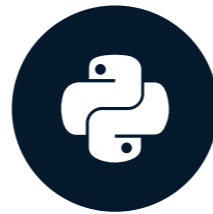


Feature engineering and selection

END-TO-END MACHINE LEARNING



Joshua Stapleton
Machine Learning Engineer

Feature engineering

Creating features

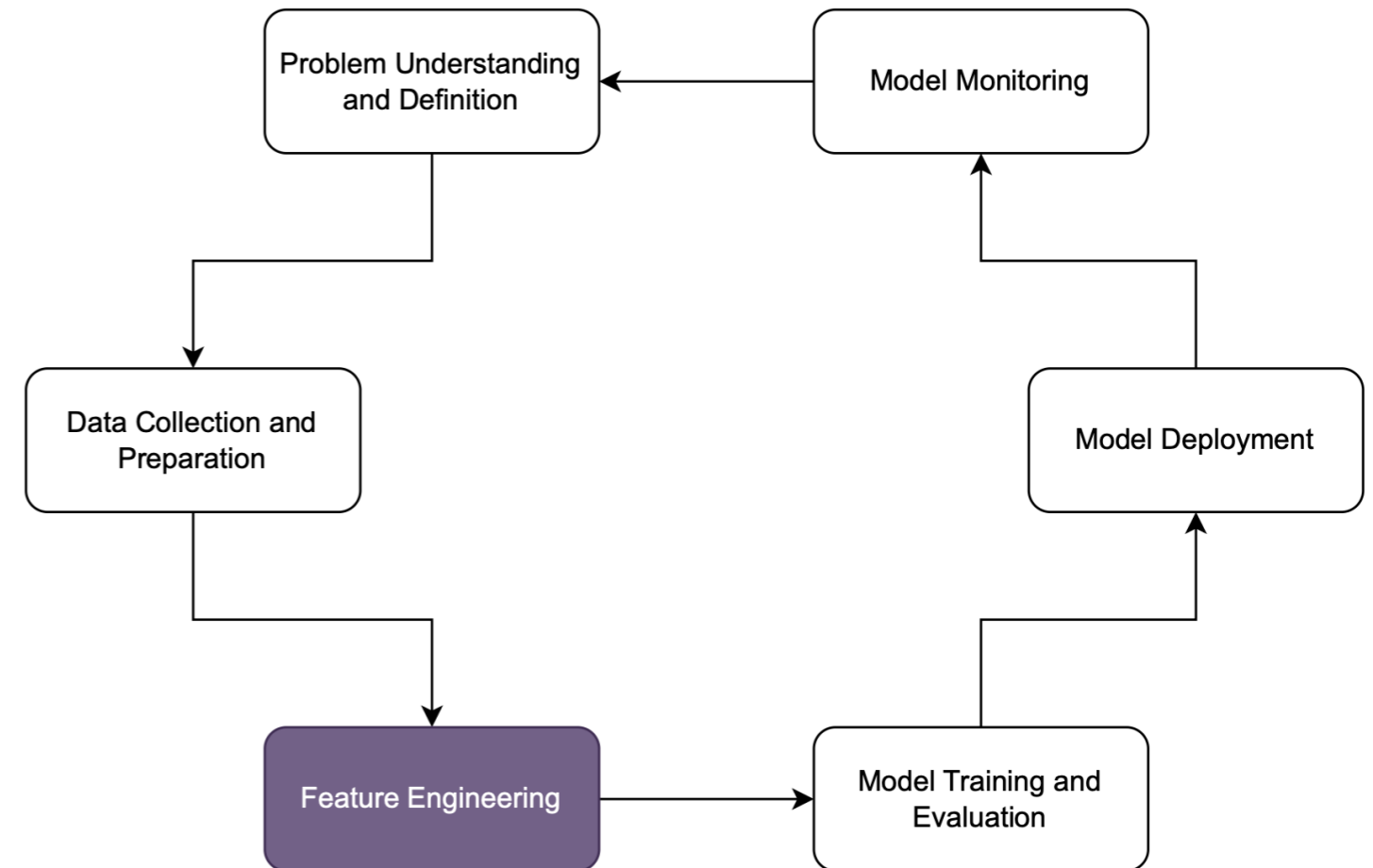
- Simplifies problem
- Improves model efficiency

