Feature engineering and selection

END-TO-END MACHINE LEARNING

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Feature engineering

Creating features

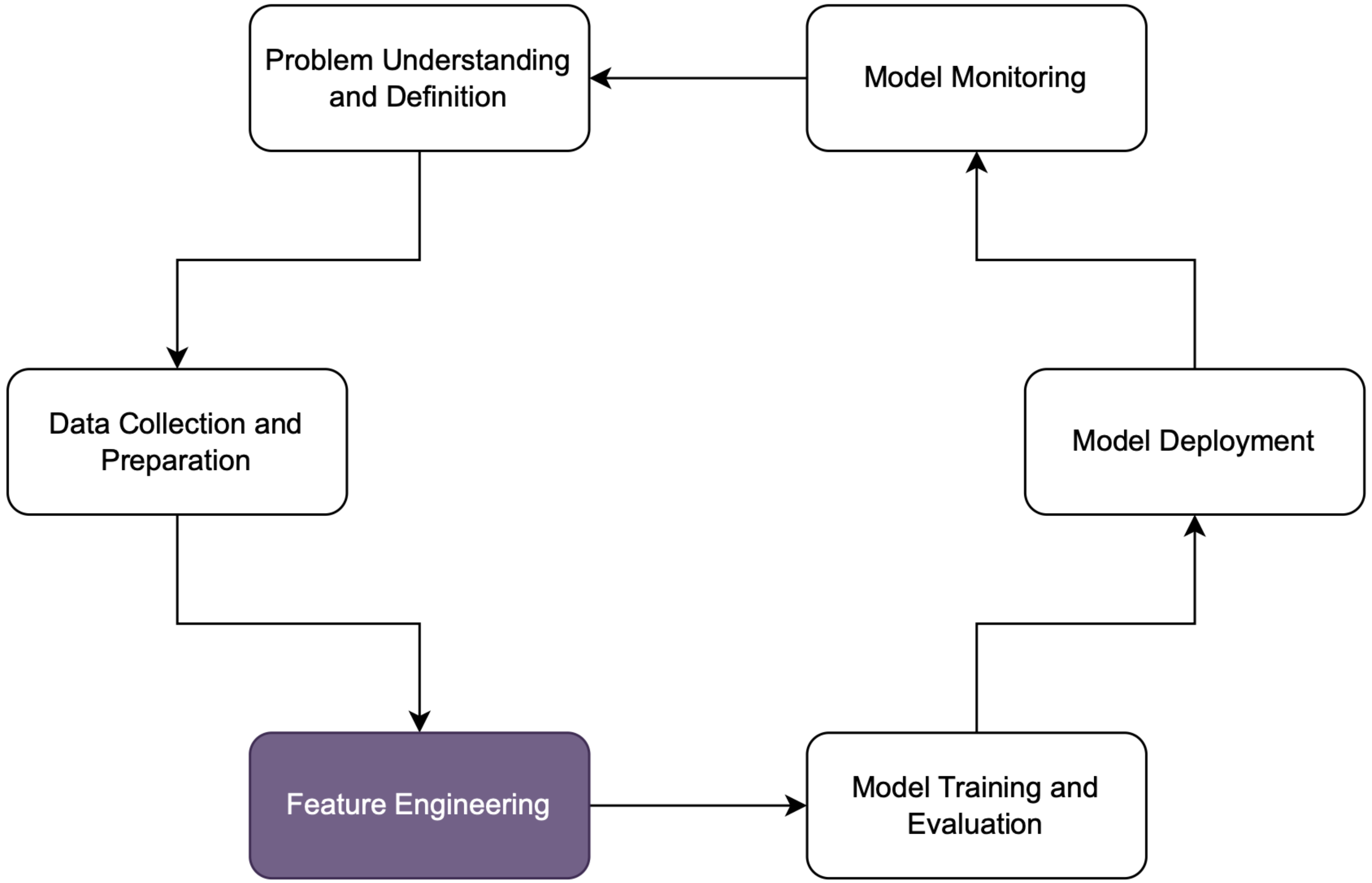
- Simplifies problem
- Improves model efficiency

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)
# Createnormalizer 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

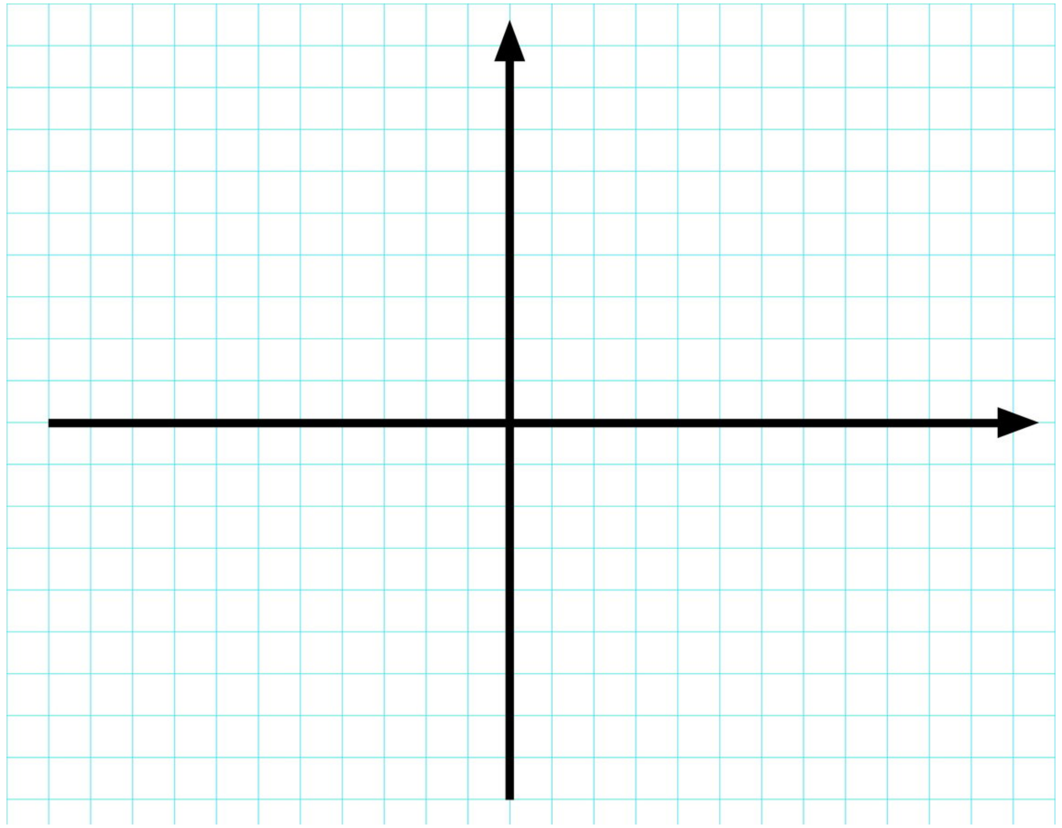
