Applied Machine Learning for Business Analytics

Lecture 9: Model Evaluation in Machine Learning

Lecturer: Zhao Rui

Logistics

- For kaggle competition, make sure your team name is student number (starting with A)
- We will keep online learning for the rest four lectures
  - 51% of you selected online learning
  - Due to covid situation
- Appreciate if you keeps video on!

Agenda

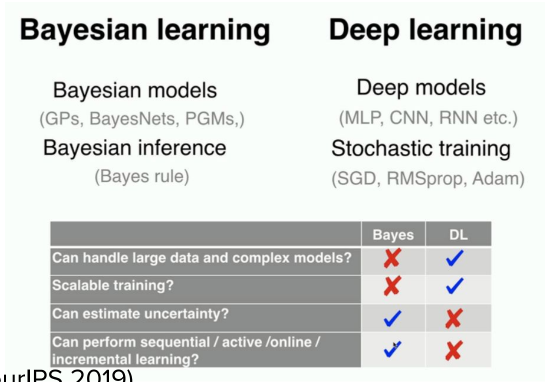
1. Baseline First
2. Model Evaluation
3. Experiment Tracking

1. Baseline First

Classical Machine Learning Algorithms

- Logistic regression
  - Very hard to beat baseline
- Naive Bayes
  - Suitable for high-dimensional data
- Tree-based models: random forest, bagging, boosting
  - XGBoost still one of the most popular winning algorithms on Kaggle
- K-nearest neighbor
  - Great for anomaly detection
- SVM
- ...

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 tc 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": 0.2184154175588652,
    "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.

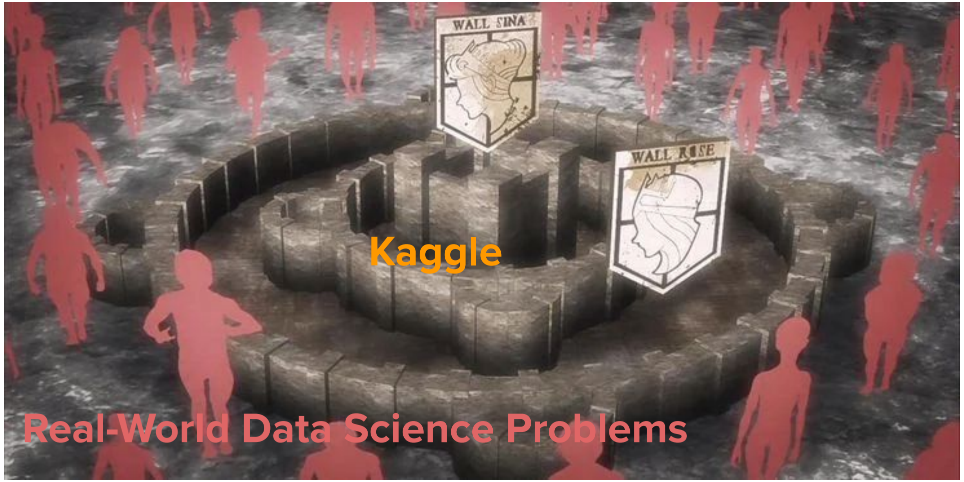
2. Model Evaluation

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

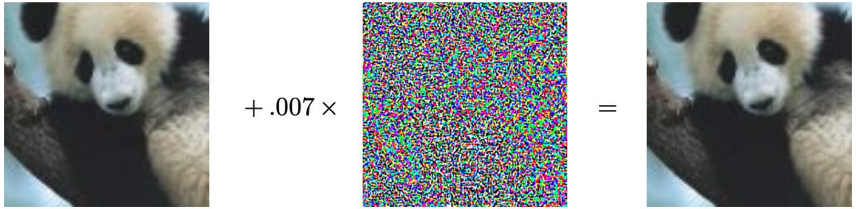
Check those FP/FN samples

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



$\boldsymbol{x}$ — "panda" 57.7% confidence

$\text{sign}(\nabla_{\boldsymbol{x}} J(\boldsymbol{\theta}, \boldsymbol{x}, y))$ — "nematode" 8.2% confidence