Techniques

- Modify pre-existing features
- Design new features

Benefits

- Easier deployment, maintenance, training
- Interpretability gain



Normalization

- Scales numeric features to $[0, 1]$
- Helpful when features have different scales/ranges.

```
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import Normalizer

# Split the data
X_train, X_test = train_test_split(df, test_size=0.2, random_state=42)
# Create normalizer object, fit on training data, normalize, and transform test set
norm = Normalizer()
X_train_norm = norm.fit_transform(X_train)
X_test_norm = norm.transform(X_test)
```

Standardization

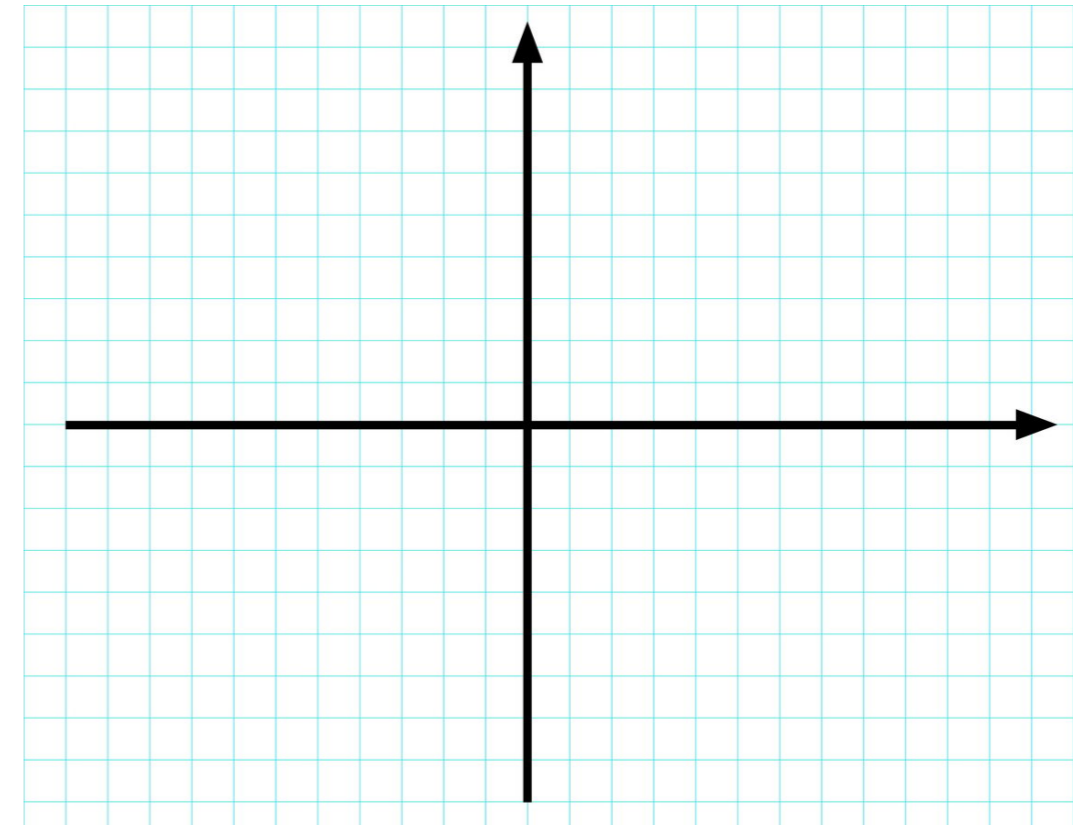
- Scales data to have mean = 0, variance = 1
- Beneficial for algorithms that assume similar mean and variance

```
from sklearn.preprocessing import StandardScaler

# Split the data
X_train, X_test = train_test_split(df, test_size=0.2, random_state=42)
# Create a scaler object and fit training data to standardize it
sc = StandardScaler()
X_train_stzd = sc.fit_transform(X_train)
# Only standardize the test data
X_test_stzd = sc.transform(X_test)
```

What constitutes a good feature?

