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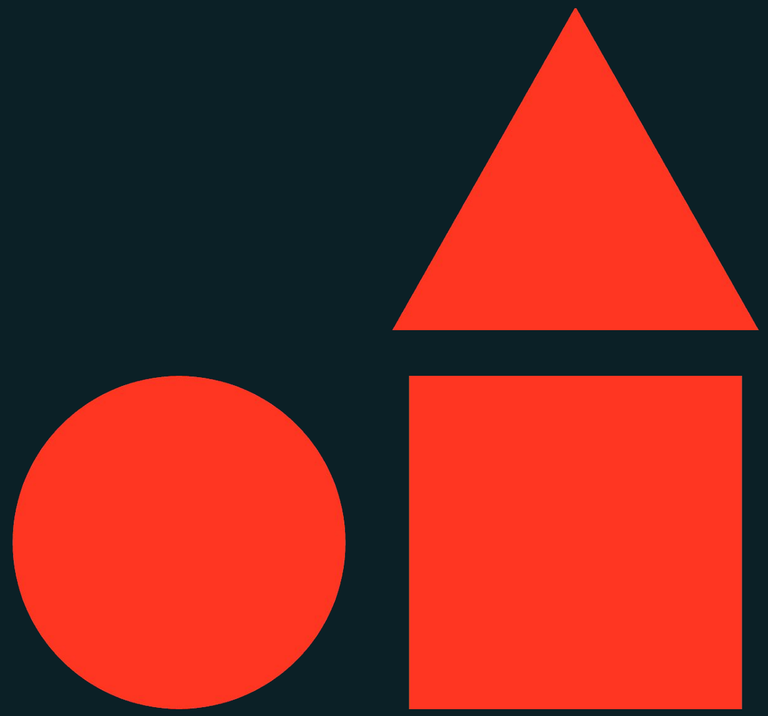
# Machine Learning Model Development



Databricks Academy

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# Course Learning Objectives

- Describe fundamental concepts of developing ML models
- Describe the main components of MLflow for model development
- Describe hyperparameter tuning and leverage Optunta for HPO
- Utilize MLflow for model tracking and development
- Leverage the AutoML API and Databricks UI for AutoML to run an experiment, identify the model based on a preferred metric, and modify a generated model

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# Learning Goals

Upon completion of this content, you should be able to:

- Describe fundamental concepts of machine learning.
- Describe the main components of MLflow for model development.
- Describe hyperparameter tuning and methods.
- Utilize MLflow for model tracking and model tuning with Optuna.
- Create an AutoML experiment, identify the best model, and modify the generated models.

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# Prerequisites/Technical Considerations

## Things to keep in mind before you work through this course

### Prerequisites

1. Knowledge of fundamental concepts of regression, classification, and clustering methods.
2. Familiarity with Databricks workspace and notebooks.
3. Intermediate level knowledge of Python.

### Technical Considerations

1. A cluster running on **DBR ML 16.3**
2. **Unity Catalog** enabled workspace

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# AGENDA

| 1. Model Development Workflow | DEMO | LAB |
|---|---|---|
| Model Development and MLflow | ✔ | ✔ |
| Evaluating Model Performance | | |
| 02. Hyperparameter Tuning | | |
| Hyperparameter Tuning Fundamentals | | |
| Hyperparameter Tuning with Optuna | ✔ | ✔ |
| 03. AutoML | | |
| Automated Model Development with AutoML | ✔ | ✔ |

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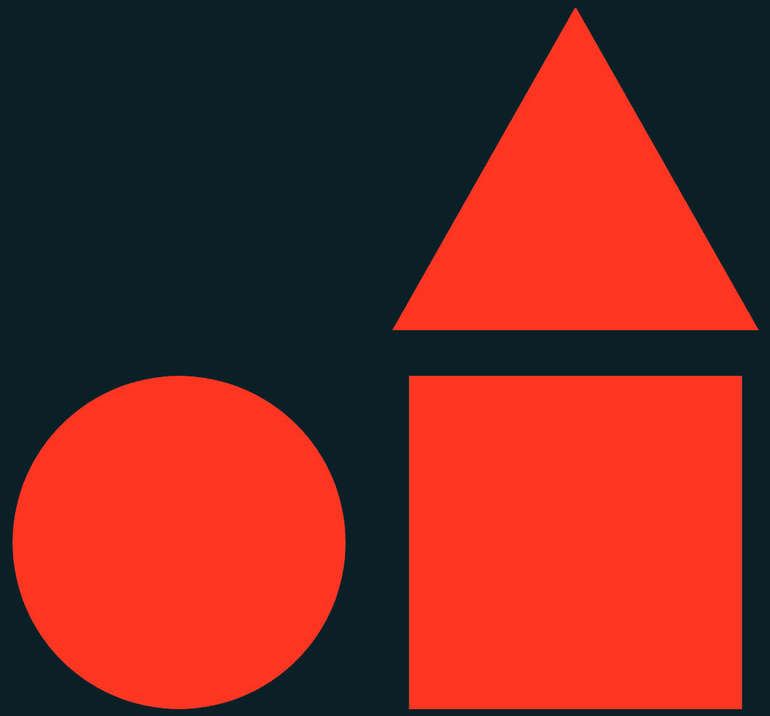
# Machine Learning Model Development



Machine Learning Model Development

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# Problem Statement

Things you'll be able to do after completing this module

- Describe principle categories of machine learning (supervised, unsupervised, reinforcement learning, etc.).
- Describe principle types of supervised learning: regression, classification, forecasting.
- Describe traditional steps of the machine learning model training workflow.
- Describe the benefits of MLflow on Databricks
- Describe Databricks Autologging.
- Review of key metrics for ML algorithms (regression, classification, clustering)

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Model Development Workflow

LECTURE

# Model Development and MLflow

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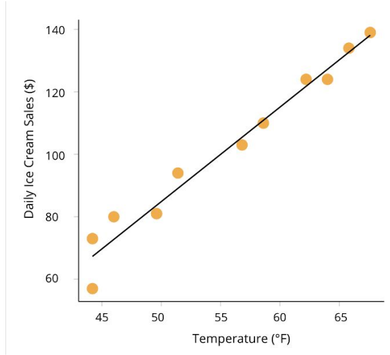
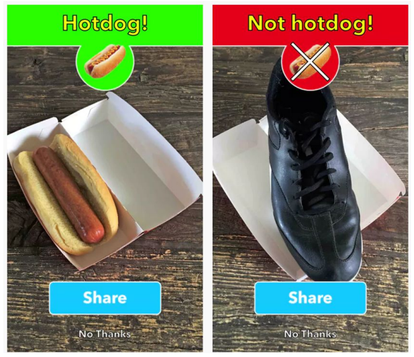
# Types of Machine Learning

## The basics of supervised, unsupervised, and reinforcement learning

### Supervised Learning

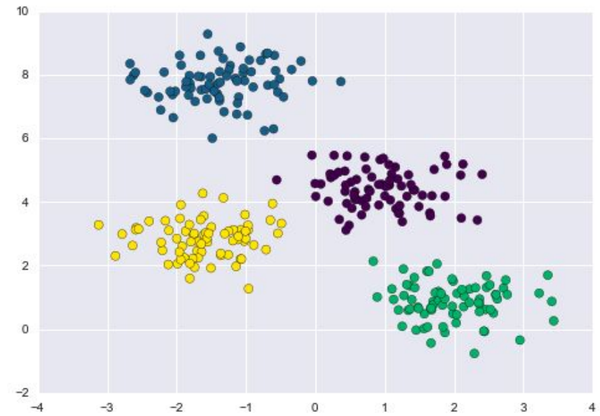
- Data has a set of input records with **associated labels**.
- Goal is to predict the output labels given an **unlabeled input**.
- Model the conditional probability: $P(Y \mid X_1, X_2, \ldots, X_n)$




### Unsupervised Learning

- Unlabeled data (no known function output)
- Clustering (group records with similar features)
- Dimensionality reduction (reduce feature space)
- Model the joint probability: $P(X_1, X_2, \ldots, X_n)$

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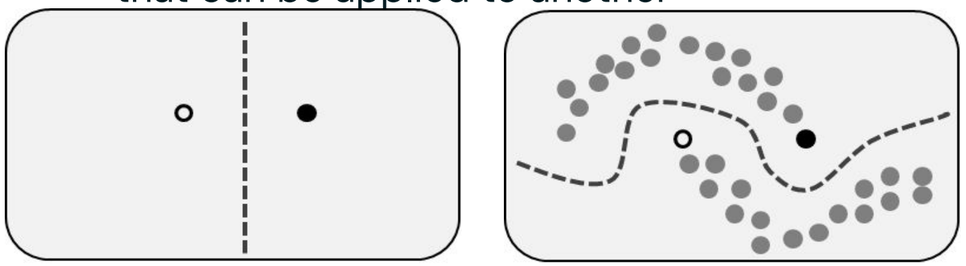
# Types of Machine Learning

## The basics of supervised, unsupervised, and reinforcement learning

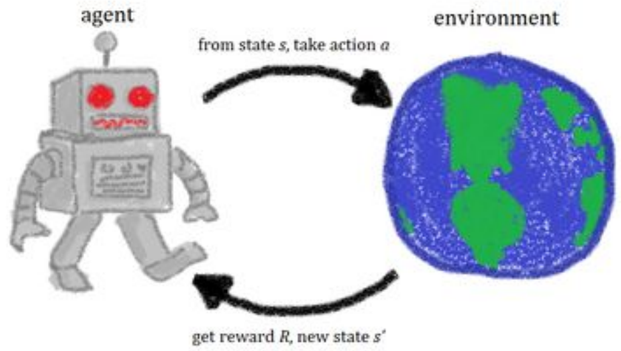
### Hybrids

- Combines supervised learning and unsupervised learning
- Labeled and unlabeled data, mostly unlabeled
- Semi-supervised:
  - Use small set of labeled data to infer labels to a larger set
- Self-supervised:
  - Learn patterns of data in one (larger) dataset that can be applied to another



### Reinforcement Learning

- States, actions, and rewards
- Useful for exploring spaces and exploiting information to maximize expected cumulative rewards
- Frequently **utilizes neural networks and deep learning**

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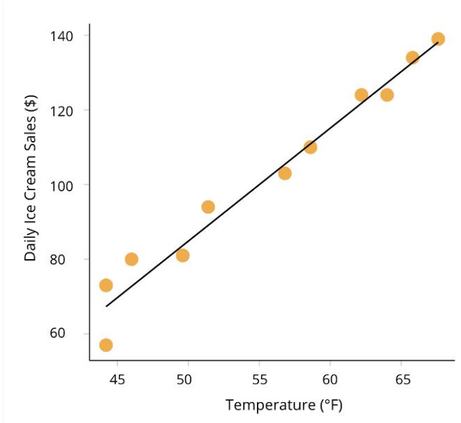
# Types of Supervised Learning

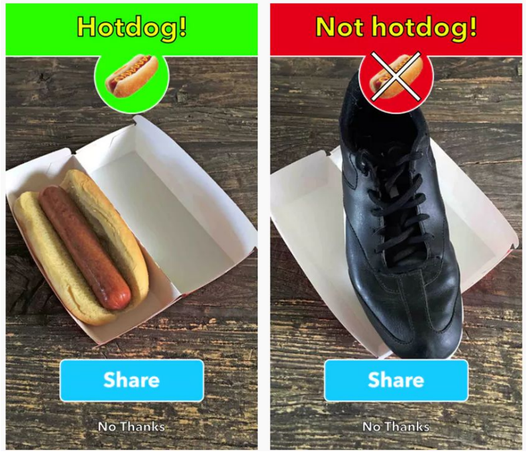
## Regression

- Predicting a **continuous** output
- **Example:** predict sales, predict number of viewers




## Classification

- Predicting a **categorical/discrete** output
- **Example:** yes/no, image classification, predict disease




## Forecasting

- Predicting future values based on **historical** data
- **Example**: demand forecasting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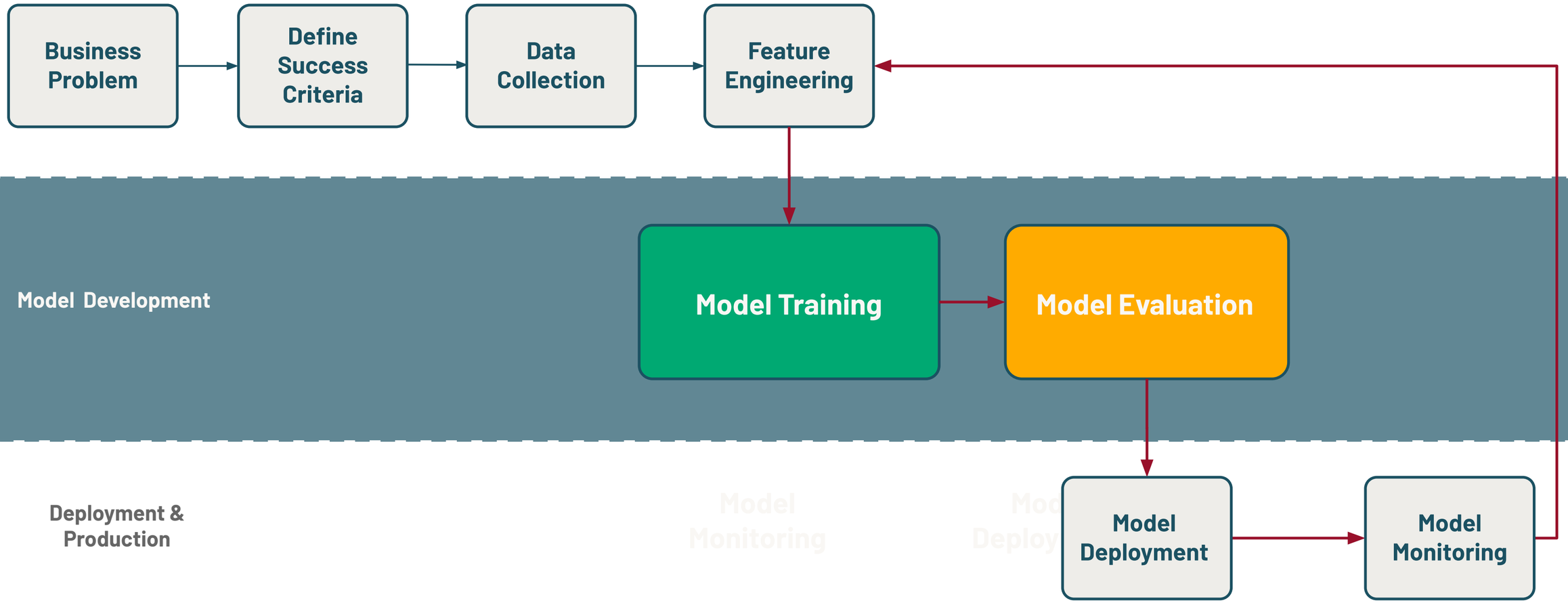
# The Machine Learning Lifecycle