```
from sklearn.preprocessing import StandardScaler


# 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

```python
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!

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Model training

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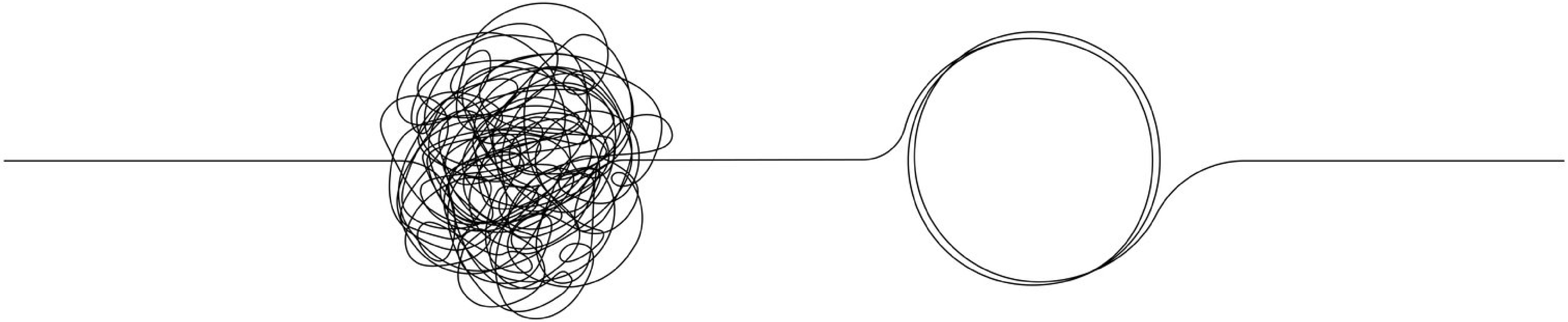
Occam's Razor

- 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.)