- Use relevant features
- Weather on the day of patient appointment should have no bearing on diagnosis
- Use dissimilar (orthogonal) features
- Two features of age in months and age in years would not be helpful



sklearn.feature_selection

```
from sklearn.ensemble import RandomForestClassifier
from sklearn.feature_selection import SelectFromModel
from sklearn.model_selection import train_test_split

# Splitting data into train and test subsets first to avoid data leakage
X_train, X_test, y_train, y_test = train_test_split(
    heart_disease_df_X, heart_disease_df_y, test_size=0.2, random_state=42)
```

sklearn.feature_selection (cont.)

```
# Define and fit the random forest model
rf = RandomForestClassifier(n_jobs=-1, class_weight='balanced', max_depth=5)
rf.fit(X_train, y_train)

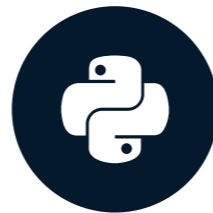
# Define and run feature selection
model = SelectFromModel(rf, prefit=True)
features_bool = model.get_support()
features = heart_disease_df.columns[features_bool]
```

Let's practice!

END-TO-END MACHINE LEARNING

Model training

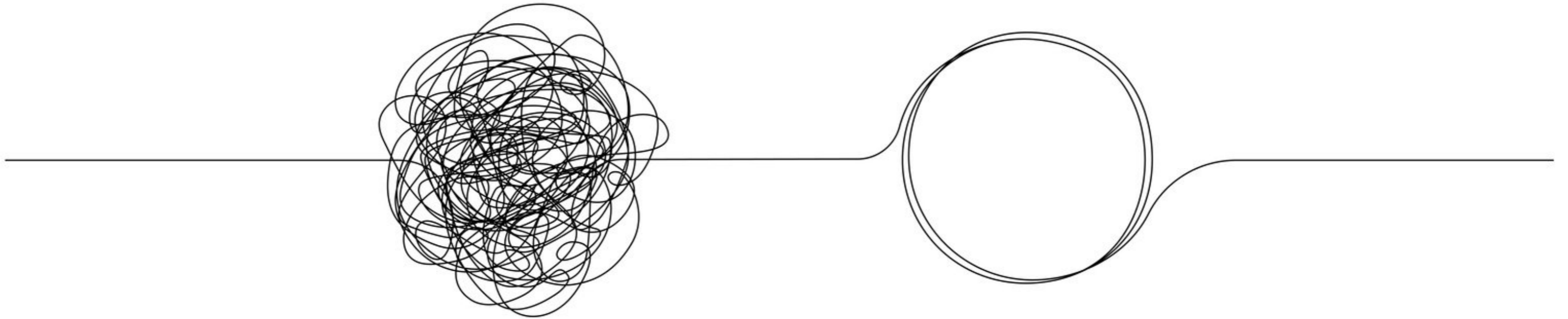
END-TO-END MACHINE LEARNING



Joshua Stapleton
Machine Learning Engineer

Occam's Razor

- Simplest satisfactory explanation is best
- Lean towards simple models when selecting



Modeling options

Logistic Regression

- Finds decision boundary between classes
- `sklearn.linear_model.LogisticRegression`

