convince your boss)
  - might reveal non-ML problems

How to identify slices?

- Manual Slices (based on subject matter expertise)
  - Classes
  - Features
  - Metadata
    - Timestamps, sources
  - Priority slices
    - Minority groups, high value customers

How to identify slices?

- Manual Slices (based on subject matter expertise)
- Slice finder
  - SliceLine
    - Use linear-algebra and pruning based method to find large slices that result in meaningful errors
  - Clustering

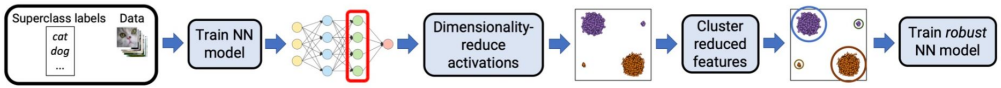
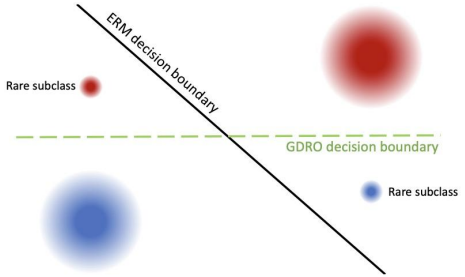


Figure 4: Schematic describing GEORGE. The inputs are the datapoints and superclass labels. First, a model is trained with ERM on the superclass classification task. The activations of the penultimate layer are then dimensionality-reduced, and clustering is applied to the resulting features to obtain estimated subclasses. Finally, a new model is trained using these clusters as groups for GDRO.



2.6 Model Calibration

Model calibration

“One of the most important tests of a forecast — I would argue that it is the single most important one — is called calibration.”

Nate Silver, **The Signal and the Noise**

What is calibration

- Assumption: the probability associated with the predicted class label should reflect its ground truth correctness likelihood
- Reality: complex models are no longer well-calibrated
  - Random Forest, SVMs, Naive Bayes, Deep Learning
- If model is well calibrated:
  - If you predict team A wins in A vs B match with 60% probability:
    - In 100 A vs. B match, A should win 60% of the time!
  - In binary classification, if the model's predictions over 100 samples whose prob. score of positive class is 0.6
    - It means 60 samples here are positive (ground truth)

Why calibration matters

- The high-level idea here is that with calibration, we can interpret the estimated probabilities as long-run frequencies.
- Estimated probabilities allow flexibility
- Model modularity

Model calibration: CTR

- The classifier is used to predict whether the user will click the add:
  - User A: ad 1 (20%) ad 2 (40%), ad 3 (8%), ad 4 (10%)
  - User B: ad 1 (30%) ad 2 (4%), ad 3 (80%), ad 4 (20%)
  - User C: ad 1 (15%) ad 2 (50%), ad 3 (10%), ad 4 (30%)
- Do we need to calibrate models if we want to rank ads for users (personalization)?

Model calibration: CTR

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  - User C: ad 1 (15%) ad 2 (50%), ad 3 (10%), ad 4 (30%)
- Do we need to calibrate models if we want to rank ads for users (personalization)?
  - **No need to calibrate. The probability are only used for comparison.**

Model calibration: CTR

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  - User C: ad 1 (15%) ad 2 (50%), ad 3 (10%), ad 4 (30%)
- Do we need to calibrate models if we want to calculate the expected number of clicks?
  - The expected clicks for ad1 is 0.2 + 0.3 + 0.15 + ...
  - The expected number can be used to estimated the revenue before we really launch the ads?

Model calibration: CTR

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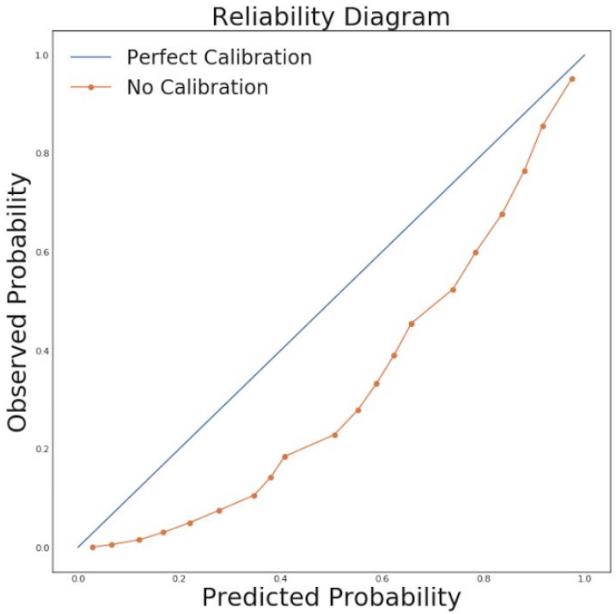
  - The expected clicks for ad1 is 0.2 + 0.3 + 0.15 + ...
  - The expected number can be used to estimated the revenue before we really launch the ads?
  - We need calibrated probabilities to estimate the expected number of clicks