```python
# 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!

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Logging experiments on MLFlow

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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

```python
# 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

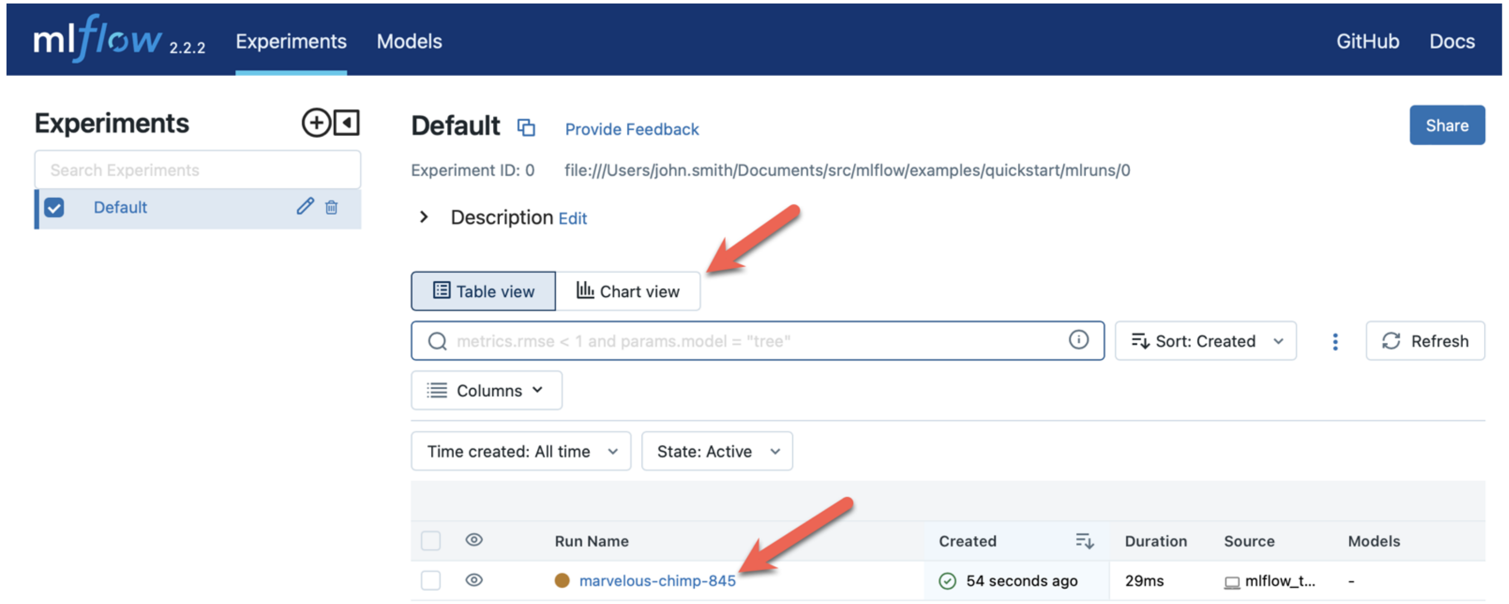
Usage:

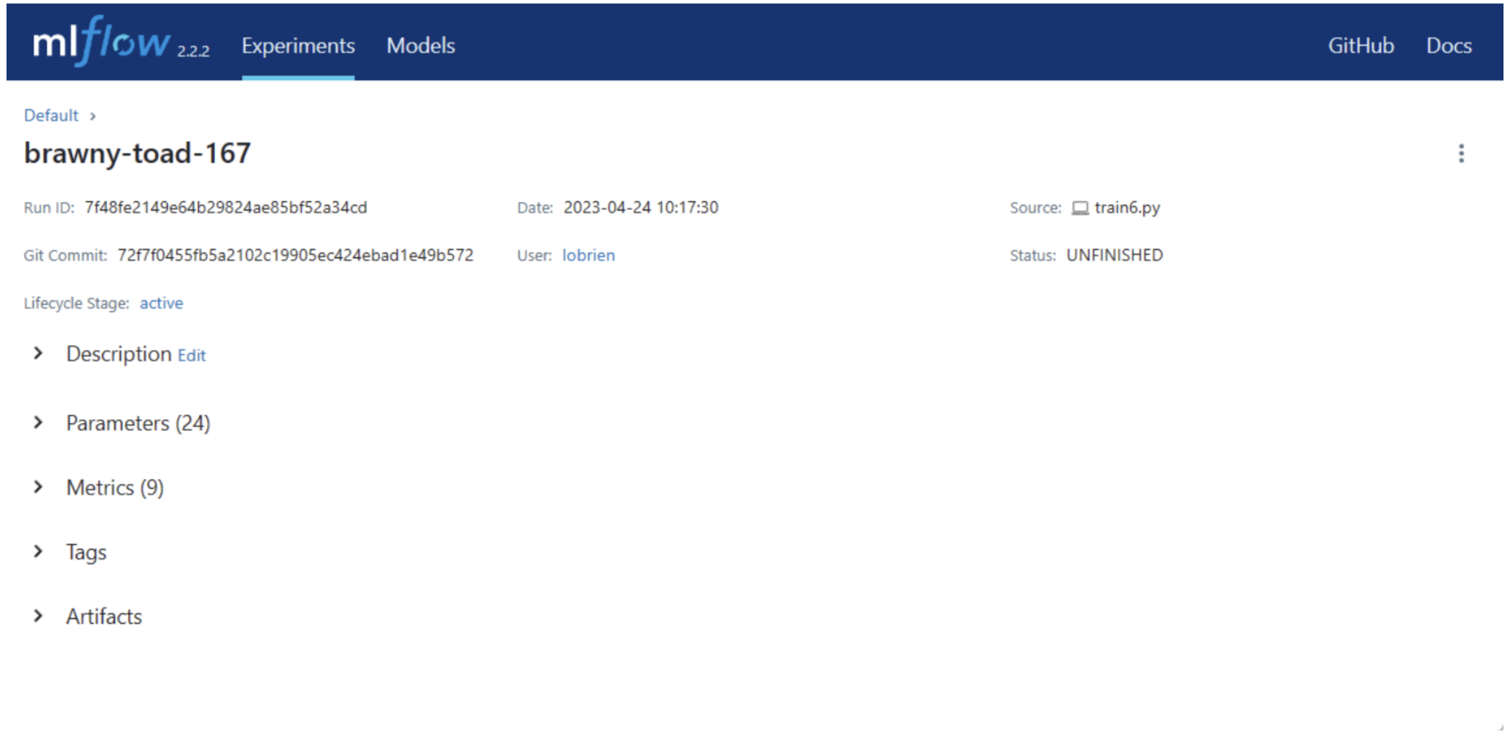
```
# Fetch the run data and print params
run_data = mlflow.get_run(run_id)
print(run_data.data.params)
print(run_data.data.metrics)