Support Vector Classifier

- Finds plane to separate classes
- `sklearn.svm.SVC`

Decision Tree

- Finds simple 'rules' to classify data
- `sklearn.tree.DecisionTreeClassifier`

Random Forest

- Combines multiple decision trees
- `sklearn.ensemble.RandomForestClassifier`

Other models

Deep learning models

- Neural Networks
- Convolutional Neural Networks
- Generative Pretrained Transformer (GPT)

K-Nearest Neighbors (KNN)

- Supervised learning algorithm

XGBoost

- Gradient boosted model
- <https://xgboost.readthedocs.io/en/stable/>

Training principles

Model:

- Uses cleaned and feature-handled dataset
- Learns patterns in training data
- Aims to predict target of heart disease diagnosis

Principles:

- Model must generalize to unseen data (outside of training set)
- 'Hold-out' some data to test model on after training completes.
- Split of training/testing is normally 70/30 or 80/20
- Can use `sklearn.model_selection.train_test_split`

Training a model

```
# Importing necessary libraries
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LogisticRegression

# Split the data into training and testing sets (80:20)
X_train, X_test, y_train, y_test = train_test_split(features, heart_disease_y,
                                                    test_size=0.2, random_state=42)

# Define the models
logistic_model = LogisticRegression(max_iter=200)

# Train the model
logistic_model.fit(X_train, y_train)
```

Getting model predictions

```
# Jane Doe's health data, for example: [age, cholesterol level, blood pressure, etc.]
jane_doe_data = [45, 230, 120, ...]

# Reshape the data to 2D, because scikit-learn expects a 2D array-like input
jane_doe_data = jane_doe_data.reshape(1, -1)

# Use the model to predict Jane's heart disease diagnosis probabilities
jane_doe_probabilities = logistic_model.predict_proba(jane_doe_data)
jane_doe_prediction = logistic_model.predict(jane_doe_data)
```

Getting model predictions (cont.)

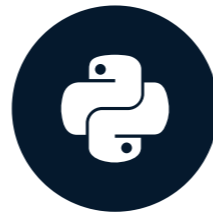
```
# Print the probabilities
print(f"Jane Doe's predicted probabilities: {jane_doe_probabilities[0]}")
print(f"Jane Doe's predicted health condition: {jane_doe_prediction[0]}")
```

```
Jane Doe's predicted health condition probabilities: [0.2 0.8]
Jane Doe's predicted health condition: 1
```

Let's practice!
END-TO-END MACHINE LEARNING

Logging experiments on MLFlow

END-TO-END MACHINE LEARNING



Joshua Stapleton
Machine Learning Engineer

MLFlow

Without MLflow...

- Many untracked, disorganized experiment runs
- Dissimilar, or incomparable runs
- Unreproducible, lost runs

With MLflow...

- Tracked, organized experiment runs
- Comparison between standardized runs
- Reproducible runs
- Share, deploy models

Creating experiments

`mlflow.set_experiment()`

- Sets experiment name
- Provides workspace for experiment runs

Usage:

```
import mlflow

# Set an experiment name, which is a workspace for your runs
mlflow.set_experiment("Heart Disease Classification")
```

Running experiments

```
# Start a new run in this experiment
with mlflow.start_run():
    # Train a model, get the prediction accuracy
    logistic_model = LogisticRegression()
    # Log parameters, eg:
    mlflow.log_param("n_estimators", logistic_model.n_estimators)
    # Log metrics (accuracy in this case)
    mlflow.log_metric("accuracy", logistic_model.accuracy)
    # Print out metrics
    print("Model accuracy: %.3f" % accuracy)
```

```
Model accuracy: 0.96
```

Retrieving experiments

```
mlflow.get_run(run_id)
```

- Metadata for specific run

```
mlflow.search_runs()
```

- Returns DataFrame of metrics for multiple runs

Usage:

```
# Fetch the run data and print params
run_data = mlflow.get_run(run_id)
print(run_data.data.params)
print(run_data.data.metrics)
```

```
# Search all runs in experiment
exp_id = run_data.info.experiment_id
runs_df = mlflow.search_runs(exp_id)
```

```
{'epochs': '20', 'accuracy': 0.95}
```