## Model development and evaluation

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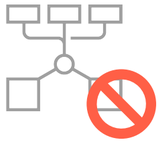
# Core Machine Learning Dev. Issues

## Modern ML lifecycle comes with many challenges



**Reproducibility and Experiment Tracking**

Difficulty in ensuring consistent results across different environments and effectively documenting and organizing experiments

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# Core Machine Learning Dev. Issues

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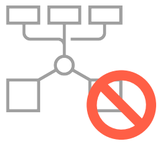

**Reproducibility and Experiment Tracking**

Difficulty in ensuring consistent results across different environments and effectively documenting and organizing experiments.

**Model Evaluation and Comparison**

Challenges in accurately comparing and selecting the best-performing model due to variations in evaluation metrics and design.

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# Core Machine Learning Dev. Issues

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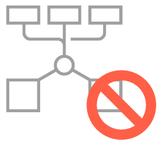

### Reproducibility and Experiment Tracking

Difficulty in ensuring consistent results across different environments and effectively documenting and organizing experiments.

### Model Evaluation and Comparison

Challenges in accurately comparing and selecting the best-performing model due to variations in evaluation metrics and design.

### Deployment and Standardization

Complexities in transitioning model, ensuring seamless integration, standardized deployment processes.

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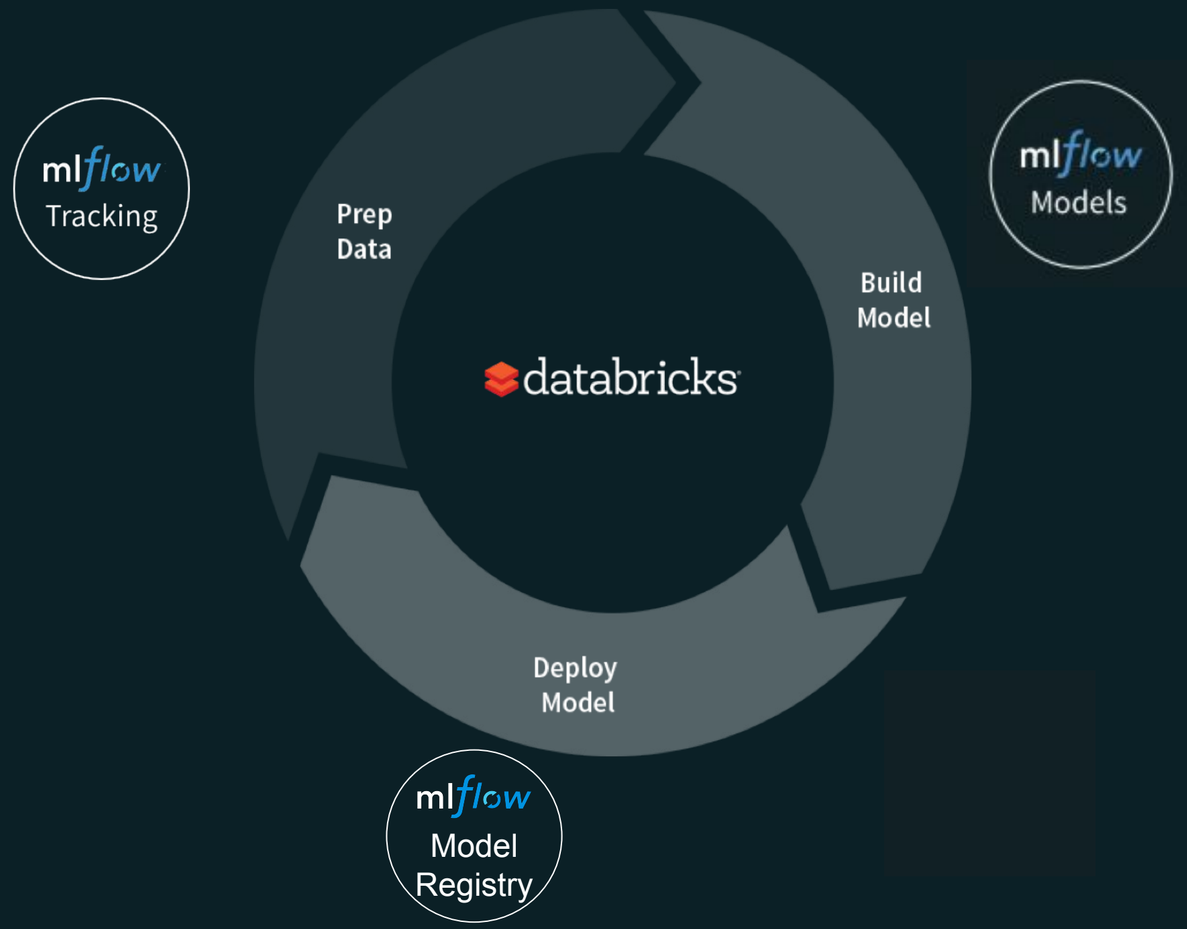
# MLflow

## MLflow addresses common ML development issues.

- Open-source platform for machine learning lifecycle
- Operationalizing machine learning
- Developed by Databricks
- Pre-installed on the Databricks Runtime for ML

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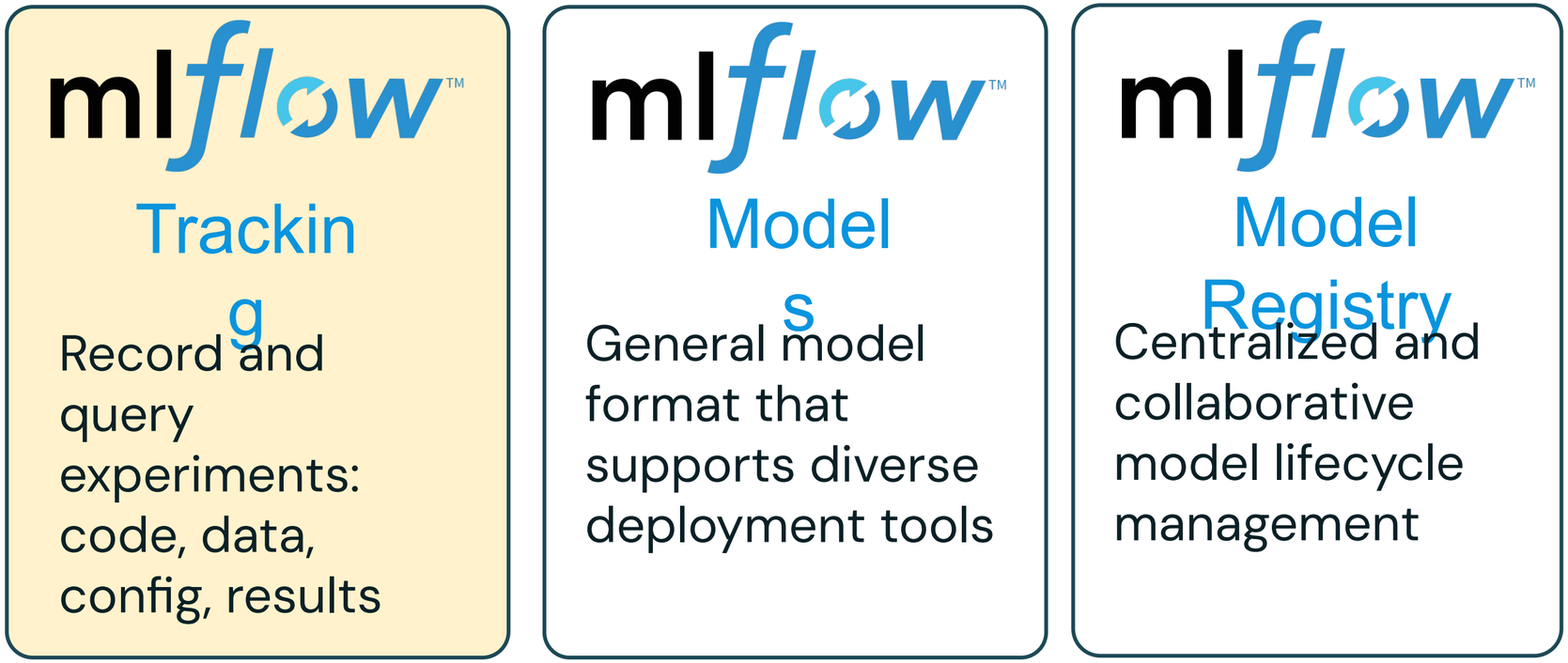
# MLflow Components

## The four components of MLflow




APIs: CLI, Python, R, Java, REST

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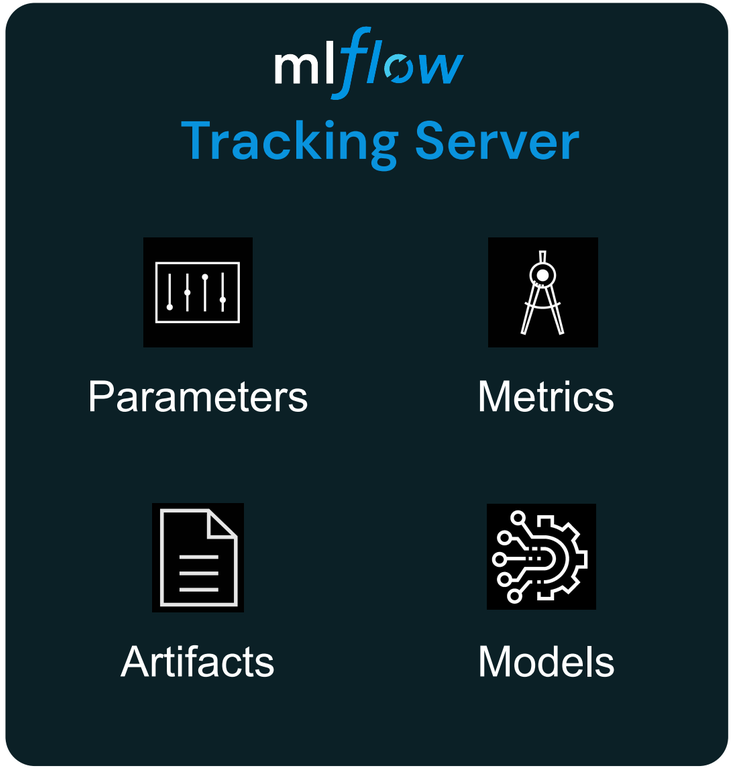
# ML*flow* Model Tracking

## Make your ML workflow more manageable and transparent

- Record experiment **parameters** such as hyperparameters and model configurations.
- Log **metrics** and compare them for performance measures.
- Store and manage output **artifacts** such as trained models and plots.
- Store model's **source code** from the run.