Allow flexibility

Reliability plot

- Plot predicted probability against your empirical probability for some quantity buckets of the data



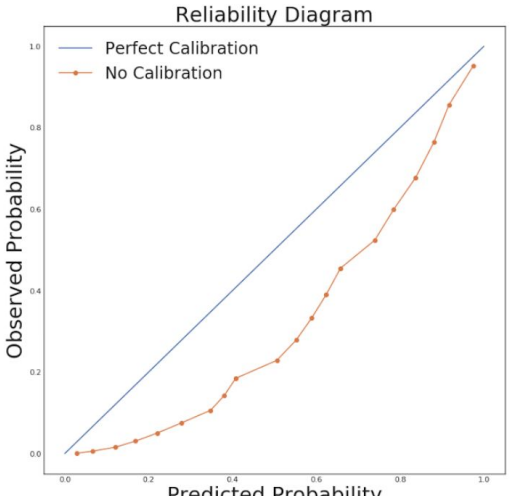
Tutorial:
https://www.youtube.com/watch?v=hWb-MIXKe-s

Reliability plot

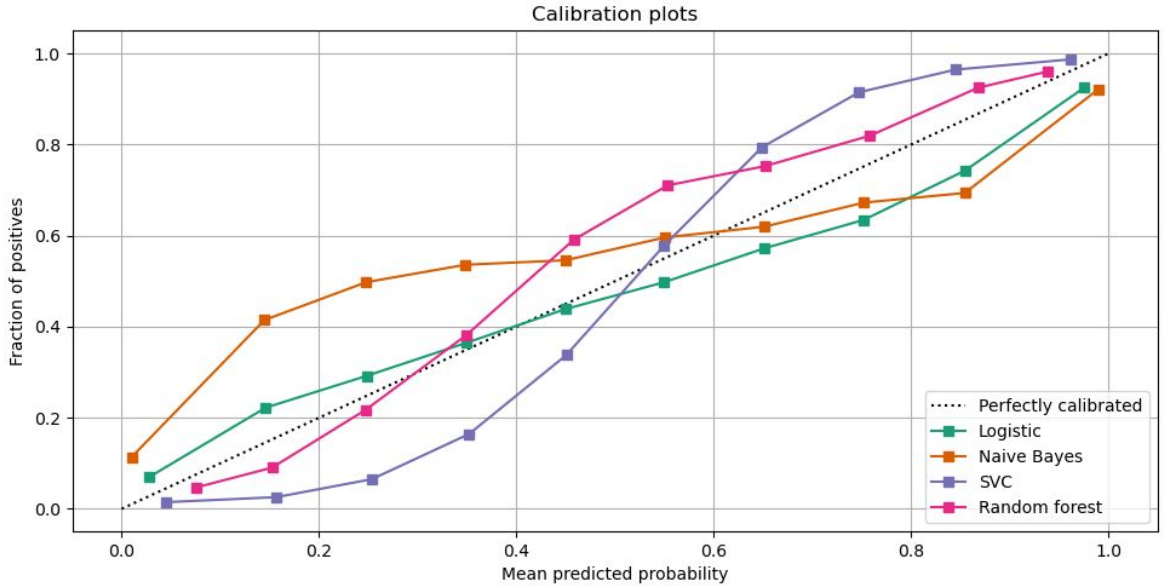
predicted_prob score	True label
0.1	1
0.1	0
0.1	1
0.1	0
0.1	0
0.2	
…	
0.8	0
0.9	1
0.9	0
0.9	1
0.9	1

Predicted Prob: 0.1 Observed Prob:?