$\boldsymbol{x} + \epsilon\text{sign}(\nabla_{\boldsymbol{x}} J(\boldsymbol{\theta}, \boldsymbol{x}, y))$ — "gibbon" 99.3 % confidence

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

Slices can be classes

- We need to check the same fine-grained metrics per class
  - As a general rule, the classes with fewer samples will have lower performance
  - We need to identify the class of data to improve the overall model performances
  - Plot the # of training samples per class vs the test performance

Source: https://madewithml.com/courses/mlops/evaluation/

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

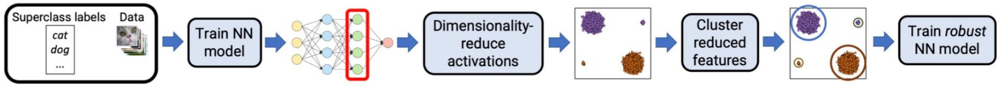
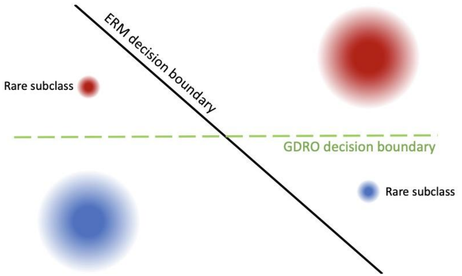


Figure 4: Schematic describing GEORGE. The inputs are the datapoints and superclass labels. First, a model is trained with ERM on the superclass classification task. The activations of the penultimate layer are then dimensionality-reduced, and clustering is applied to the resulting features to obtain 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)?

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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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- 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

Model calibration: Email Spam Detection

- In complex machine learning systems, models' prob. scores are used as inputs to other machine learning models.
  - Email spam detection
    - Model A predicts the importance of the email and feed the prob(important) as the feature to the model b to predict the spam
  - Do we need to calibrate model A?

Model calibration: Email Spam Detection

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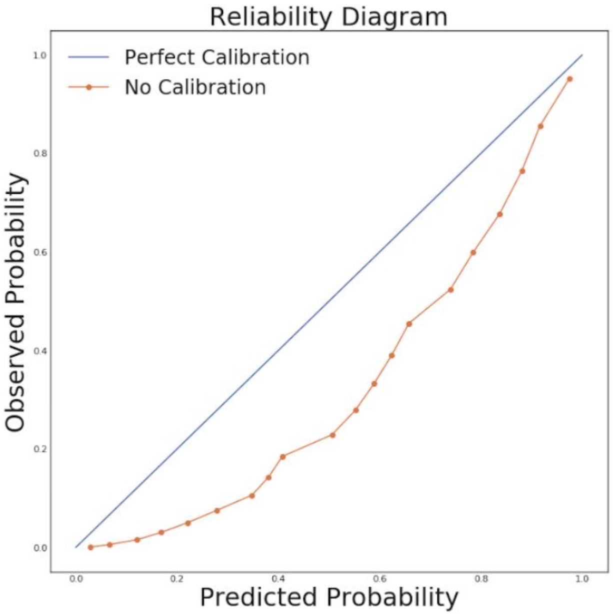
  - Email spam detection
    - Model A predicts the importance of the email and feed the prob(important) as the feature to the model b to predict the spam
  - Do we need to calibrate model A?
  - We need calibrated probabilities
    - If the model a is miscalibrated and starts assigning too high of prob. Score for emails being important, the model b will under-predict spam

Reliability Plot

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



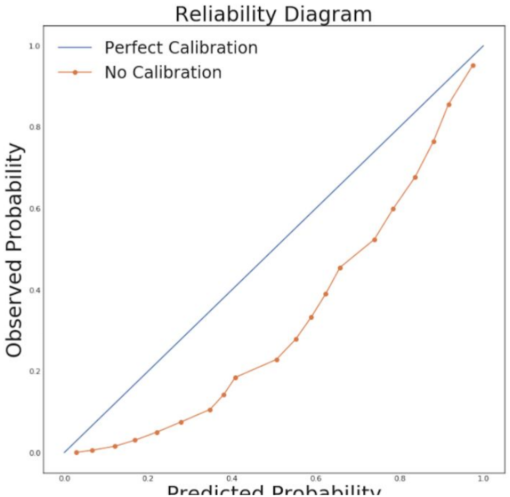
Tutorial:
https://www.youtube.com/watch?v=hWb-MIXKe-s