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# Model Tracking and Custom Logging

## Supports for custom logging

Custom logging for;

- **Parameters** (such as custom model hyperparameters),
- Custom **metrics**
- **Artifacts** (such as the trained model and additional files) within the context of the run.

```python
# Log metrics
y_pred = model.predict(X_test)
super_score = custom_score(y_test, y_pred)
mlflow.log_metric('super_score', super_score)

# Log artifacts (e.g., model file)
model_path = 'random_forest_model.pkl'
mlflow.sklearn.log_model(model, model_path)
mlflow.log_artifact(model_path)

# Log params
mlflow.log_params({'param1': 123, 'param2': 'abc'})
```

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# Model Tracking and Autologging

Ensure reproducibility

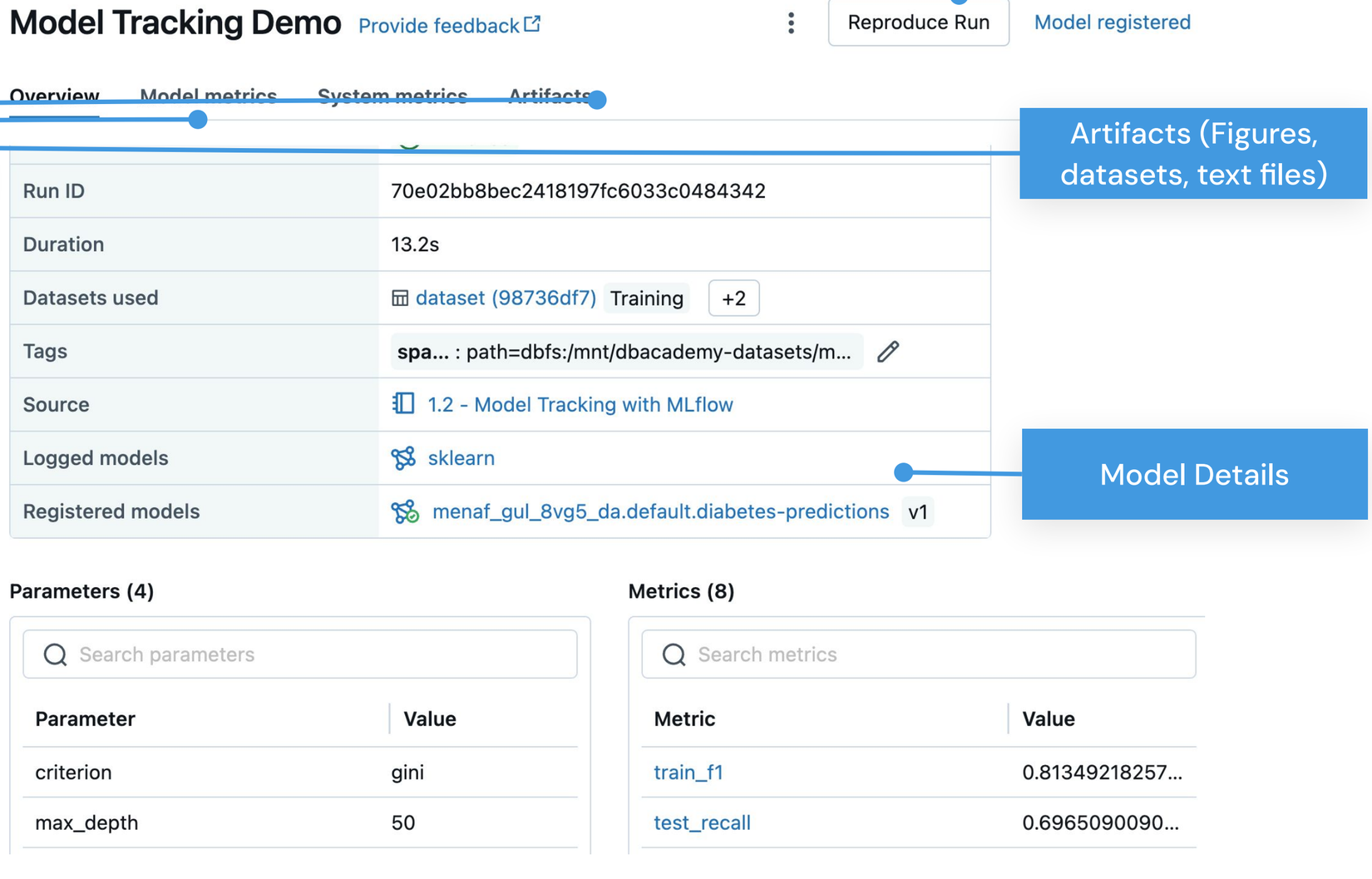
Inspect, Visualize and Compare Metrics

Artifacts (Figures, datasets, text files)

Model Details

`mlflow.autolog()`

**Automatically track ML development** with one line of code: parameters, metrics, data lineage, model, and environment.

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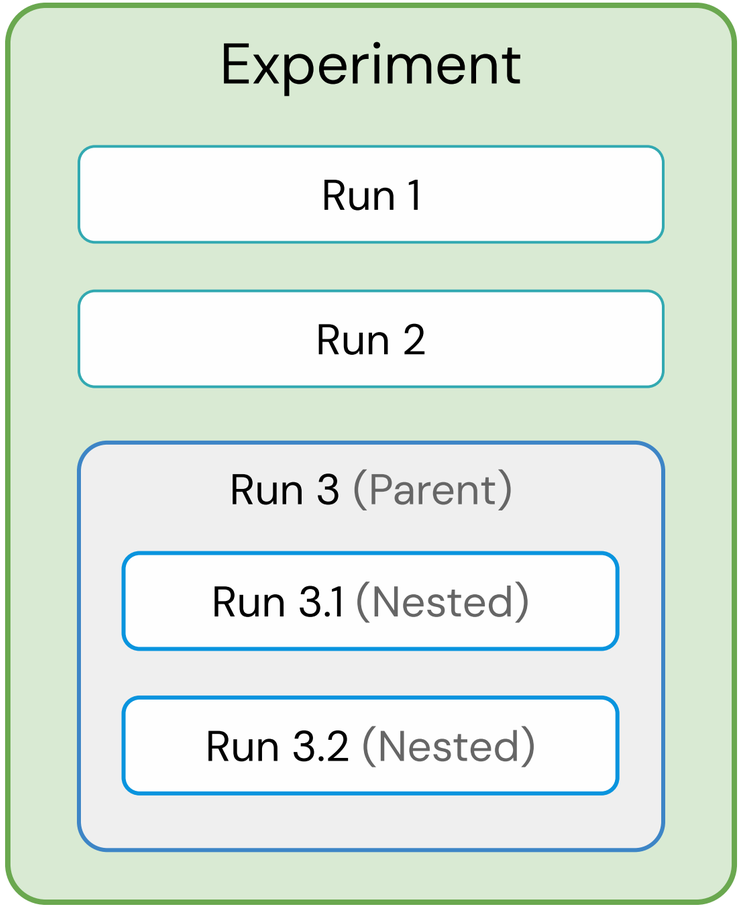
# MLflow Concepts

**Experiment** → Runs → Metadata / Artifacts

**MLflow experiment:**

- A higher-level organizational unit that **encompasses a set of runs**.
- Groups and organizes related runs, typically conducted to explore different configurations, parameters, or algorithms.
- Two options
  - Notebook Experiment: tied to the notebook
  - Workspace experiment: Manually specify the path. Multiple notebooks can create runs in it.

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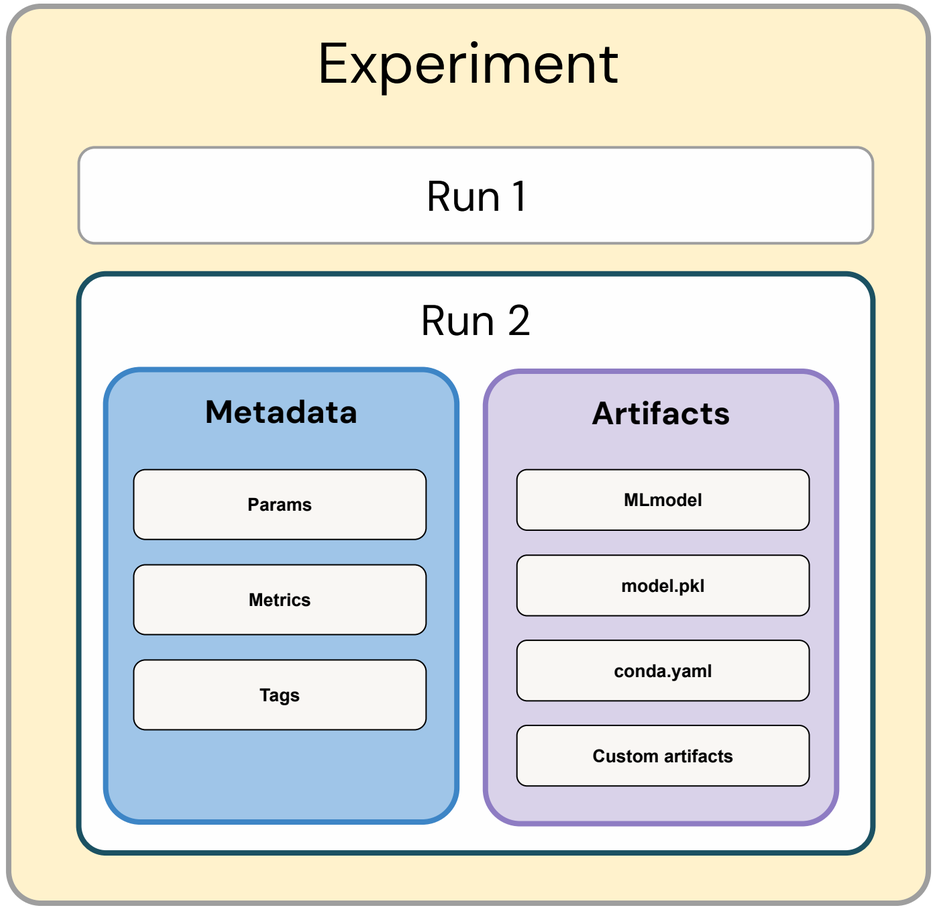
# ML*flow* Concepts

Experiment → **Runs** → Metadata / Artifacts

**MLflow run:**

- Executions of data science code.
- Belongs to only one experiment.
- Contains
  - Metadata
  - Artifacts
- Has a default Py Func flavor which is wrapper around the native model.

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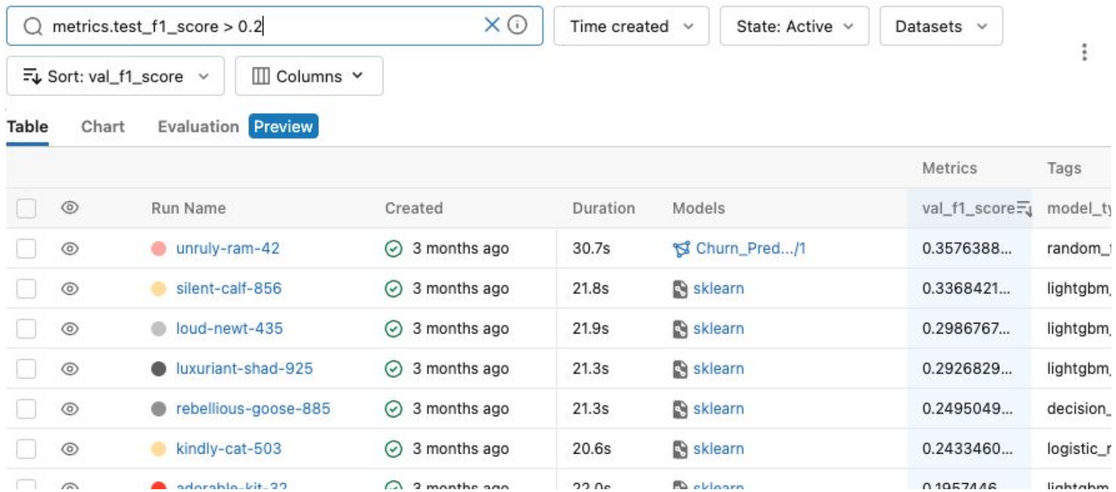
# Examining Past Runs

## Via MLflow UI

- List and filter runs by metrics
- Built in to Databricks platform




## Via MLflow API

- `MlflowClient` Object
- List experiments
- Search runs by metrics, model etc.

```python
from mlflow import MlflowClient

runs = MlflowClient().search_runs(
    experiment_ids="0",
    filter_string="params.model = 'random_forest'",
    max_results=5,
    order_by=["metrics.accuracy DESC"],
)
```

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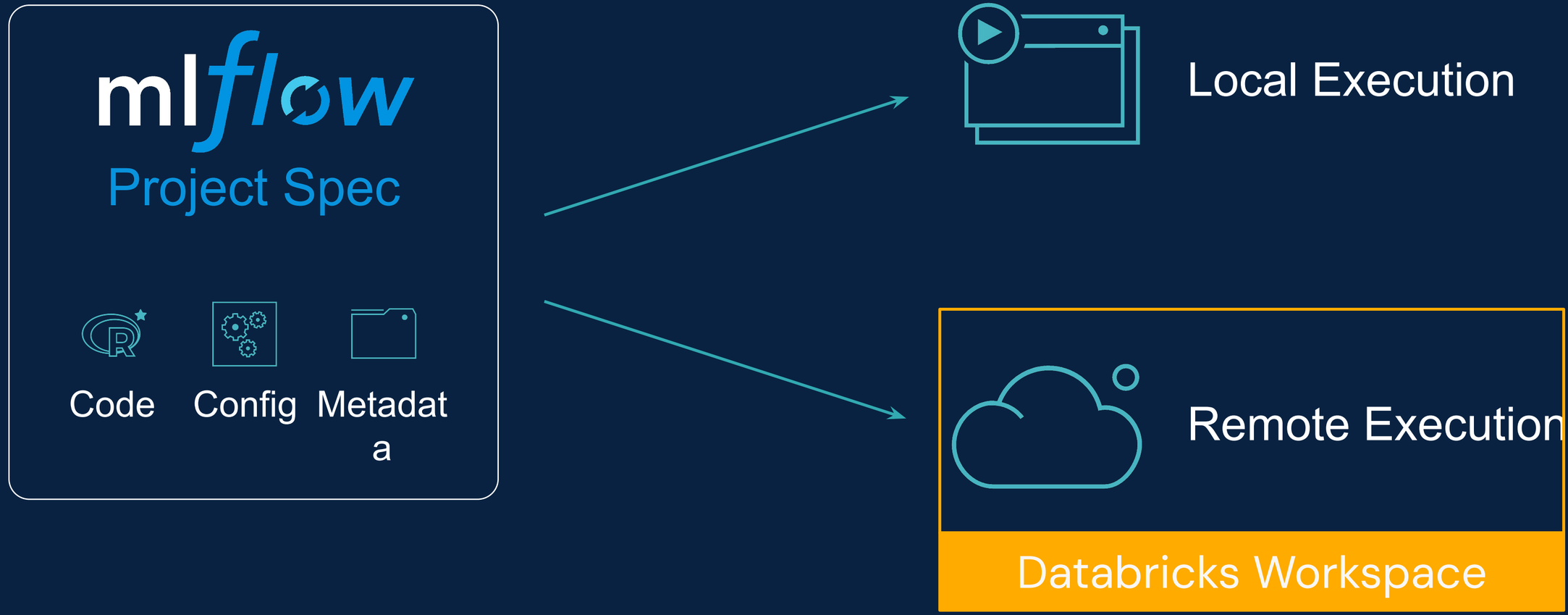
# mlflow Projects