Predicted Prob: 0.9 Observed Prob:?



Case



Which machine learning model is the best calibrated one?

Source: https://scikit-learn.org/stable/modules/calibration.html

Calibration methods

- View the classifier as a black-box and learn a calibration function which transforms your prob. output to be calibrated
  - Do you remember some previous methods we discussed?
- Different approaches for the calibration function:
  - Platt's scaling (Sklearn)
    - sklearn.calibration.CalibratedClassifierCV
    - https://github.com/gpleiss/temperature_scaling
  - Isotonic Regression (Sklearn)
  - Tensorflow Lattices

3. Experiment Tracking

Key terms

- ML experiment:
  - The process of developing the ML model
- Experiment run:
  - each trial in an ML experiment
- Run artifact:
  - Any file that is associated with an ML run like models, images, in-memory objects and etc.
- Experiment metadata
- Experiment Tracking is the process to manage all experiments and their meta-data
  - Parameters
  - Metrics
  - Models
  - Other Artifacts

Experiment tracking

- In the life cycle of machine learning, we will train and evaluate tons of different machine learning models (representations, architectures, and hyperparameters)
- Experiment tracking is the process to manage all **experiments** and their meta-data
  - Source code
  - Environment
  - Data
  - Model
  - Hyperparameters
  - Metrics
  - Other Artifacts

Why experiment tracking matters

- With tracking, we can
  - Organize all the necessary components of a specific experiments
    - Where is my phone?
  - Reproduce past results using saved experiments
  - Log iterative improvements across time, data, ideas, teams, etc

Before tracking tools

TABLE II
CLASSIFICATION ACCURACIES (%) FOR COMPARED METHODS ON THE WHOLE FIVE ADOPTED DATASETS. BOLD FACE INDICATES HIGHEST ACCURACIES

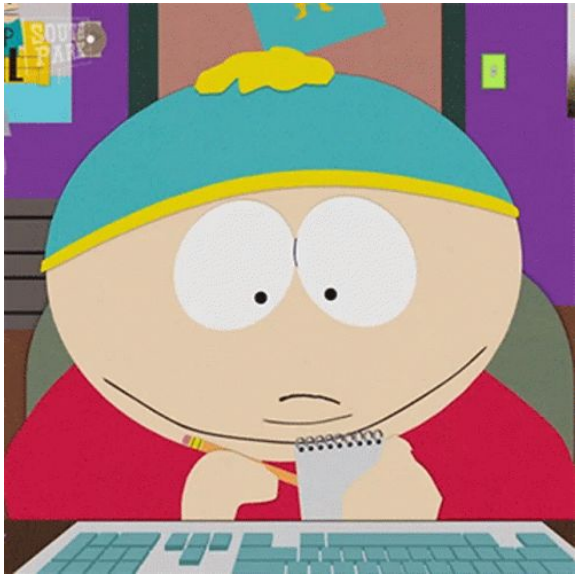
Category	Method	Datasets				
		MR	Subj	CR	MPQA	TREC
Text Classification Models	NBSVM	79.4	93.2	81.8	86.3	-
	MNB	79.0	93.6	80.0	86.3	-
	G-Dropout	79.0	93.4	82.1	86.1	-
	F-Dropout	79.1	93.6	81.9	86.3	-
CNN and its Variants	CNN	81.3	93.5	83.9	89.4	93.0
	CNN_{600}	79.3	92.0	81.6	87.5	91.9
	DCNN	-	-	-	-	93.0
	DSCNN	82.2	93.2	-	-	**95.6**
	P.V.	75.9	92.2	77.9	75.4	91.5
Other Deep Compositional Models	RAE	77.7	-	-	86.4	-
	MV-RNN	79.9	-	-	-	-
	RNN	77.2	90.9	71.8	88.6	83.8
	LSTM	79.5	93.3	80.4	88.8	89.4
	GRUs	80.5	93.5	82.1	89.0	91.8
	AdaSent	**83.1**	**95.5**	**86.3**	**93.3**	91.8
Our Models	$TopCNN_{word}$	81.7	93.4	84.9	89.9	92.5
	$TopCNN_{sen}$	81.3	93.4	84.8	90.3	92.0
	$TopCNN_{word\&sen}$	82.3	94.3	85.6	91.1	93.6
	$TopCNN_{ens}$	**83.0**	95.0	**86.4**	91.8	94.1
	$TopLSTMs_{word}$	81.2	94.1	82.6	89.6	91.5
	$TopLSTMs_{sen}$	80.6	93.7	81.6	89.1	90.5
	$TopLSTMs_{word\&sen}$	80.8	94.0	82.3	89.5	91.4
	$TopLSTMs_{ens}$	81.9	94.5	82.9	90.8	91.9