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

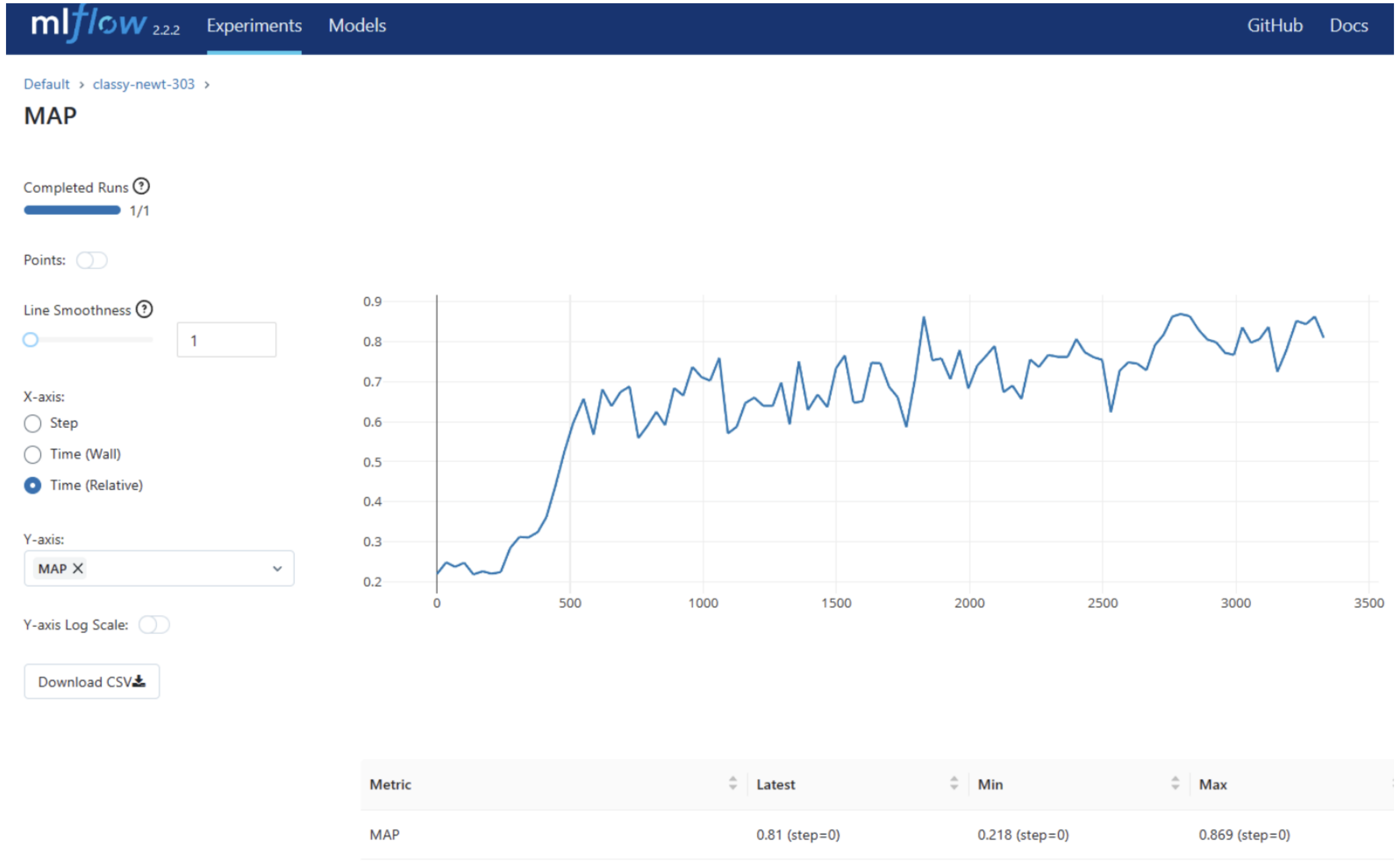
```
{'epochs': '20', 'accuracy': 0.95}
```

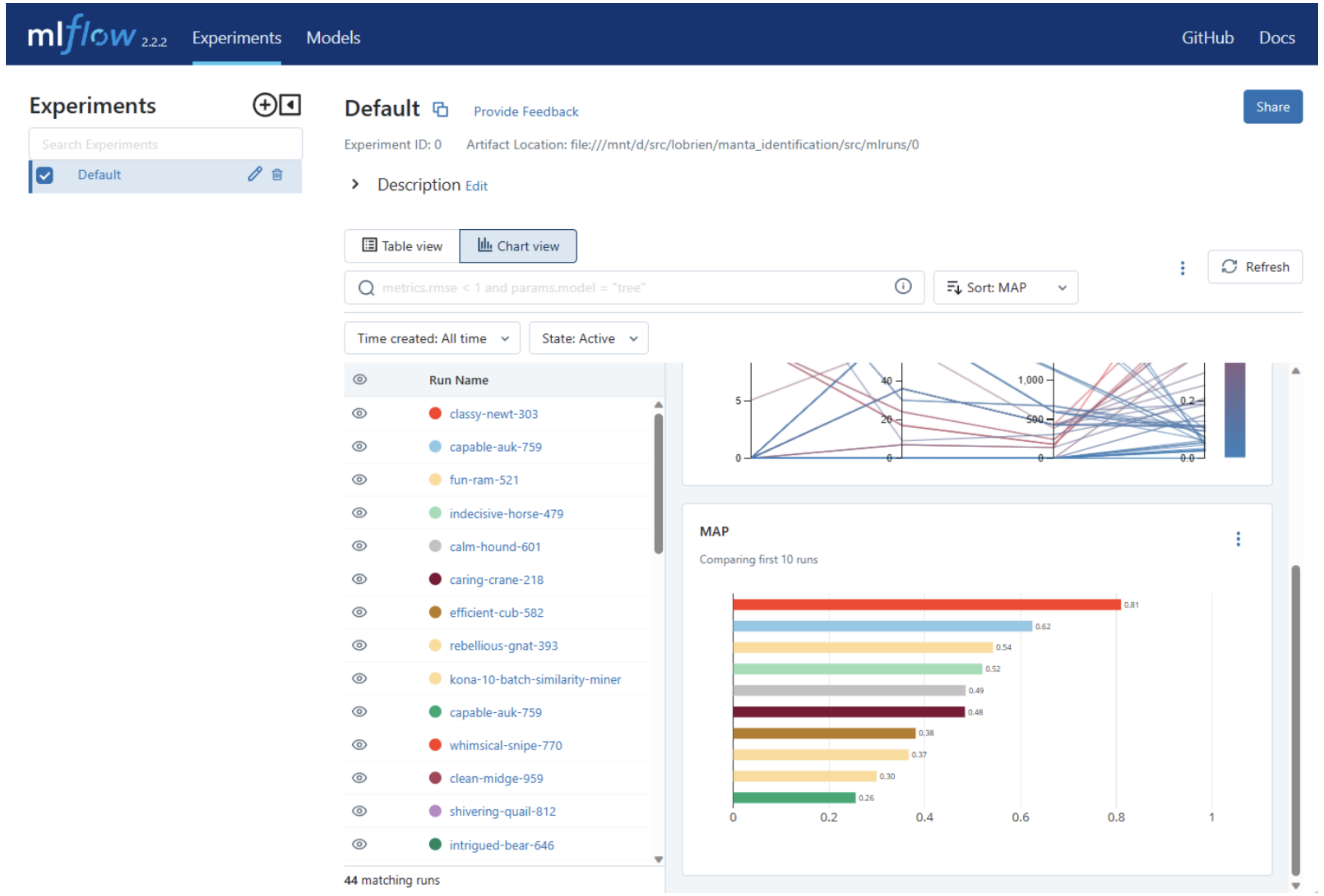
MLFlow UI


mlflow 2.2.2
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
metrics.rmse < 1 and params.model = "tree"