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# MLflow Project

Package in a reusable and reproducible manner

Key aspects:

- **Packaging**: entire project and dependencies
- **Reproducibility**
- **Easy execution**: Via CLI and APIs
- **Versioning and sharing**


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# Example ML*flow* Project

```
my_project/
├── MLproject
│
│
│
│
├── conda.yaml
├── main.py
└── model.py
    ...
```

```
conda_env: conda.yaml

entry_points:
  main:
    parameters:
      training_data: path
      lambda: {type: float, default: 0.1}
    command: python main.py {training_data} {lambda}
```

```
$ mlflow run git://<my_project>
```

```
mlflow.run("git://<my_project>", ...)
```

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Model Development Workflow

LECTURE

# Evaluating Model Performance

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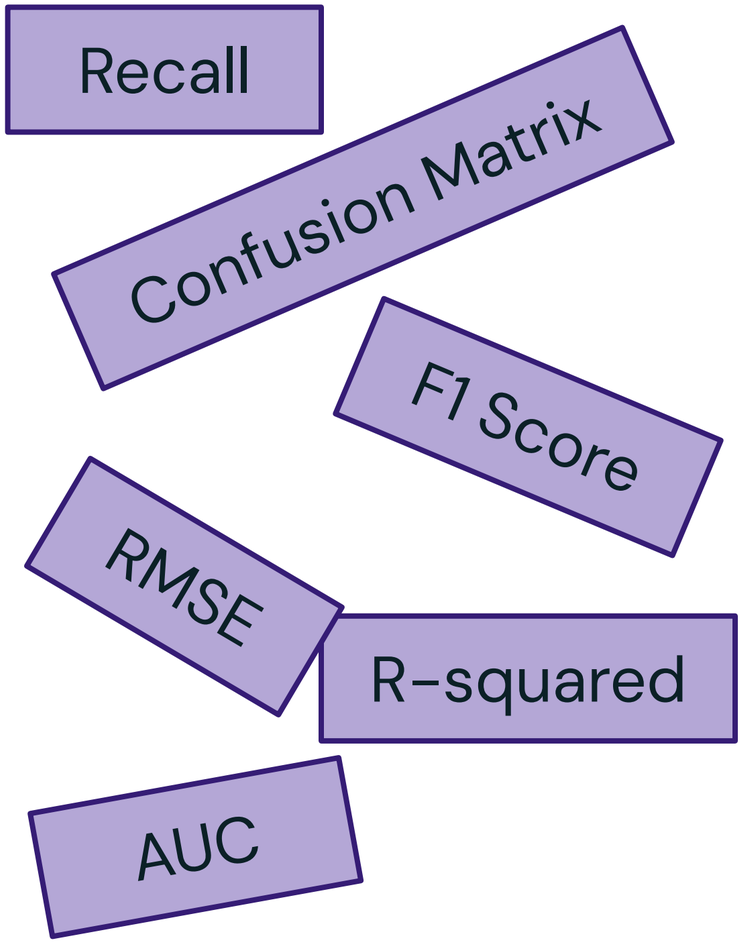
# Purpose of Computing Evaluation Metrics

- Evaluation metrics provide a numerical representation of how well a model is doing.
- Metrics enable the comparison of different models or different versions of the same model.
- Evaluation metrics guide the fine-tuning of models.
- Metrics prove an objective basis for choosing between different models or approaches.

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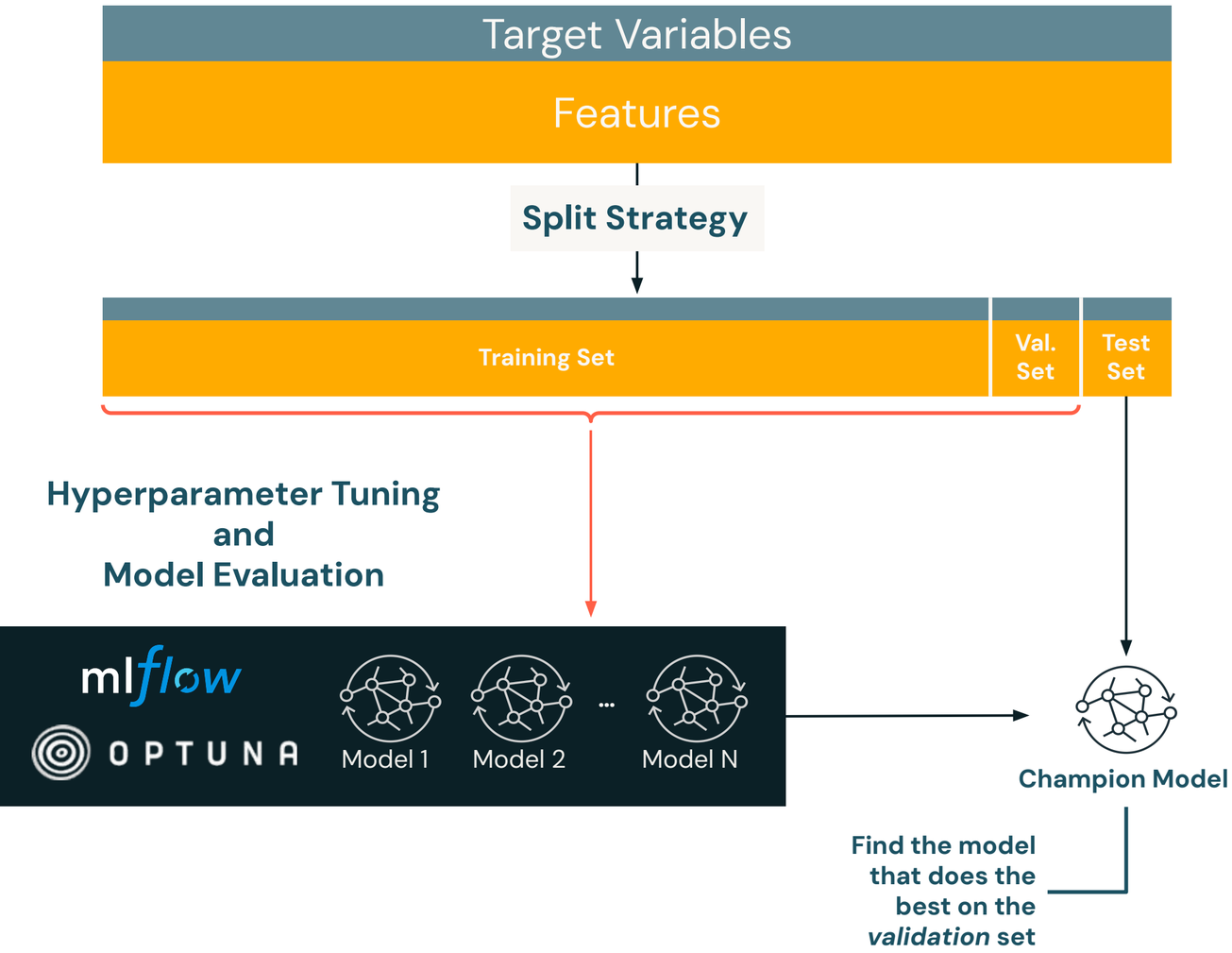
# How to Build and Evaluate Models?




| Dataset Type | Purpose | Usage | Model Impact |
|---|---|---|---|
| **Training** | Training data for model | Minimize loss during optimization | Direct impact on internal model parameters |
| **Validation** | Hyperparameter tuning | Used for preventing overfitting | Indirect impact on model parameters |
| **Test** | Evaluate generalizability | Assesses real-world performance on unseen data | No influence on model training or selection |

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# Review of Common Metrics

## Supervised Learning - Regression

| Metric | Description | Values | Code |
|---|---|---|---|
| | | | |
| | | | |
| | | | |
| | | | |

More Details: Appendix A

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# Review of Common Metrics

## Supervised Learning – Regression

| Metric | Description | Values | Code |
|---|---|---|---|
| $R^2$ | Measures how well the model explains the variation in the target variable. | Range: $(-\infty, 1]$<br>Larger is better | `from sklearn.metrics import r2_score`<br>`r2 = r2_score(y_true, y_pred)` |
| | | | |
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More Details: Appendix A

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## Supervised Learning - Regression

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| Mean Absolute Error | Measures the average absolute difference between actual and predicted values. | Range: $[0, \infty)$<br>Lower is better | `from sklearn.metrics import mean_absolute_error`<br>`mae = mean_absolute_error(y_true, y_pred)` |
| | | | |
| | | | |

More Details: Appendix A

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| Mean Squared Error | Measures the average of squared differences between actual and predicted values. Squaring gives higher weight to large errors. | Range: $[0, \infty)$<br>Lower is better | `from sklearn.metrics import mean_squared_error`<br>`mse = mean_squared_error(y_true, y_pred)` |
| | | | |

More Details: Appendix A

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# Review of Common Metrics

## Supervised Learning - Regression

| Metric | Description | Values | Code |
|---|---|---|---|
| $R^2$ | Measures how well the model explains the variation in the target variable. | Range: $(-\infty, 1]$<br>Larger is better | `from sklearn.metrics import r2_score`<br>`r2 = r2_score(y_true, y_pred)` |
| Mean Absolute Error | Measures the average absolute difference between actual and predicted values. | Range: $[0, \infty)$<br>Lower is better | `from sklearn.metrics import mean_absolute_error`<br>`mae = mean_absolute_error(y_true, y_pred)` |
| Mean Squared Error | Measures the average of squared differences between actual and predicted values. Squaring gives higher weight to large errors. | Range: $[0, \infty)$<br>Lower is better | `from sklearn.metrics import mean_squared_error`<br>`mse = mean_squared_error(y_true, y_pred)` |
| Root Mean Squared Error | Similar to MSE but takes the square root, making it more interpretable to the original units. | Range: $[0, \infty)$<br>Lower is better | `from sklearn.metrics import mean_squared_error`<br>`mse = mean_squared_error(y_true, y_pred,squared=False)` |

More Details: Appendix A

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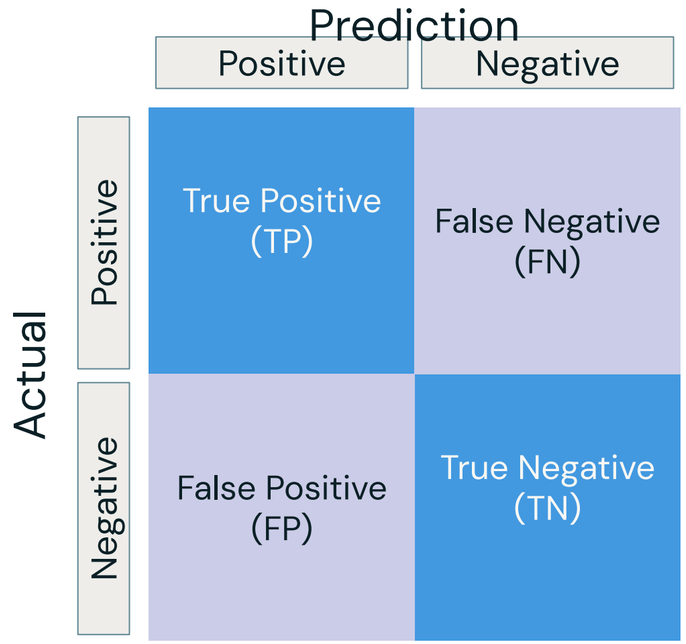
# Review of Common Metrics

## Supervised Learning - Classification

| Metric | Description |
|---|---|
| Accuracy | |
| Precision | |
| Recall (Sensitivity) | |
| F1 Score | |




Confusion Matrix

```
from sklearn.metrics import confusion_matrix
cm = confusion_matrix(y_true, y_pred)
```

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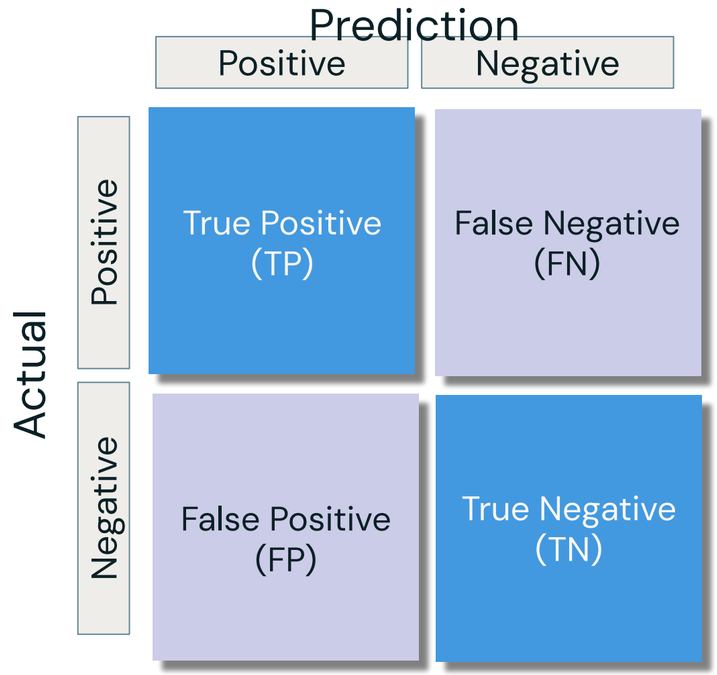
# Review of Common Metrics