Source:
https://dr.ntu.edu.sg/bitstream/10356/83235/1/Topic-Aware%20Deep%20Compositional%20Models%20for%20Sentence%20Classification.pdf

Before tracking tools

```
(rmse, mae, r2) = eval_metrics(test_y, predicted_qualities)
print("Elasticnet model (alpha=%f, l1_ratio=%f):" % (alpha, l1_ratio))
print("  RMSE: %s" % rmse)
print("  MAE: %s" % mae)
print("  R2: %s" % r2)
```

```
Elasticnet model (alpha=1.500000, l1_ratio=0.900000):
  RMSE: 0.8327481314145982
  MAE: 0.6751289812215555
  R2: 0.017435513620481347
Elasticnet model (alpha=0.500000, l1_ratio=0.020000):
  RMSE: 0.7364106074415193
  MAE: 0.5673052761841408
  R2: 0.23162398391500494
Elasticnet model (alpha=0.010000, l1_ratio=0.500000):
  RMSE: 0.6778557583356976
  MAE: 0.5190564939146215
  R2: 0.3489590462840657
```



Before tracking tools

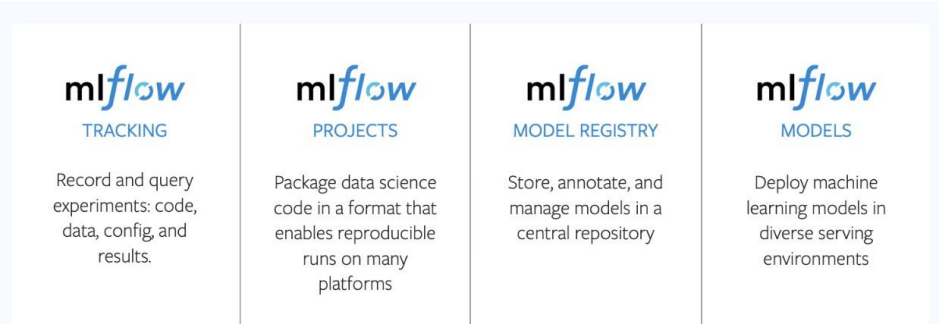
- Even we use spreadsheets:
  - Error prone
  - No standard format
  - Visibility & Collaboration

Tracking tools

- MLFow: 100% Free and open-source
  - Used by Azure, Facebook, Databricks
- Comet ML
  - Used by Google AI, HuggingFace
- Neptune
  - Used by NewYorkers
- Weights and Biases
  - Used by Open AI

MLflow

- Definition: “An open source platform for the machine learning lifecycle”
- It is a python package with four main modules:
  - **Tracking**
  - Models
  - Model Registry
  - Projects




```
# Install MLflow
pip install mlflow
```

Source: https://mlflow.org/docs/latest/index.html
MLflow make experiments tracking manageable with minimal code.

Track experiments using MLflow

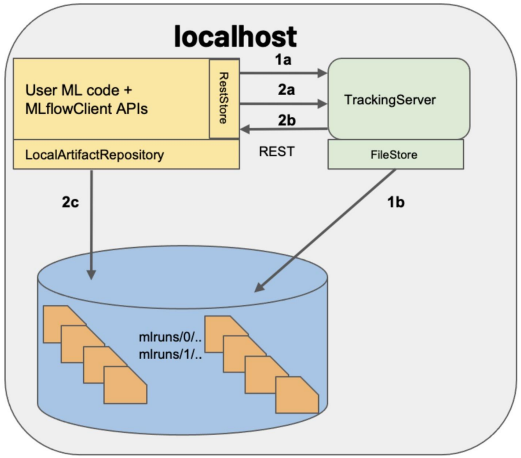
- MLflow Tracking module can organize the experiments into runs, and to keep track of
  - Parameters
  - Metrics
  - Metadata
  - Artifacts
  - Models
- In each run, MLflow will automatically logs extra information including:
  - Source code
  - Version of the code
  - Start and end time
  - Author
- MLflow server also provides GUI to manage and check all of stored data