Reliability Plot

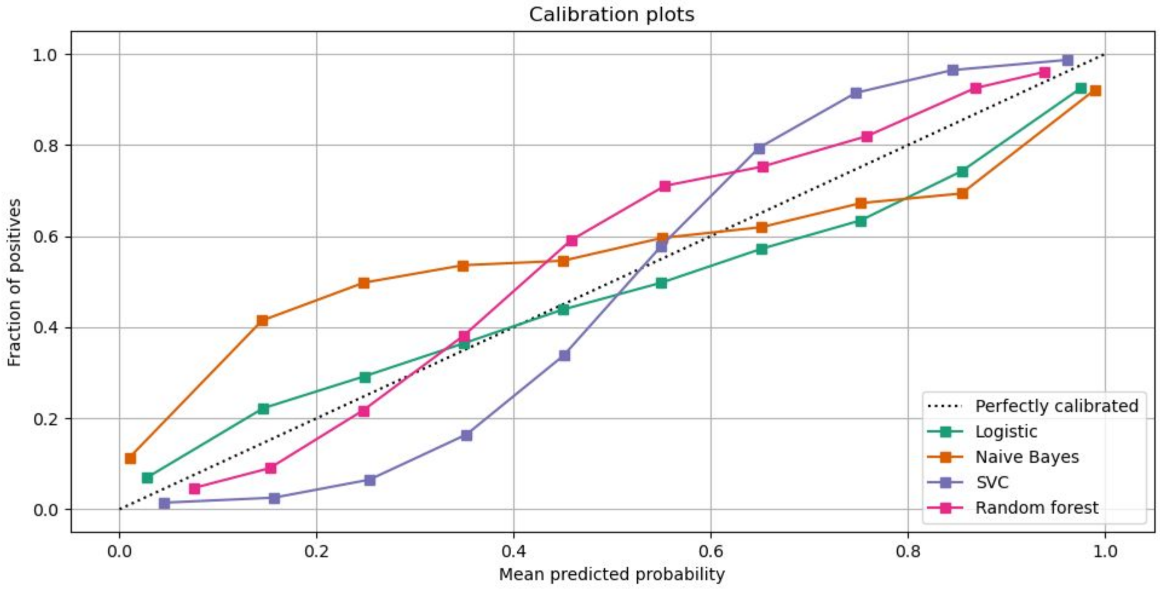
predicted_prob score	True label
0.1	1
0.1	0
0.1	1
0.1	0
0.1	0
0.2	
…	
0.8	0
0.9	1
0.9	0
0.9	1
0.9	1

Predicted Prob: 0.1 Observed Prob:?

Predicted Prob: 0.9 Observed Prob:?



Case



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

Which machine learning model is the best calibrated one?

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

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
    - 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
- 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