## Supervised Learning – Classification

| Metric | Description |
|---|---|
| Accuracy | Measures the proportion of correctly classified instances. It can be misleading for imbalance datasets. |
| Precision | |
| Recall (Sensitivity) | |
| F1 Score | |




Confusion Matrix

```
from sklearn.metrics import accuracy_score
accuracy = accuracy_score(y_true, y_pred)
```

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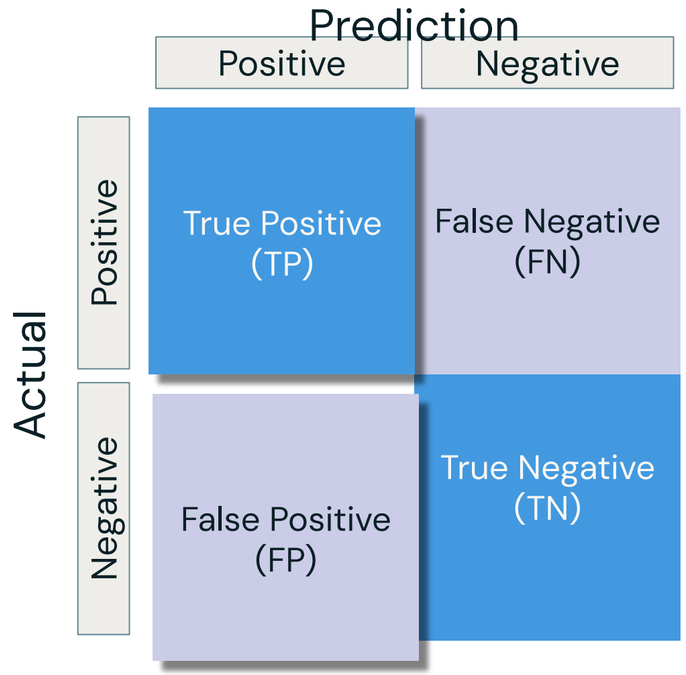
# Review of Common Metrics

## Supervised Learning – Classification

| Metric | Description |
|---|---|
| Accuracy | Measures the proportion of correctly classified instances. It can be misleading for imbalance datasets. |
| Precision | Measures how many predicted positives are actually correct. Important when false positives are costly. |
| Recall (Sensitivity) | |
| F1 Score | |




Confusion Matrix

```
from sklearn.metrics import precision_score
precision = precision_score(y_true, y_pred)
```

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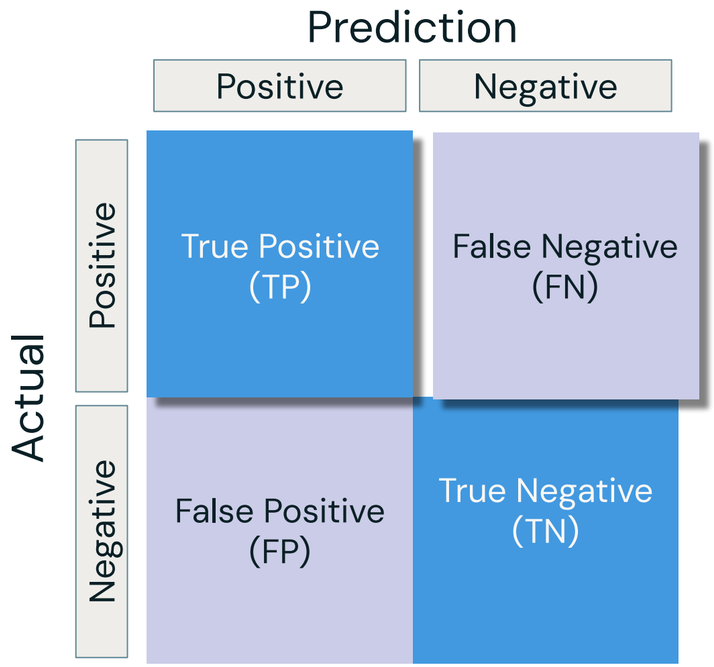
# Review of Common Metrics

## Supervised Learning – Classification

| Metric | Description |
|---|---|
| Accuracy | Measures the proportion of correctly classified instances. It can be misleading for imbalance datasets. |
| Precision | Measures how many predicted positives are actually correct. Important when false positives are costly. |
| Recall (Sensitivity) | Measures how many actual positives were correctly identified. Important when false negatives are costly. |
| F1 Score | |




Confusion Matrix

```
from sklearn.metrics import recall_score
recall = recall_score(y_true, y_pred)
```

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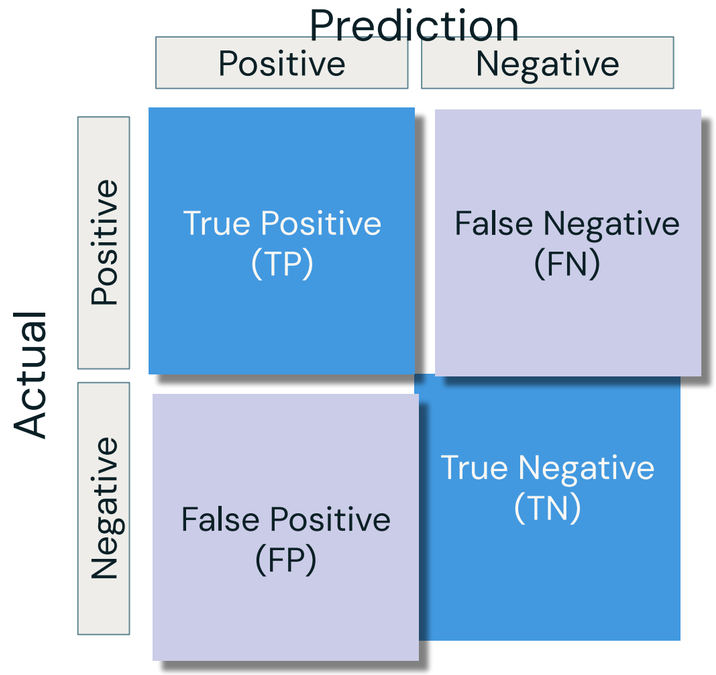
# Review of Common Metrics

## Supervised Learning – Classification

| Metric | Description |
|---|---|
| Accuracy | Measures the proportion of correctly classified instances. It can be misleading for imbalance datasets. |
| Precision | Measures how many predicted positives are actually correct. Important when false positives are costly. |
| Recall (Sensitivity) | Measures how many actual positives were correctly identified. Important when false negatives are costly. |
| F1 Score | Measures the proportion of correctly classified instances. It can be misleading for imbalance datasets. |




Confusion Matrix

```
from sklearn.metrics import f1_score
f1 = f1_score(y_true, y_pred)
```

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# Precision, Recall, F1-Score

## Which one to choose?

### Precision

Suitable when minimizing false positives is crucial, even at the expense of missing some positive instances.

**Example:** In a **spam email classifier**, high precision ensures that emails marked as spam are indeed spam, reducing the chances of incorrectly classifying important emails as spam.

### Recall

Appropriate when capturing all positive instances is vital, even if it means tolerating some false positives.

**Example:** In a **medical diagnosis system**, high recall ensures identifying all patients with a certain disease, even if it leads to a few false alarms.

### F1 Score

Useful when seeking a balance between precision and recall.

**Example:** In a search engine **ranking algorithm**, F1 score might be used to evaluate how well the algorithm retrieves relevant documents while minimizing irrelevant ones.

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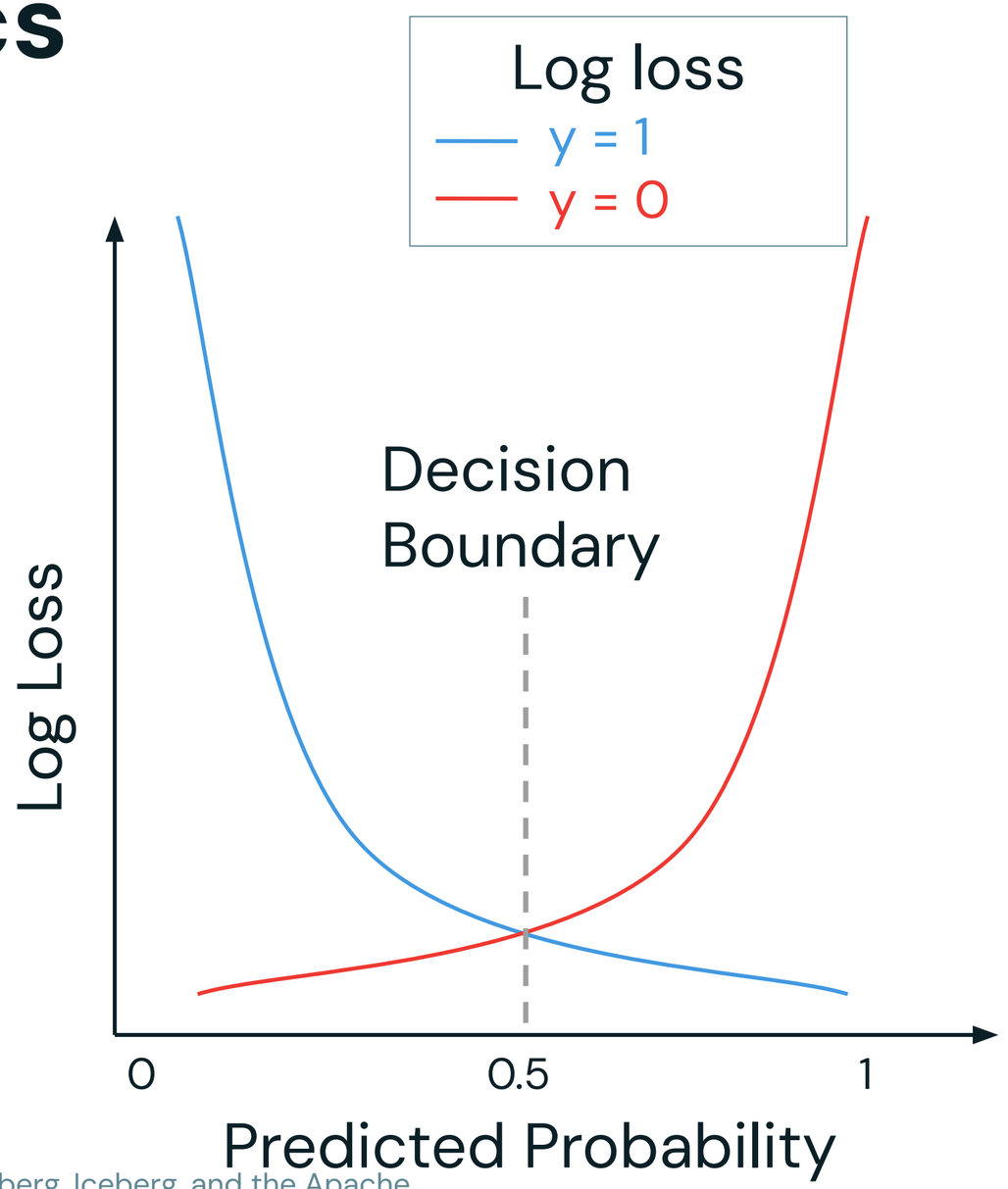
# Review of Common Metrics

## Supervised Learning – Classification

| Metric | Description |
|---|---|
| Log loss (Cross-Entropy Loss) | Measures by comparing predicted probabilities to the actual class labels. Penalizes confident but incorrect predictions heavily. Lower values indicate better calibrated models. |
| ROC/AUC | |

```
from sklearn.metrics import log_loss
ll_value = log_loss(y_true, y_pred)
```

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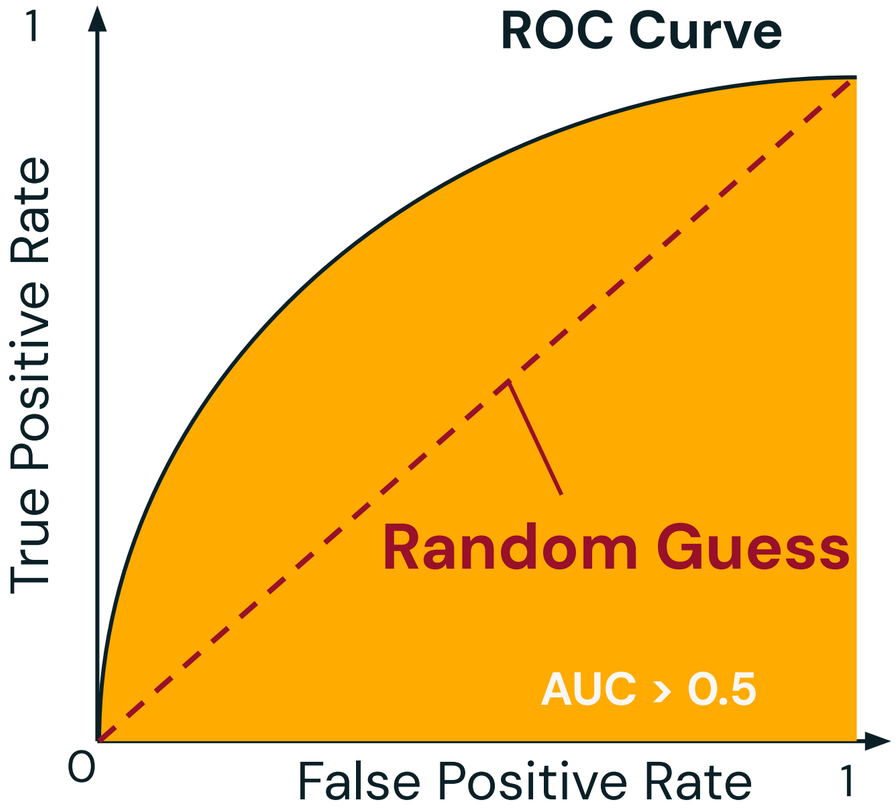
# Review of Common Metrics