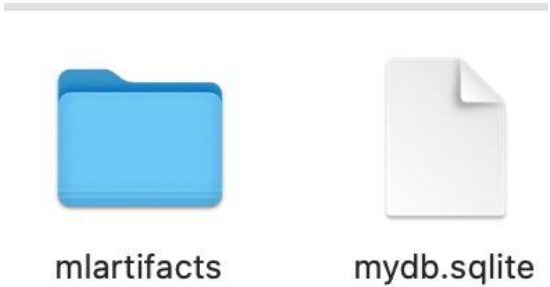
Storage location of MLflow

- Storage Location:
  - Local files
    - ./mlruns folders (local filesystem)
  - SQLite
  - Postgre SQL
  - S3 database
  - More details could be found:
    - https://mlflow.org/docs/latest/tracking.html#how-runs-and-artifacts-are-recorded

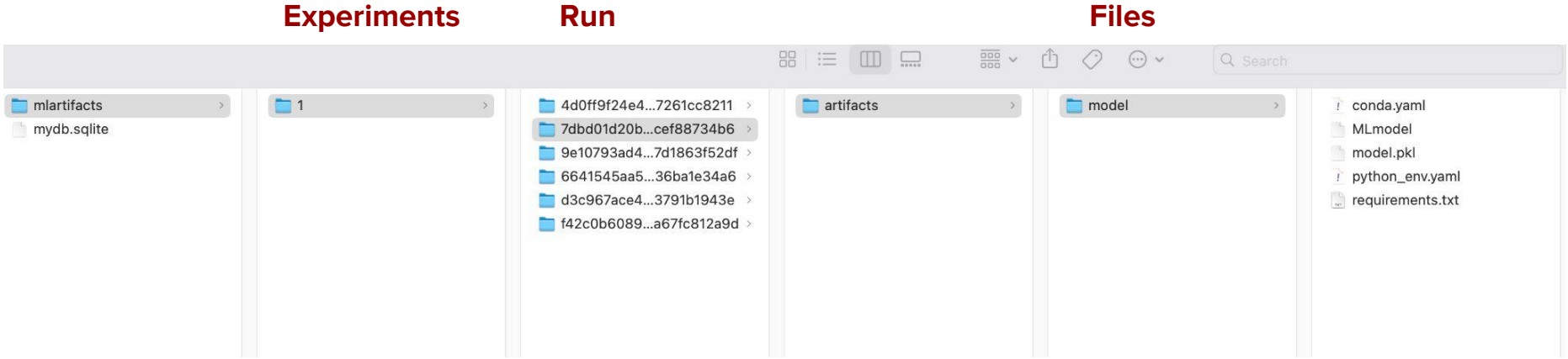
Setup MLflow on localhost with tracking server

```
(bt5153env) rz@RuisPeralMacPro mlflow_folder % mlflow server --backend-store-uri sqlite:///mydb.sqlite
2023/01/29 22:56:25 INFO mlflow.store.db.utils: Creating initial MLflow database tables...
2023/01/29 22:56:25 INFO mlflow.store.db.utils: Updating database tables
INFO  [alembic.runtime.migration] Context impl SQLiteImpl.
INFO  [alembic.runtime.migration] Will assume non-transactional DDL.
```