MLFlow UI

mlflow2.2.2

Experiments

Models

GitHub

Docs

Experiments

Search Experiments

✓

Default

Default

Provide Feedback

Share

Experiment ID: 0

file:///Users/john.smith/Documents/src/mlflow/examples/quickstart/mlruns/0

> Description

Edit

Table view

Chart view

Q metrics.rmse < 1 and params.model = "tree"

Sort: Created

Refresh

Columns

Time created: All time

State: Active

<input type="checkbox"/>	<input type="checkbox"/>	Run Name	Created	Duration	Source	Models
<input type="checkbox"/>	<input type="checkbox"/>	<div><div></div>marvelous-chimp-845</div>	<div><div>✓</div>54 seconds ago</div>	29ms	<div><div></div>mlflow_t...</div>	-

mlflow2.2.2

Experiments

Models

GitHub

Docs

Default

>

brawny-toad-167

Run ID: 7f48fe2149e64b29824ae85bf52a34cd

Date: 2023-04-24 10:17:30

Source:

train6.py

Git Commit: 72f7f0455fb5a2102c19905ec424ebad1e49b572

User: lobrien

Status: UNFINISHED

Lifecycle Stage: active

> Description

Edit

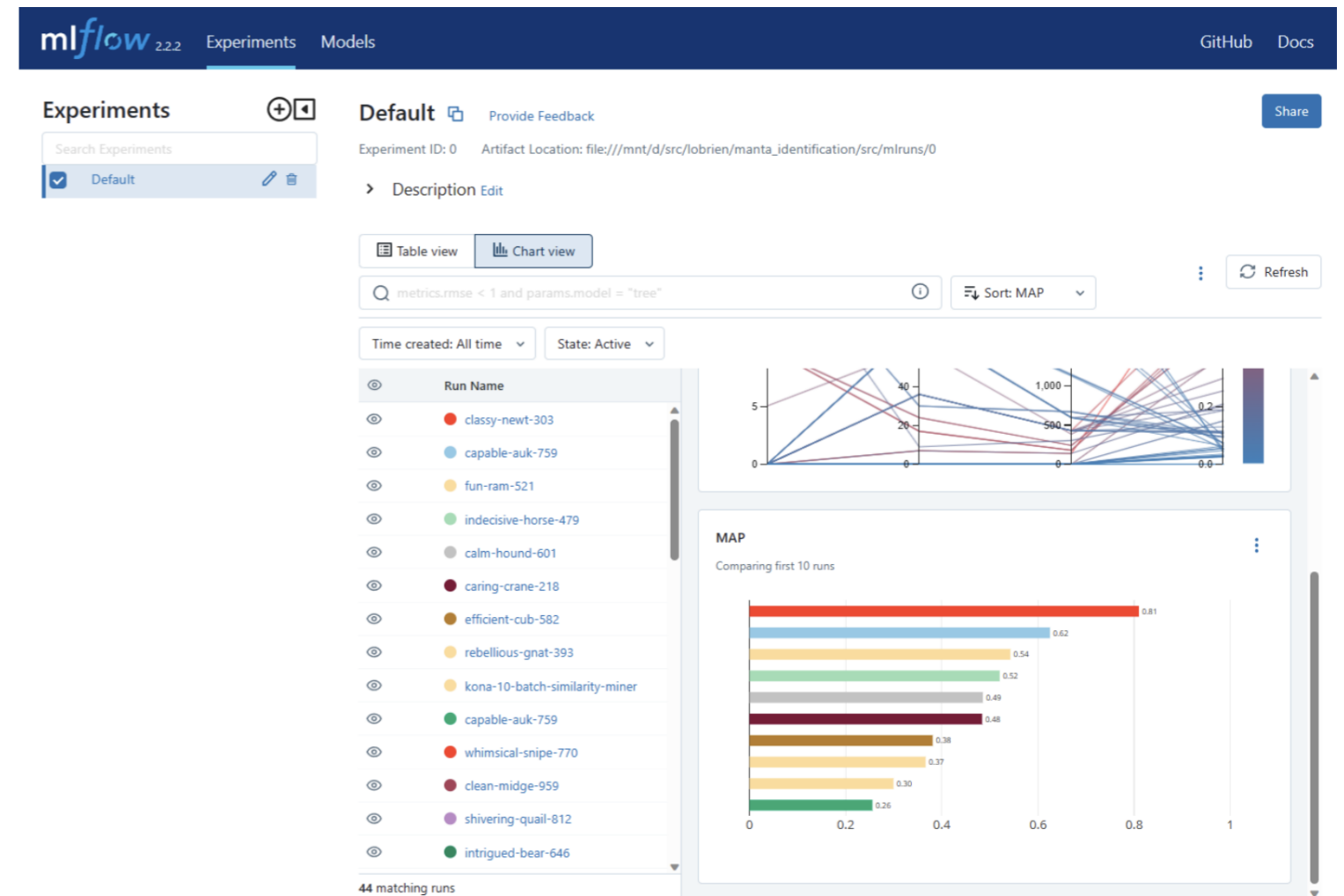
> Parameters (24)