## Supervised Learning – Classification

| Metric | Description |
|---|---|
| Log loss (Cross-Entropy Loss) | Measures by comparing predicted probabilities to the actual class labels. Penalizes confident but incorrect predictions heavily. Lower values indicate better calibrated models. |
| ROC/AUC | Measures the model's ability to distinguish between classes across different thresholds. AUC (Area Under the Curve) closer to 1 indicates a better model. |

```
from sklearn.metrics import roc_auc_score
auc_score = roc_auc_score(y_true, y_pred)
```

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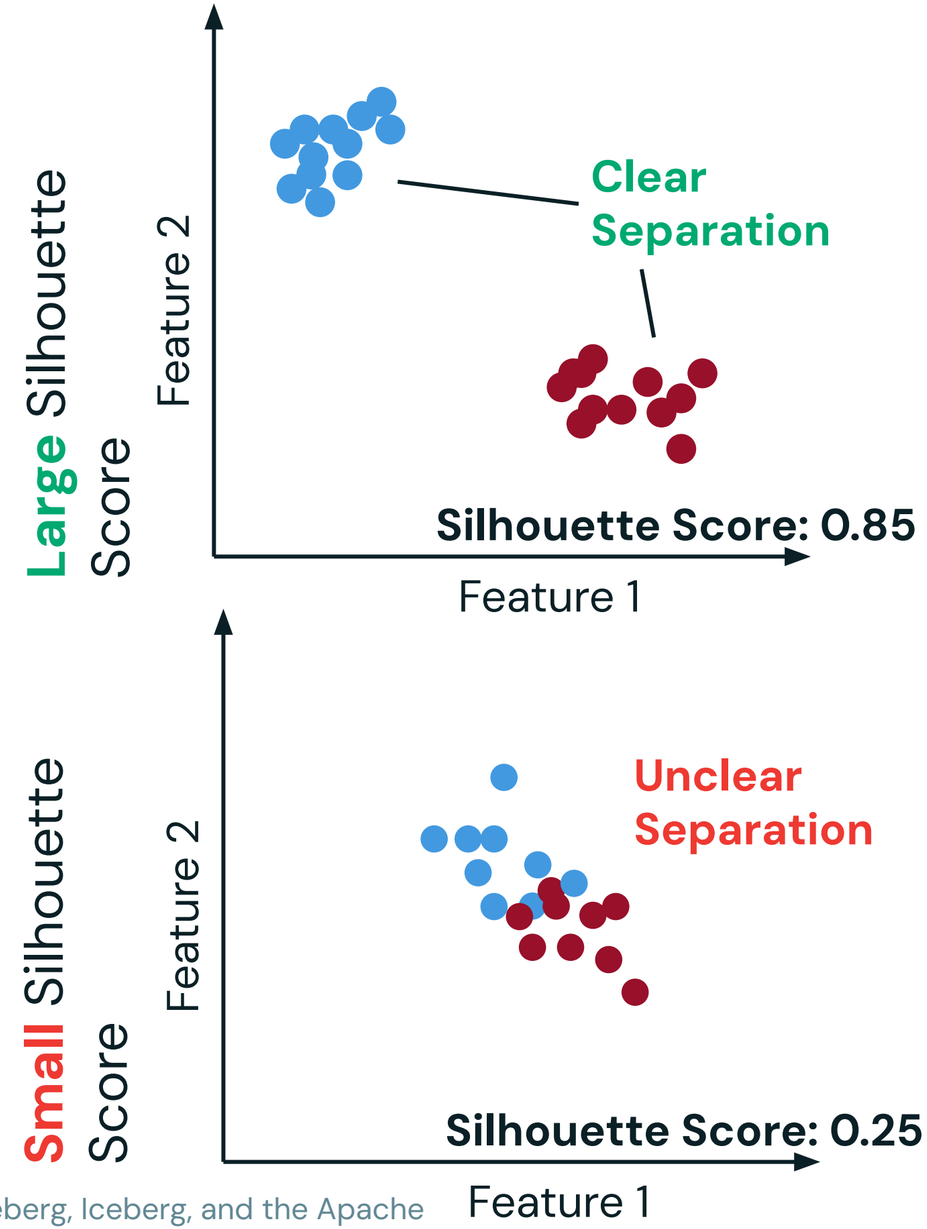
# Review of Common Metrics

## Unsupervised Learning - Clustering

| Metric | Description |
| --- | --- |
| Silhouette Score | Measures how well-defined clusters are. Higher values indicate better separation. |
| Elbow Method | |

```
from sklearn.metrics import silhouette_score
From sklearn.cluster import KMeans
kmeans = KMeans(n_clusters=2, random_state=42, n_init=10)
Labels = kmeans.fit_predict(X)
s_score = silhouette_score(X, labels)
```

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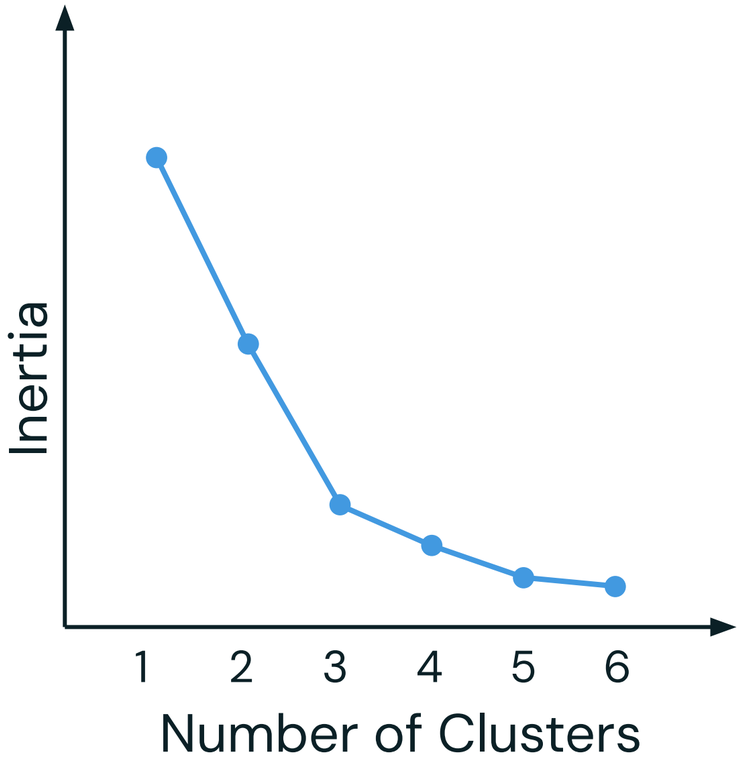
# Review of Common Metrics

## Unsupervised Learning - Clustering

| Metric | Description |
| --- | --- |
| Silhouette Score | Measures how well-defined clusters are. Higher values indicate better separation. |
| Elbow Method | Plots variance within clusters vs the number of clusters to find the elbow point where adding more clusters doesn't improve separation. |

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# Review of Common Metrics

## Unsupervised Learning – Clustering

| Metric | Description |
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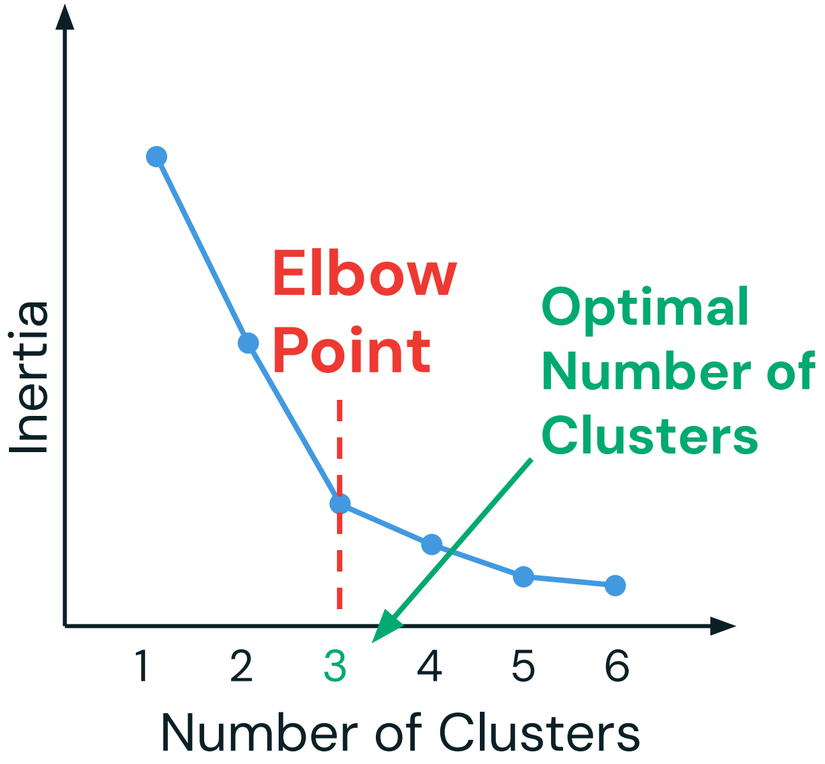


1

```
from sklearn.metrics import silhouette_score
From sklearn.cluster import KMeans

k_values = range(1, 7)
```

2

```
inertia_values = [KMeans(n_clusters=k,
random_state=42, n_init=10).fit(X).inertia_ for k
in k_values]

knee_locator = KneeLocator(k_values,
inertia_values, curve="convex",
direction="decreasing")

optimal_k = knee_locator.elbow
```

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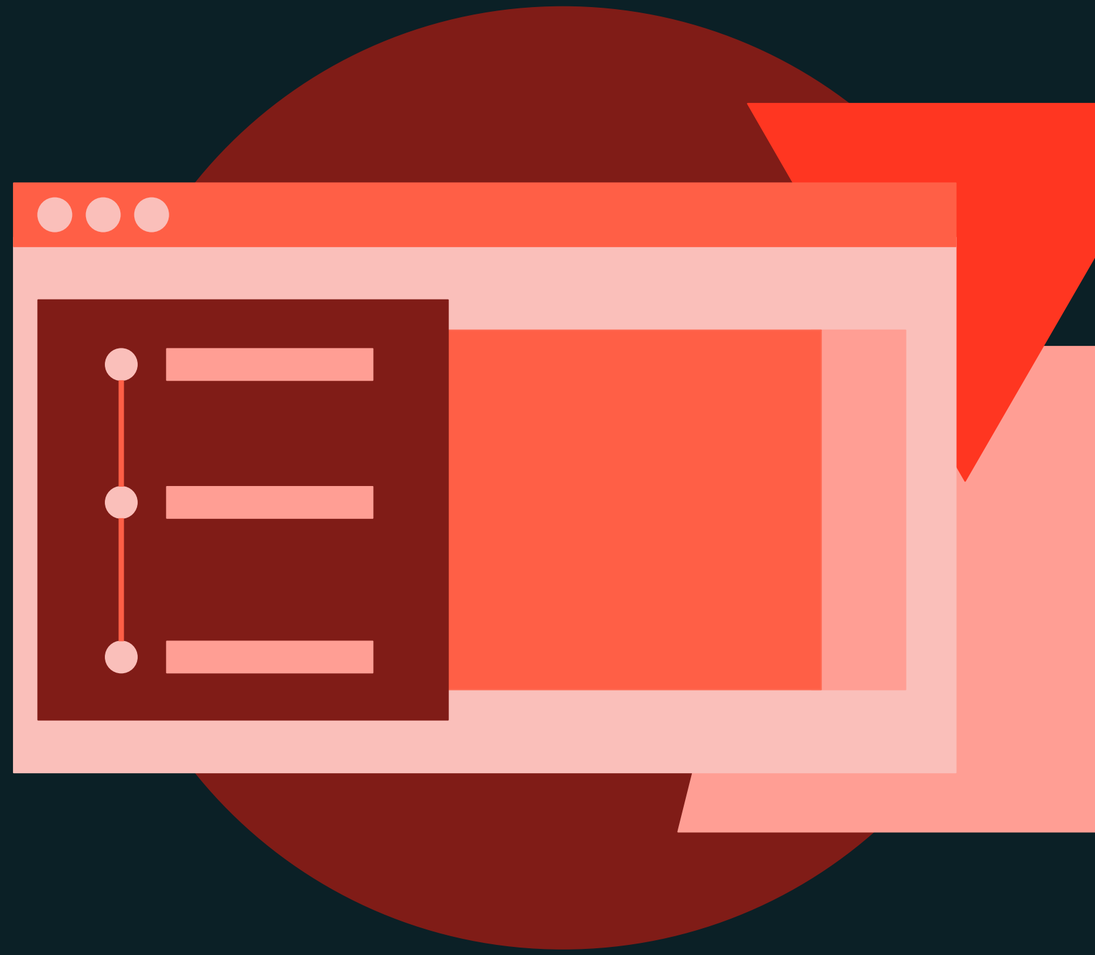
Model Development Workflow