Sort: Created
Refresh
Columns
Time created: All time
State: Active
Run Name
Created
Duration
Source
Models
marvelous-chimp-845
54 seconds ago
29ms
mlflow_t...
-


mlflow 2.2.2
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

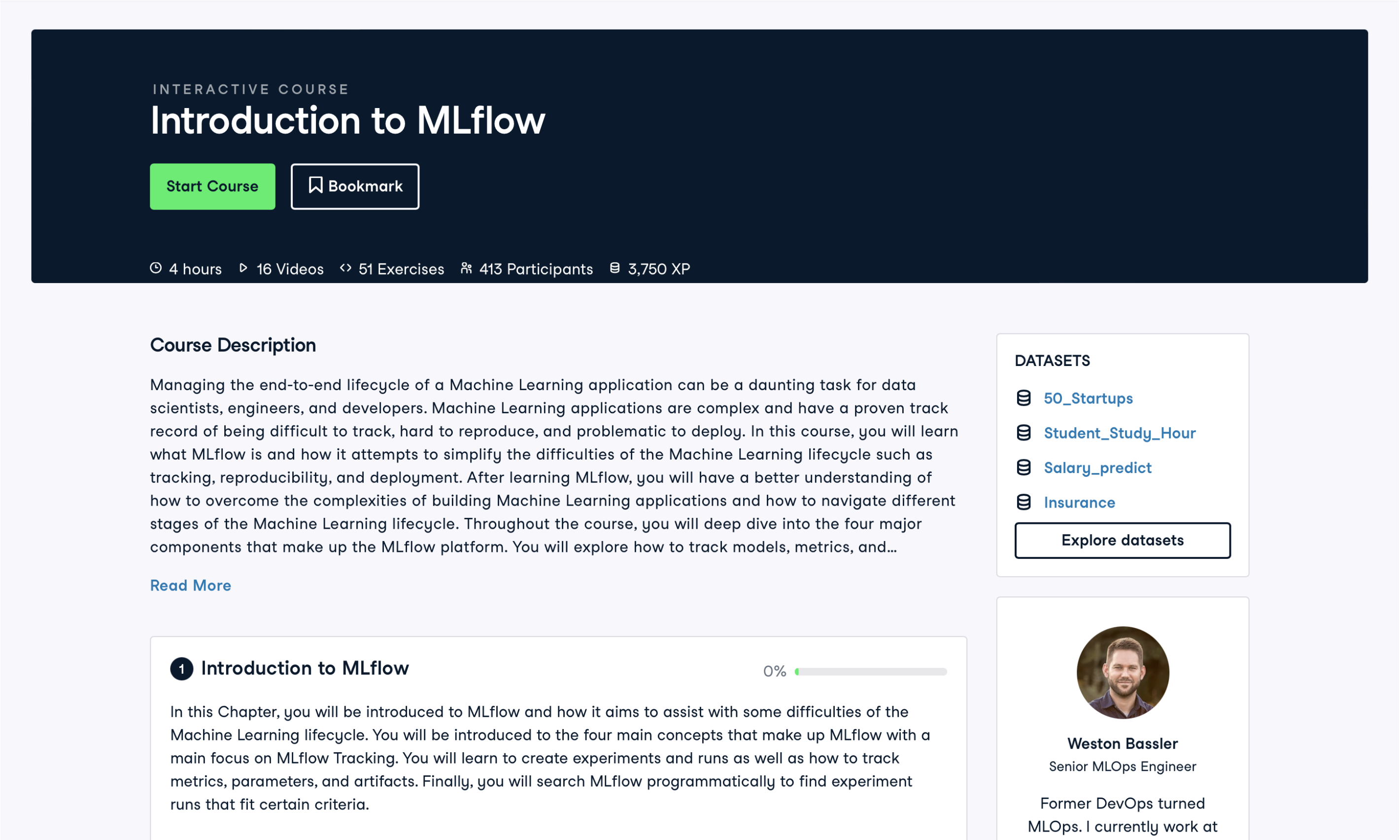
MLFlow UI (cont.)