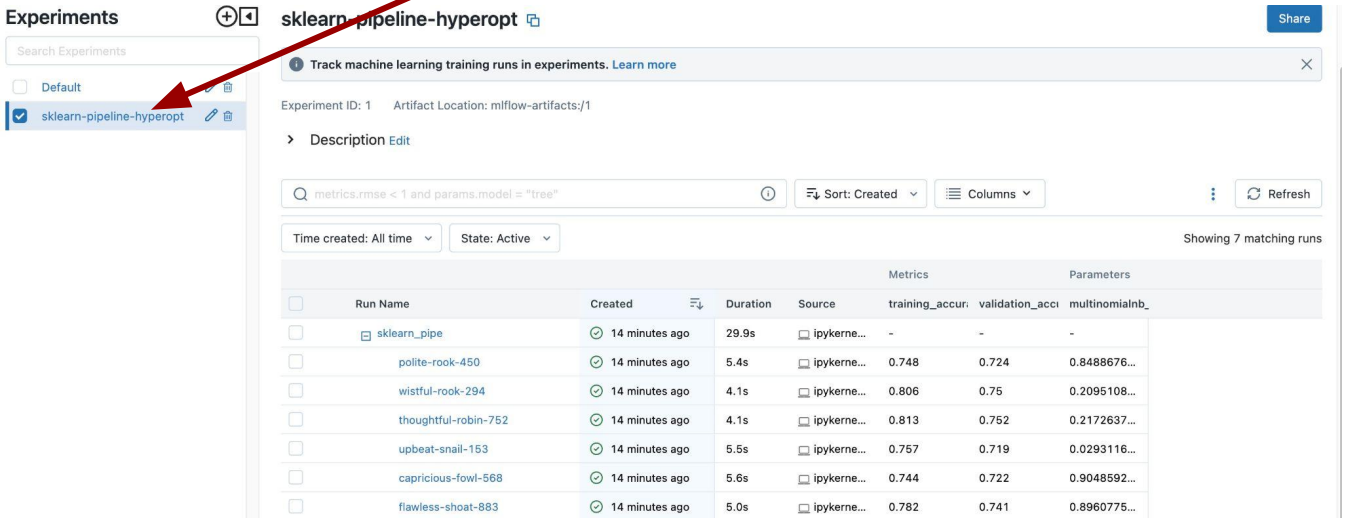


MLflow on localhost with tracking server



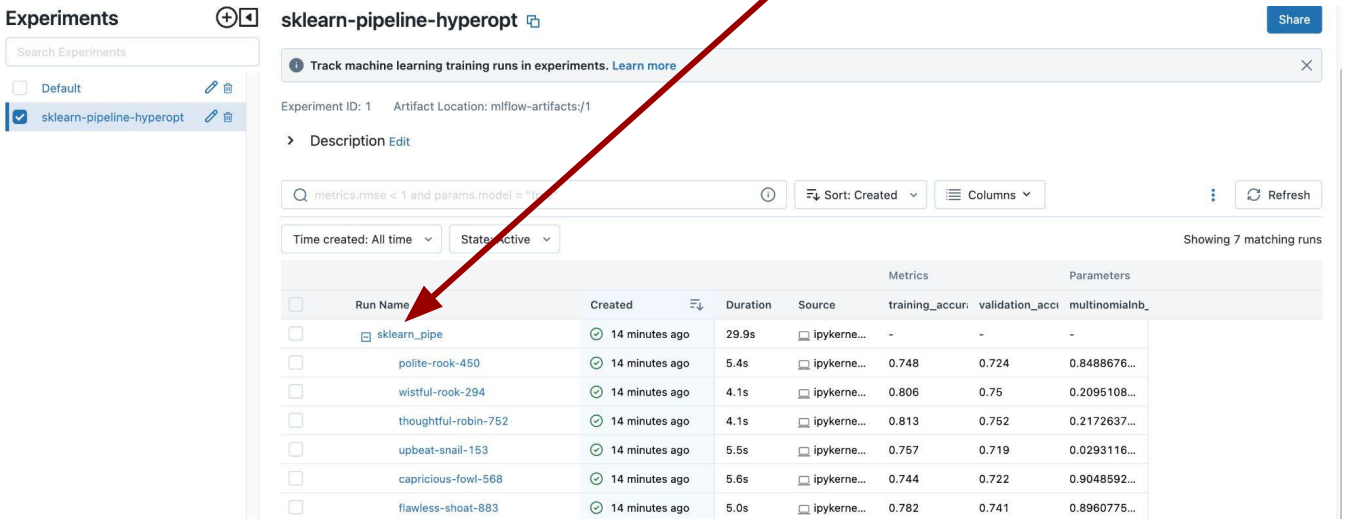
Track experiments - after MLflow

```
try:
    EXPERIMENT_ID = mlflow.create_experiment('sklearn-pipeline-hyperopt')
except:
    EXPERIMENT_ID = dict(mlflow.get_experiment_by_name('sklearn-pipeline-hyperopt'))['experiment_id']
```



Track experiments - after MLflow

```
with mlflow.start_run(experiment_id=EXPERIMENT_ID, run_name='sklearn_pipe'):
    xgboost_best_params = fmin(
        fn=train_model,
        space=param_hyperopt,
        algo=tpe.suggest,
        trials=trials,
        max_evals=6
)
```