DEMONSTRATION

# Supervised Learning



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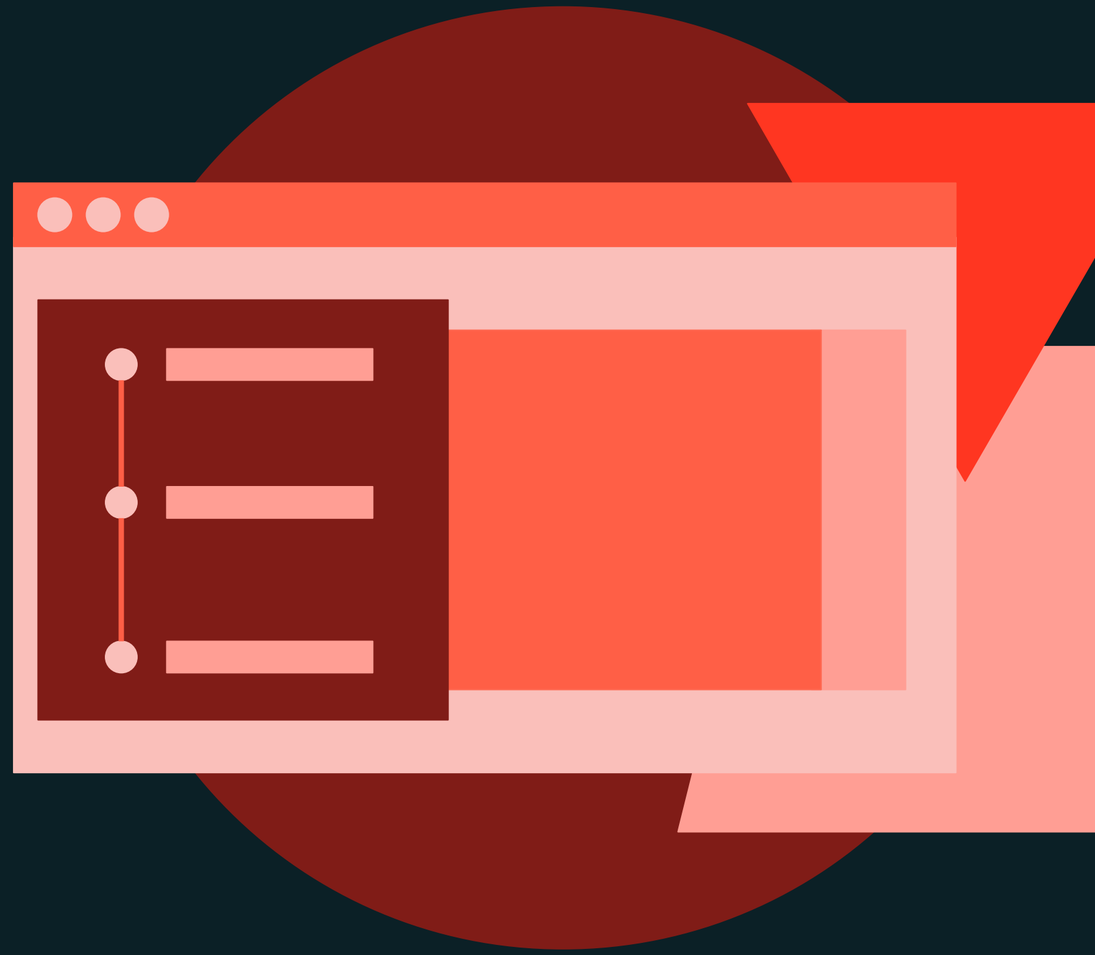
Model Development Workflow

DEMONSTRATION

# Unsupervised Learning



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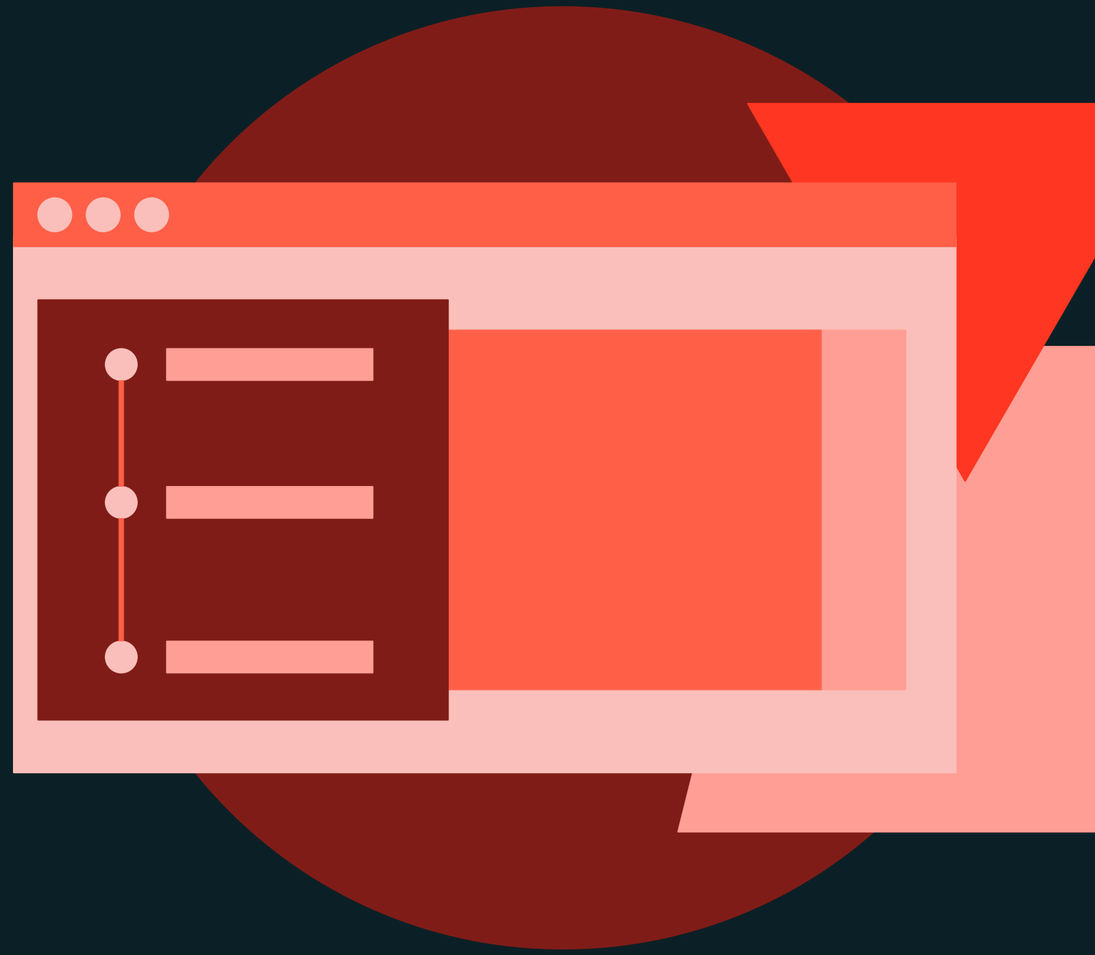
Model Development Workflow

DEMONSTRATION

# Model Tracking with MLflow



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Model Development Workflow

LAB EXERCISE

# Model Development Tracking with MLflow

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# AppendixA

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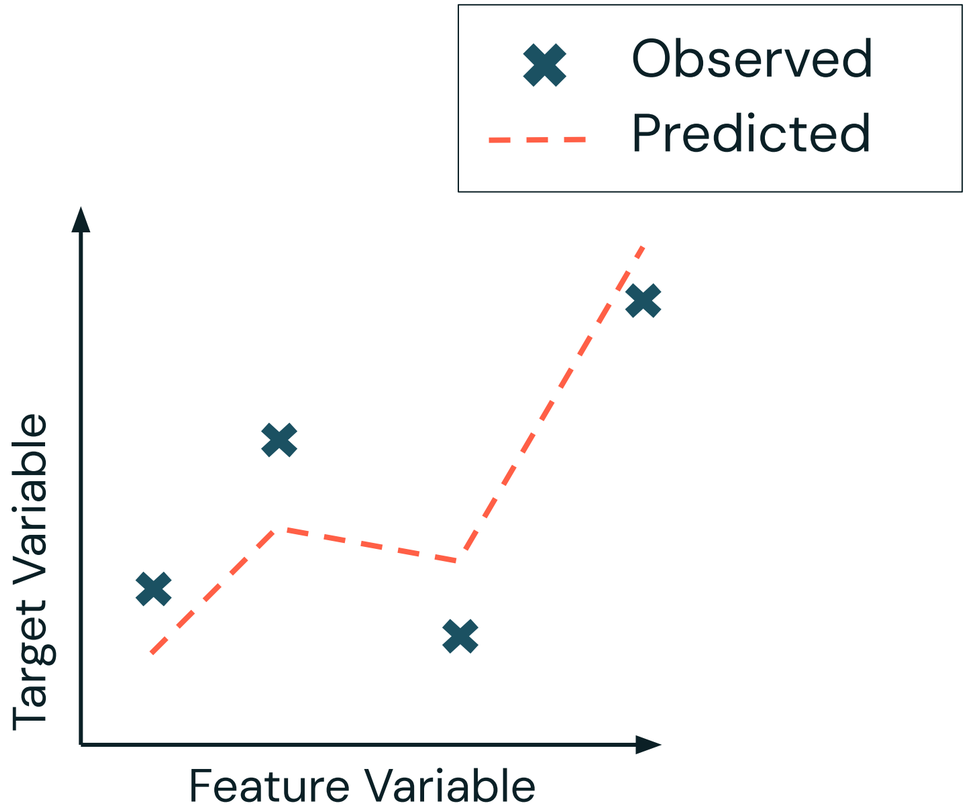
# Review of Some Common Metrics

## Supervised Learning – Regression

| Metric | Description |
|---|---|
| $R^2$ | |
| Mean Absolute Error | |
| Mean Squared Error | |
| Root Mean Squared Error | |

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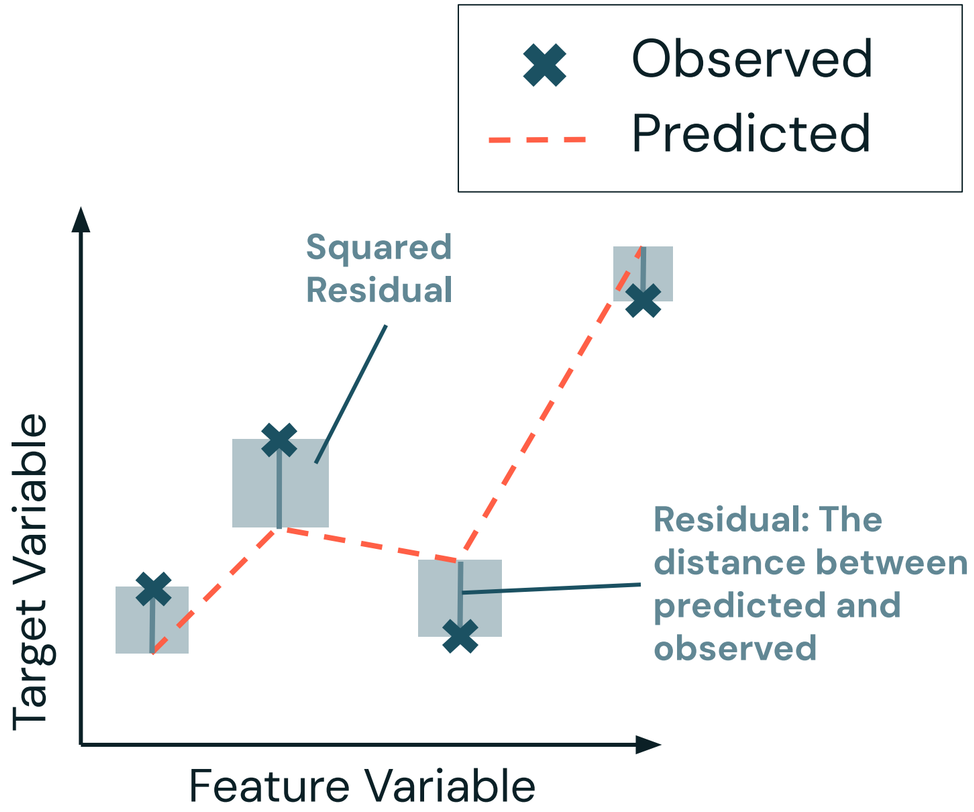
# Review of Some Common Metrics

## Supervised Learning – Regression

| Metric | Description |
|---|---|
| $R^2$ | Measures the proportion of variance explained by the model. Higher values indicate a better fit. |
| Mean Absolute Error | |
| Mean Squared Error | |
| Root Mean Squared Error | |

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# Review of Some Common Metrics