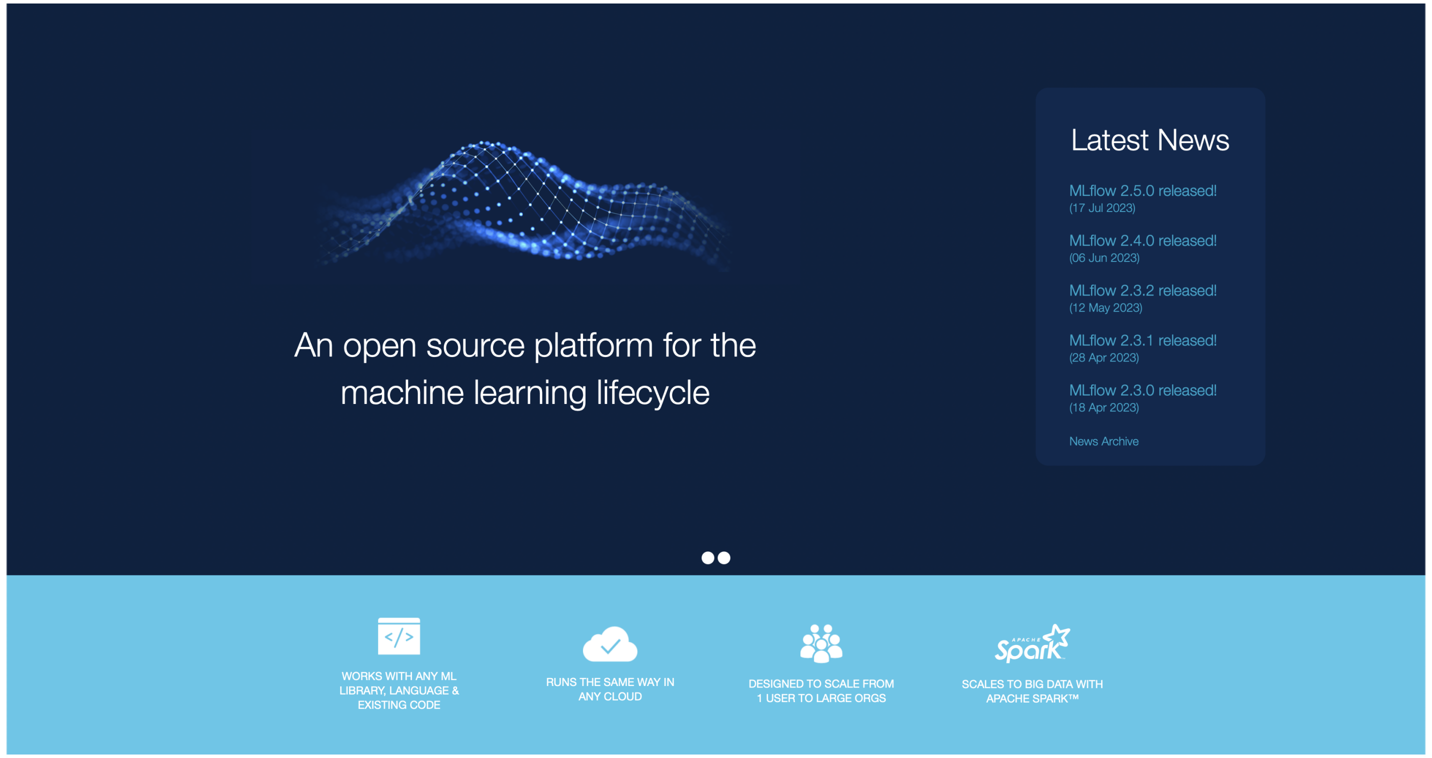


MLflow resources

- Introduction to MLflow



- MLflow's official website



Let's practice!