> Metrics (9)

> Tags

> Artifacts

MLFlow UI (cont.)



MLflow resources

- Introduction to MLflow

INTERACTIVE COURSE

Introduction to MLflow

Start Course

Bookmark

4 hours

16 Videos

51 Exercises

413 Participants

3,750 XP

Course Description

Managing the end-to-end lifecycle of a Machine Learning application can be a daunting task for data scientists, engineers, and developers. Machine Learning applications are complex and have a proven track record of being difficult to track, hard to reproduce, and problematic to deploy. In this course, you will learn what MLflow is and how it attempts to simplify the difficulties of the Machine Learning lifecycle such as tracking, reproducibility, and deployment. After learning MLflow, you will have a better understanding of how to overcome the complexities of building Machine Learning applications and how to navigate different stages of the Machine Learning lifecycle. Throughout the course, you will deep dive into the four major components that make up the MLflow platform. You will explore how to track models, metrics, and...

[Read More](#)

1 Introduction to MLflow

0%

In this Chapter, you will be introduced to MLflow and how it aims to assist with some difficulties of the Machine Learning lifecycle. You will be introduced to the four main concepts that make up MLflow with a main focus on MLflow Tracking. You will learn to create experiments and runs as well as how to track metrics, parameters, and artifacts. Finally, you will search MLflow programmatically to find experiment runs that fit certain criteria.

DATASETS


50_Startups

Student_Study_Hour

Salary_predict

Insurance

Explore datasets




Weston Bassler


Senior MLOps Engineer


Former DevOps turned MLOps. I currently work at


- MLflow's official website




An open source platform for the machine learning lifecycle


WORKS WITH ANY ML LIBRARY, LANGUAGE & EXISTING CODE


RUNS THE SAME WAY IN ANY CLOUD


DESIGNED TO SCALE FROM 1 USER TO LARGE ORGS


SCALES TO BIG DATA WITH APACHE SPARK™

Latest News

MLflow 2.5.0 released!
(17 Jul 2023)


MLflow 2.4.0 released!
(06 Jun 2023)

MLflow 2.3.2 released!
(12 May 2023)

MLflow 2.3.1 released!
(28 Apr 2023)

MLflow 2.3.0 released!
(18 Apr 2023)

[News Archive](#)