Log metrics - after MLFlow

			Metrics			
Run Name	Created	Duration	training_accuracy	training_f1_micro	validation_accuracy	validation_f1_micro
sklearn_pipe	14 minutes ago	29.9s	-	-	-	-
polite-rook-450	14 minutes ago	5.4s	0.748	0.748	0.724	0.724
wistful-rook-294	14 minutes ago	4.1s	0.806	0.806	0.75	0.75
thoughtful-robin-752	14 minutes ago	4.1s	0.813	0.813	0.752	0.752
upbeat-snail-153	14 minutes ago	5.5s	0.757	0.757	0.719	0.719
capricious-fowl-568	14 minutes ago	5.6s	0.744	0.744	0.722	0.722
flawless-shoat-883	14 minutes ago	5.0s	0.782	0.782	0.741	0.741

```
# Logging each metric
for name, metric in list(zip(metric_names, training_metrics_values)):
    mlflow.log_metric(f'training_{name}', metric)
for name, metric in list(zip(metric_names, validation_metrics_values)):
    mlflow.log_metric(f'validation_{name}', metric)
```

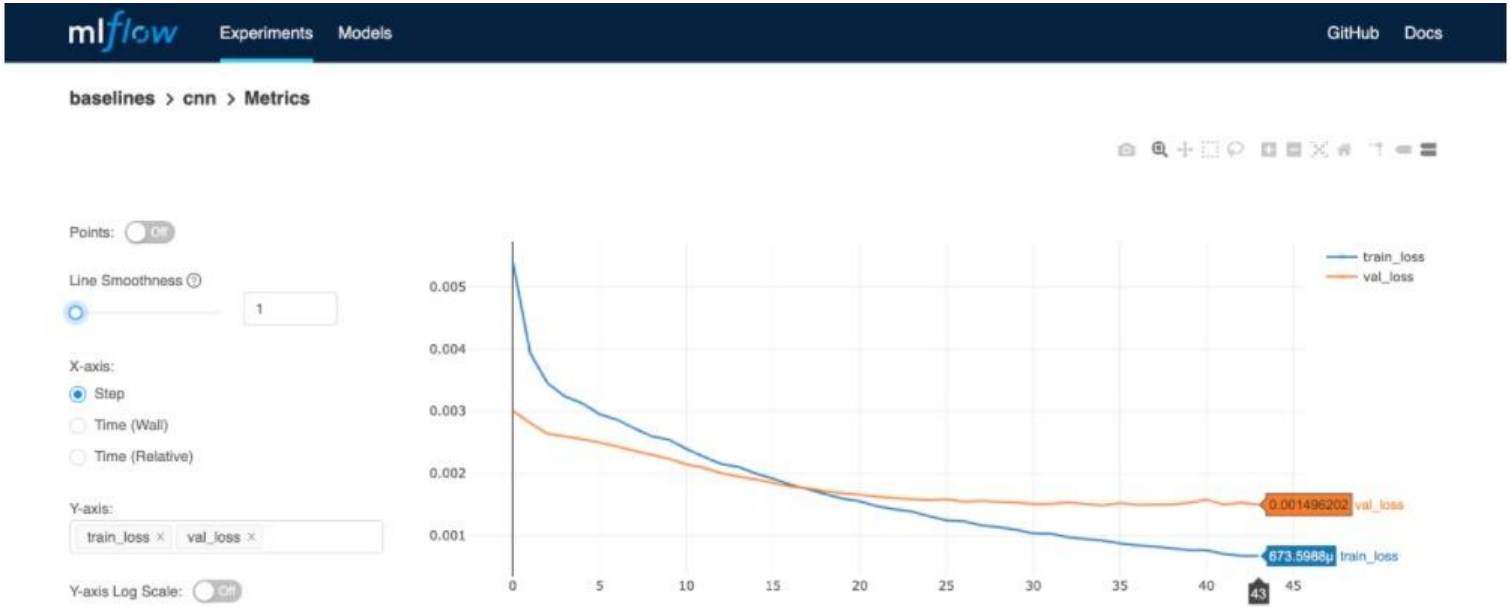