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Model evaluation and visualization

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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 positives (FP)

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

False negatives (FN)

- Model prediction = negative, actual classification = positive
- The model predicted no heart disease, the patient had 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
- Balanced accuracy = (TP + 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

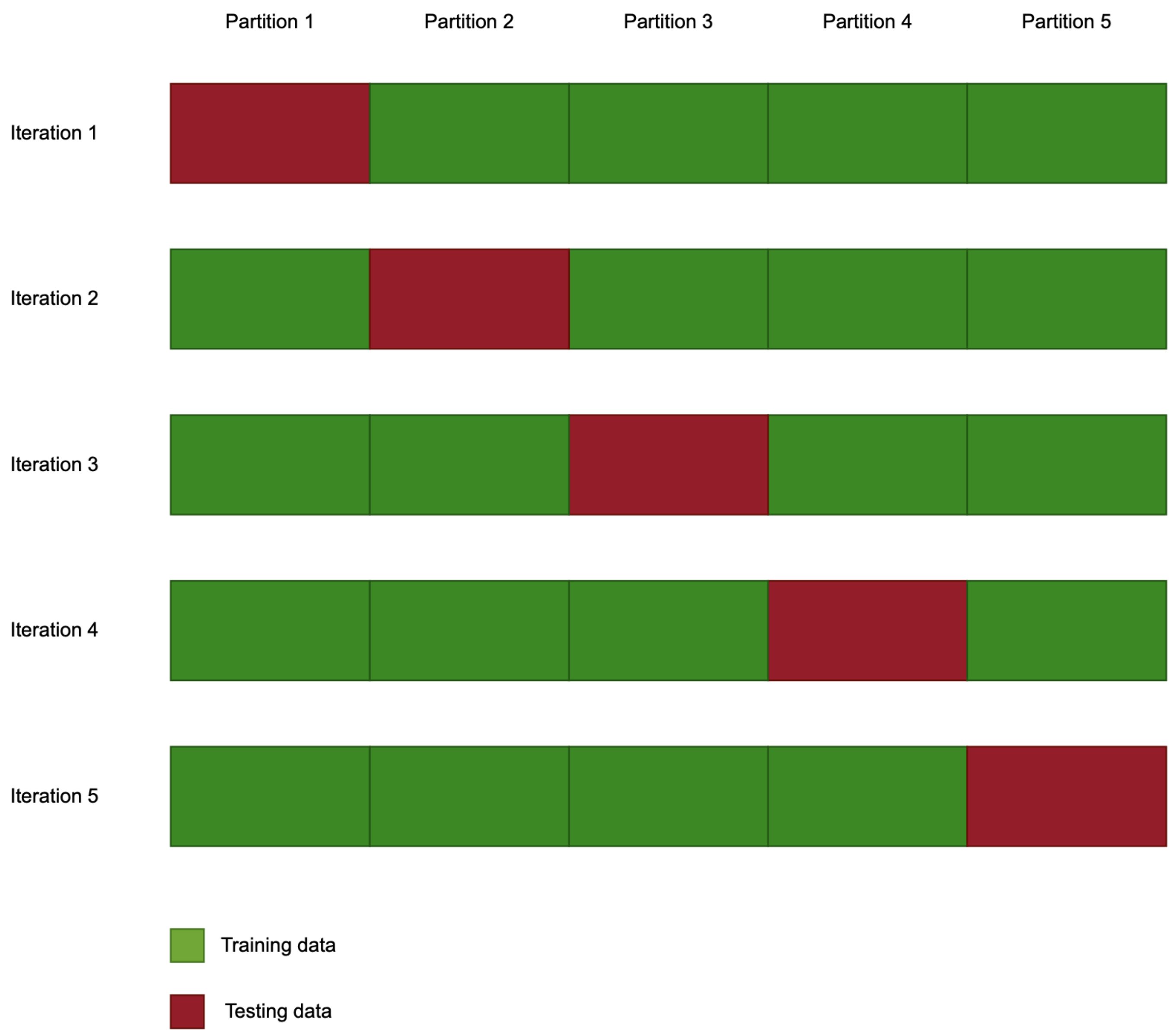
Cross validation

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!

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