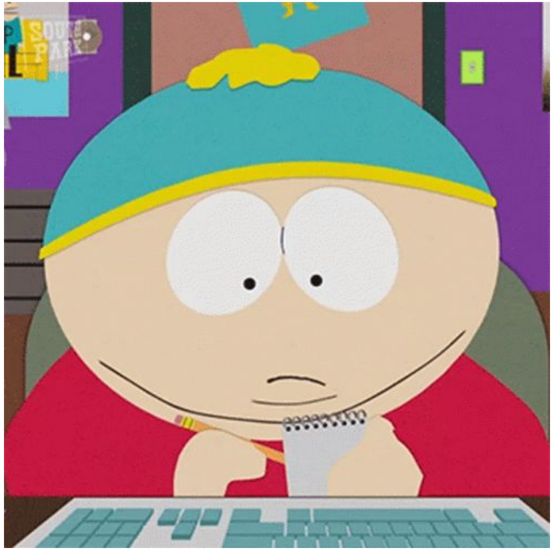
Category	Method	Datasets				
		MR	Subj	CR	MPQA	TREC
Text Classification Models	NBSVM	79.4	93.2	81.8	86.3	-
	MNB	79.0	93.6	80.0	86.3	-
	G-Dropout	79.0	93.4	82.1	86.1	-
	F-Dropout	79.1	93.6	81.9	86.3	-
CNN and its Variants	CNN	81.3	93.5	83.9	89.4	93.0
	CNN_{600}	79.3	92.0	81.6	87.5	91.9
	DCNN	-	-	-	-	93.0
	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
```



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

Track Experiments - After MLFlow

Description Edit

Refresh | Compare | Delete | Download CSV | Start Time | All time

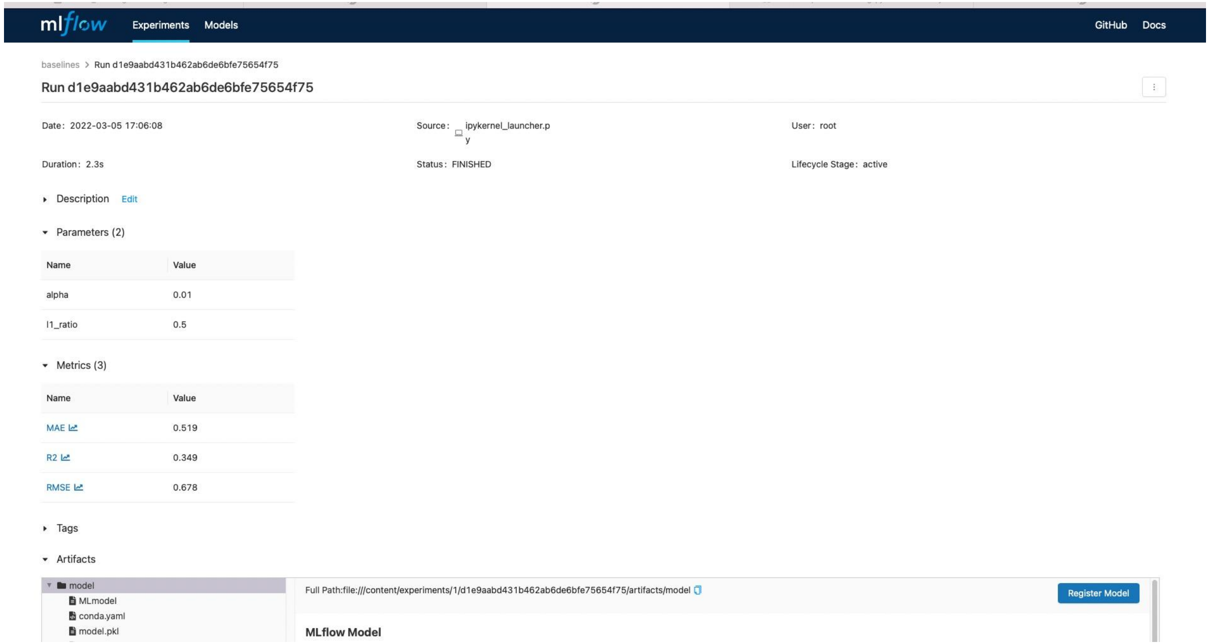
Columns | Only show differences | metrics.rmse < 1 and params.model = "tree" | Search | Filter | Clear

Showing 3 matching runs

								Metrics			Parameters	
	Start Time	Duration	Run Name	User	Source	Version	Models	MAE	R2	RMSE	alpha	l1_ratio
	36 minutes ago	2.3s	-	root	ipykernel_	-	sklearn	0.519	0.349	0.678	0.01	0.5
	36 minutes ago	2.2s	-	root	ipykernel_	-	sklearn	0.567	0.232	0.736	0.5	0.02
	36 minutes ago	2.4s	-	root	ipykernel_	-	sklearn	0.675	0.017	0.833	1.5	0.9

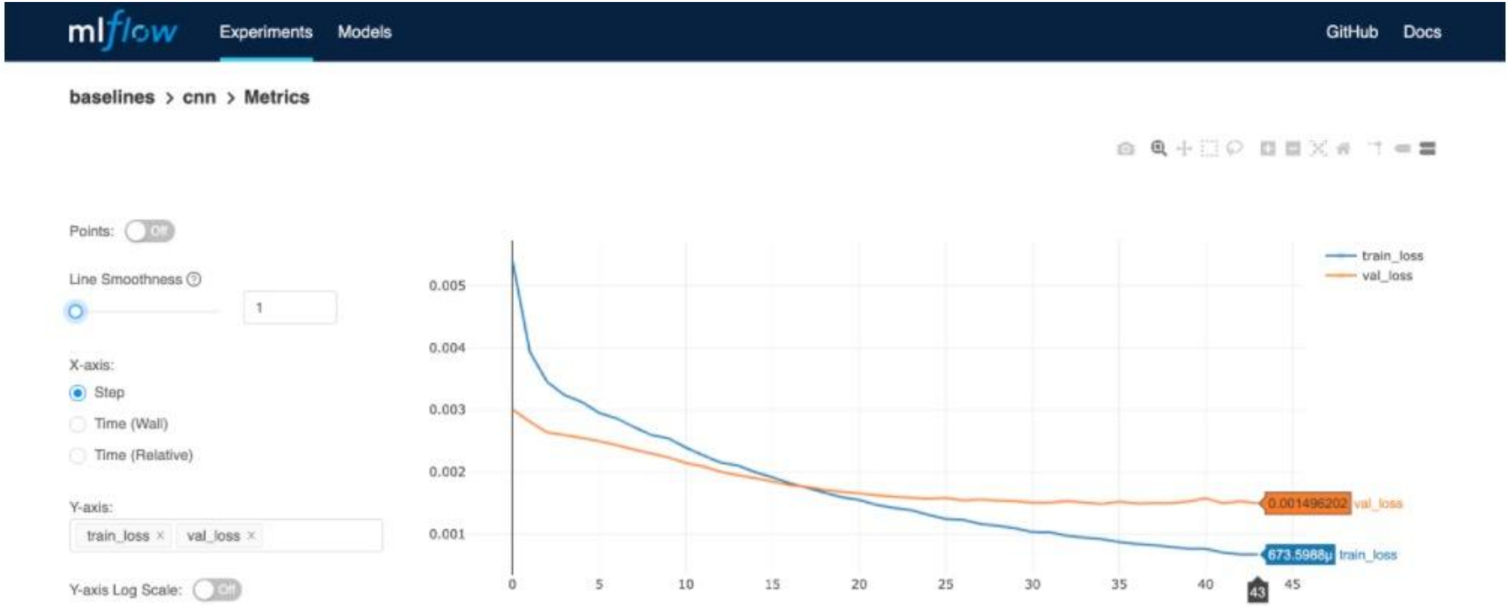
Load more

Track Experiments - After MLFlow



Track Experiments - After MLFlow

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



Reproduce A Model - After MLFlow

▾ Artifacts

- conda.yaml
- model.pkl
- requirements.txt

MLflow Model

The code snippets below demonstrate how to make predictions using the logged model. You can also register it to the model registry to version control

Model schema

Input and output schema for your model. Learn more

Name	Type

No schema. See MLflow docs for how to include input and output schema with your model.

Make Predictions

Predict on a Spark DataFrame:

```
import mlflow
logged_model = 'runs:/d1e9aabd431b462ab6de6bfe75654f75/model'

# Load model as a Spark UDF. Override result_type if the model does not return double values.
loaded_model = mlflow.pyfunc.spark_udf(spark, model_uri=logged_model, result_type='double')

# Predict on a Spark DataFrame.
columns = list(df.columns)
df.withColumn('predictions', loaded_model(*columns)).collect()
```

Predict on a Pandas DataFrame:

```
import mlflow
logged_model = 'runs:/d1e9aabd431b462ab6de6bfe75654f75/model'

# Load model as a PyFuncModel.
loaded_model = mlflow.pyfunc.load_model(logged_model)

# Predict on a Pandas DataFrame.
import pandas as pd
loaded_model.predict(pd.DataFrame(data))
```