Log parameters - after MLFlow

Run Name	Created	Duration	countvectorize	countvectorize	multinomialnb
sklearn_pipe	14 minutes ago	29.9s	-	-	-
polite-rook-450	14 minutes ago	5.4s	1	\b\w\w+\b	0.8488676...
wistful-rook-294	14 minutes ago	4.1s	3	'([a-z]+)'	0.2095108...
thoughtful-robin-752	14 minutes ago	4.1s	1	'([a-z]+)'	0.2172637...
upbeat-snail-153	14 minutes ago	5.5s	4	\b\w\w+\b	0.0293116...
capricious-fowl-568	14 minutes ago	5.6s	3	\b\w\w+\b	0.9048592...
flawless-shoat-883	14 minutes ago	5.0s	2	'([a-z]+)'	0.8960775...

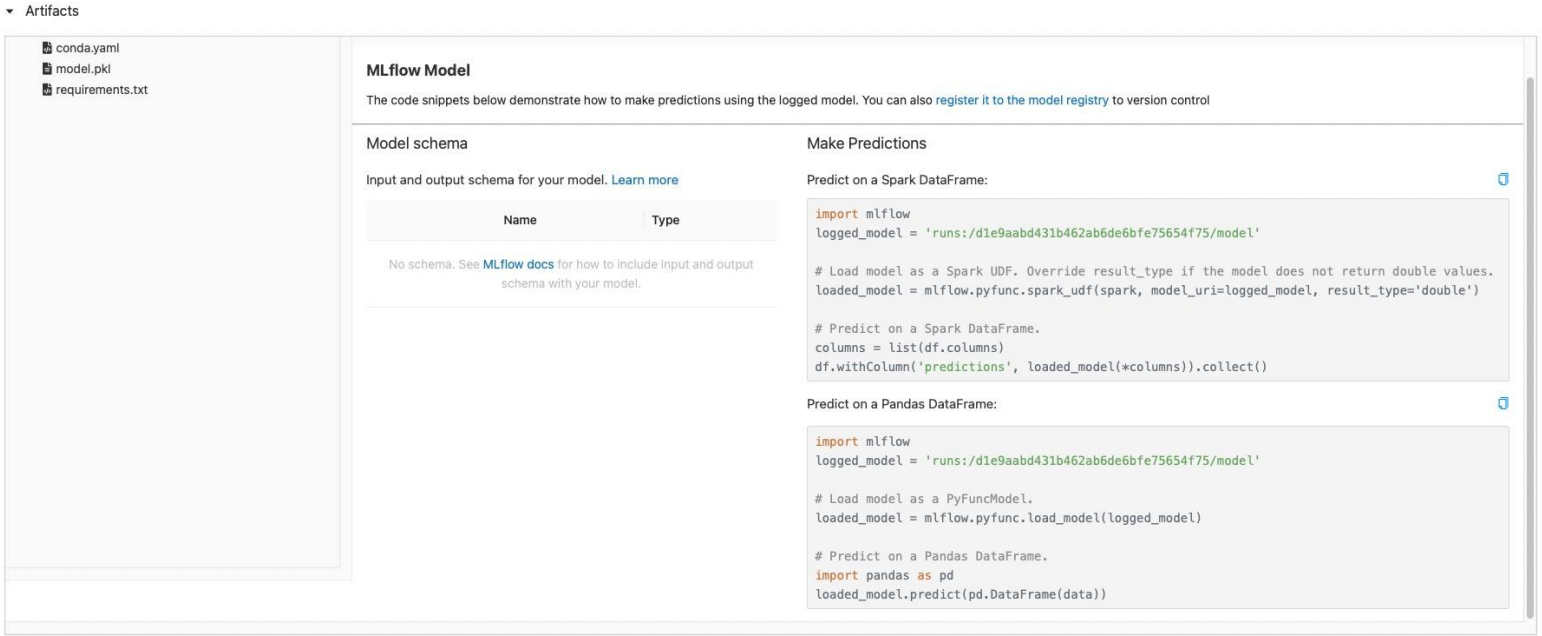
```
# Logging each hyper-parameters
for name in hyparams_list:
    mlflow.log_param(name, params[name])
```

Track experiments - after MLFlow

- For Deep Learning, the epoch performances can also be traced



Reproduce a model - after MLFlow



Next Class: Model Deployment