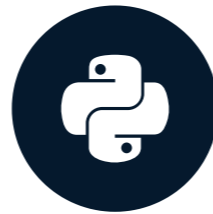
 datacamp

END-TO-END MACHINE LEARNING

Let's practice!
END-TO-END MACHINE LEARNING

Model evaluation and visualization

END-TO-END MACHINE LEARNING



Joshua Stapleton
Machine Learning Engineer

Accuracy

- Correct accuracy metrics are vital to robust model evaluation
- Easy to misinterpret or obscure results

Standard accuracy:

- Standard accuracy = num correct answers / num answers
- Standard accuracy can be unhelpful

Example:

```
# achieves ~99% accuracy for imbalanced dataset of 99 positive and 1 negative
for patient_datapoint in heart_disease_dataset:
    model.prediction(patient_datapoint) = 'positive'
```

Confusion matrix

True positives (TP)

- Model prediction = actual classification = positive
- The model predicted heart disease, the patient had heart disease

False negatives (FN)

- Model prediction = negative, actual classification = positive
- The model predicted no heart disease, the patient had heart disease

False positives (FP)

- Model prediction = positive, actual classification = negative
- The model predicted heart disease, the patient did not have heart disease

True negatives (TN)

- Model prediction = actual classification = negative
- The model predicted no heart disease, the patient did not have heart disease

Balanced accuracy

- Better metric than plain accuracy for most binary classification models
- Provides weighted average across both classes
- $\text{Balanced accuracy} = (\text{TP} + \text{TN}) / 2$

```
from sklearn.metrics import balanced_accuracy_score

# Assume y_test is the true labels and y_pred are the predicted labels
y_pred = model.predict(X_test)
bal_accuracy = balanced_accuracy_score(y_test, y_pred)
print(f"Balanced Accuracy: {bal_accuracy:.2f}")
```

Balanced Accuracy: 0.85

Confusion matrix usage

	Actual: Heart disease	Actual: No heart disease
Predicted: Heart disease	TP: 20	FP: 5
Predicted: No heart disease	FN: 3	TN: 24

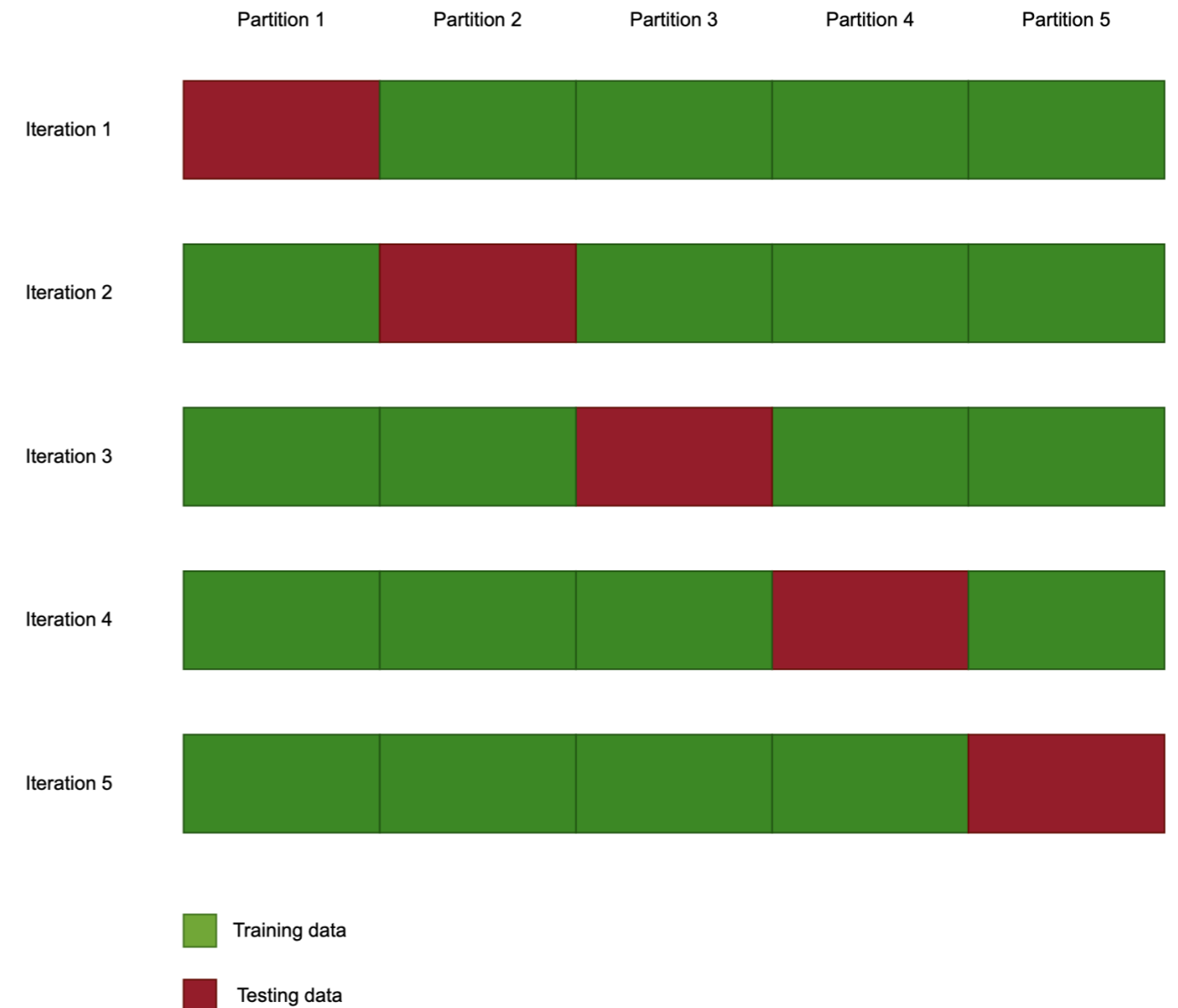
Cross validation

Cross-validation

- Resampling procedure
- Ensures robustness of results

k-fold cross-validation

- Param 'k' = number of splits for dataset
- Resample new train/test split for each modeling run



Cross validation usage

- Straightforward implementation of k-fold cross validation using sklearn
- Model-agnostic scoring

Usage:

```
from sklearn.model_selection import cross_val_score, KFold

# split the data into 10 equal parts
kfold = KFold(n_splits=5, shuffle=True, random_state=42)

# get the cross validation accuracy for a given model
cv_results = cross_val_score(model, heart_disease_X,
                              heart_disease_y, cv=kfold, scoring='balanced_accuracy')
```

Hyperparameter tuning

Hyperparameter:

- Global model parameter (doesn't change during training)
- Adjust to improve model performance

```
# Hyperparameters to test
C_values = [0.001, 0.01, 0.1, 1, 10, 100, 1000]

# Manually iterate over the hyperparameters
for C in C_values:
    model = LogisticRegression(max_iter=200, C=C)
    model.fit(X_train, y_train)
    accuracy = cross_val_score(model, X, y, cv=kfold, scoring='balanced_accuracy')
    print(f"C = {C}: Bal Acc: {accuracy.mean():.4f} (+/- {accuracy.std():.4f})")
```

Hyperparameter tuning example

Example output for hyperparameter tuning:

```
C = 0.001: Bal Acc: 0.6200 (+/- 0.0215)
C = 0.01: Bal Acc: 0.7325 (+/- 0.0234)
C = 0.1: Bal Acc: 0.7923 (+/- 0.0202)
C = 1: Bal Acc: 0.8050 (+/- 0.0191)
C = 10: Bal Acc: 0.8034 (+/- 0.0185)
C = 100: Bal Acc: 0.8021 (+/- 0.0187)
C = 1000: Bal Acc: 0.8017 (+/- 0.0188)
```

Let's practice!
END-TO-END MACHINE LEARNING