## Supervised Learning – Regression

| Metric | Description |
|---|---|
| $R^2$ | Measures the proportion of variance explained by the model. Higher values indicate a better fit. |
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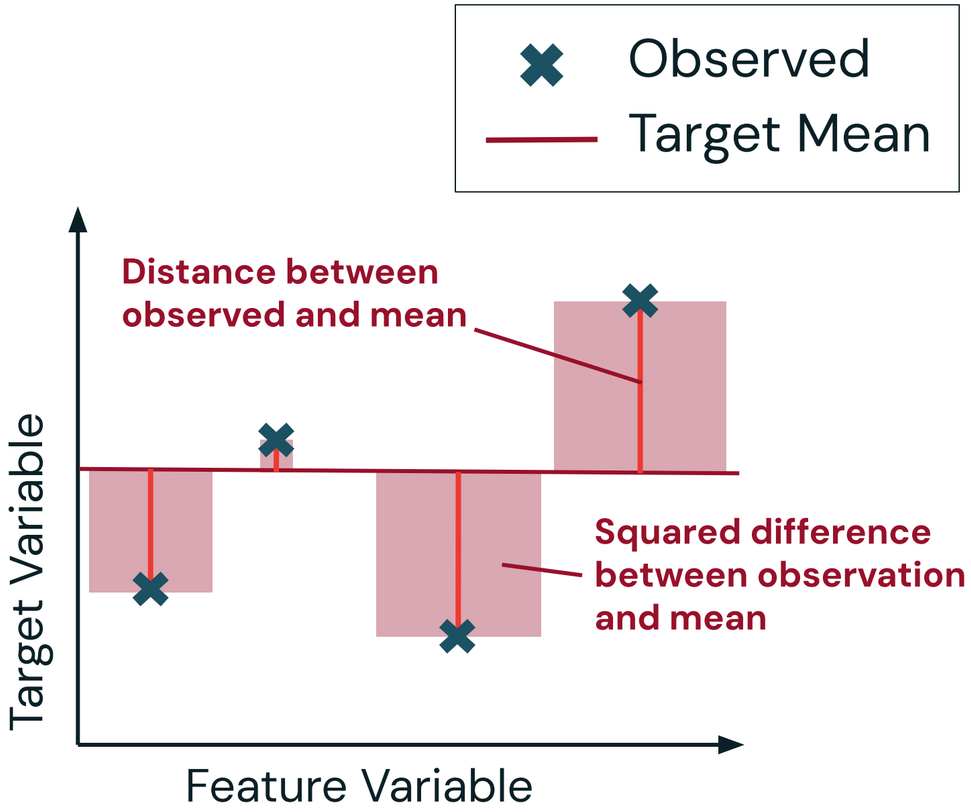
| Mean Squared Error | |
| Root Mean Squared Error | |

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# Review of Some Common Metrics

## Supervised Learning – Regression

| Metric | Description |
|---|---|
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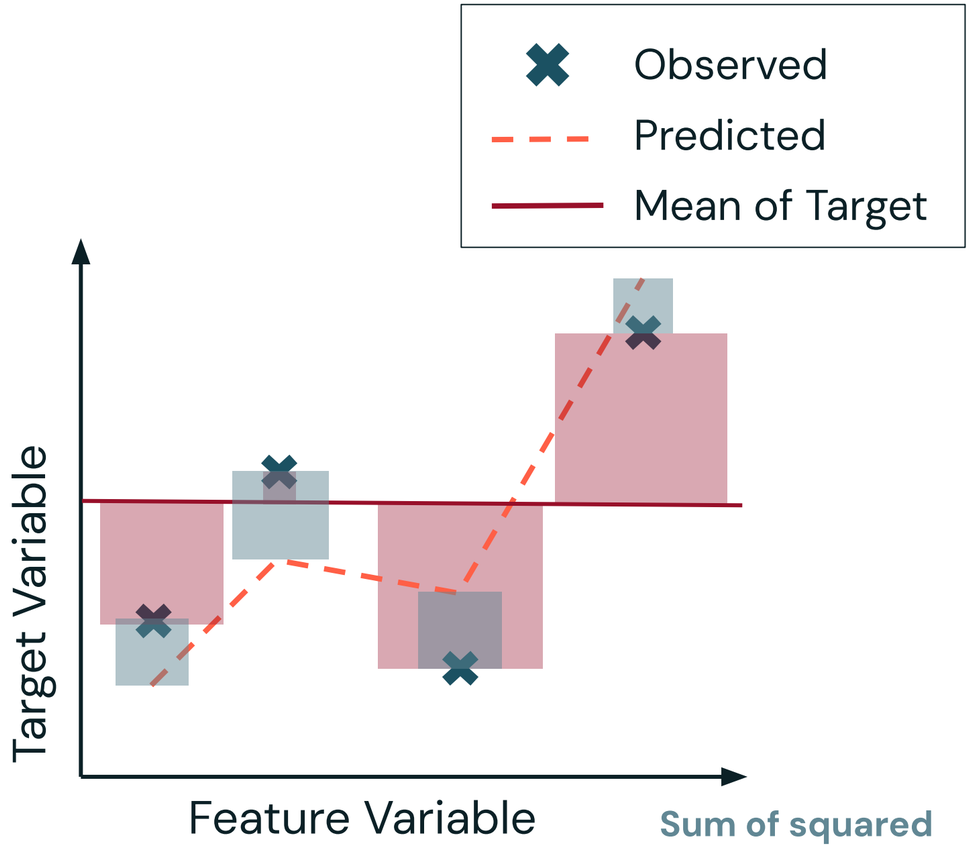
| Mean Squared Error | |
| Root Mean Squared Error | |




Sum of squared residual

$$R^2 = 1 - \frac{SS_{\text{res}}}{SS_{\text{tot}}}$$

Total sum of squares

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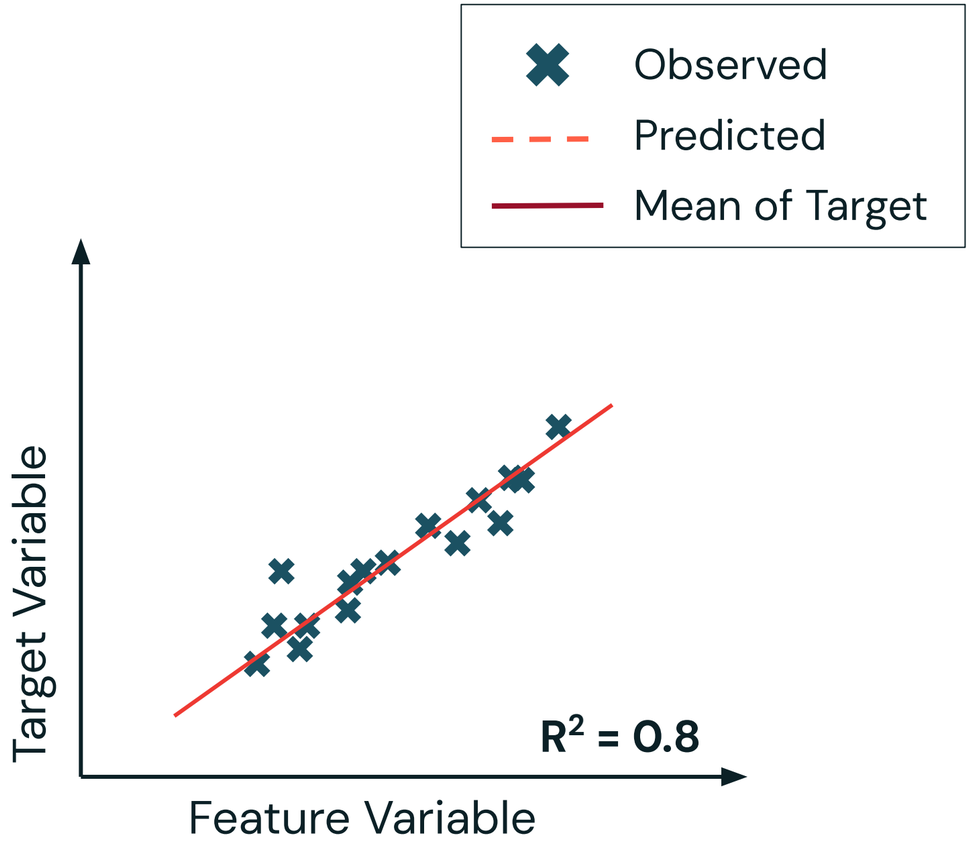
# Review of Some Common Metrics

## Supervised Learning – Regression

| Metric | Description |
| --- | --- |
| $R^2$ | Measures the proportion of variance explained by the model. Higher values indicate a better fit. |
| Mean Absolute Error | |
| Mean Squared Error | |
| Root Mean Squared Error | |

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# Review of Some Common Metrics

## Supervised Learning – Regression

| Metric | Description |
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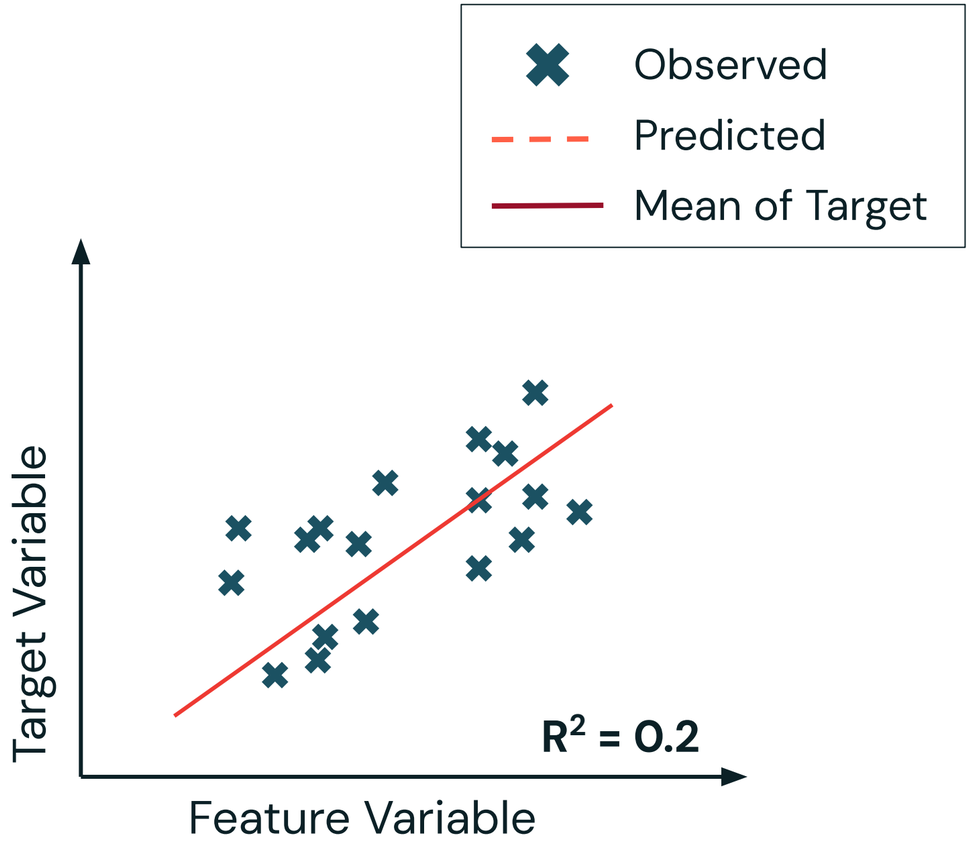


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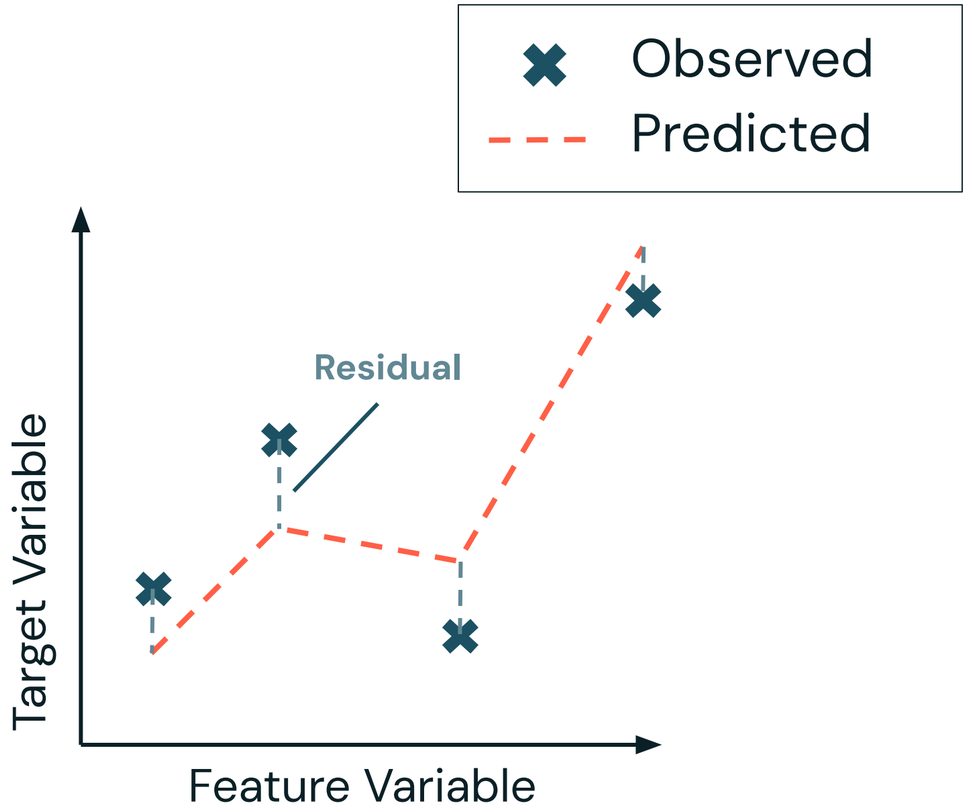
# Review of Some Common Metrics

## Supervised Learning – Regression

| Metric | Description |
|---|---|
| $R^2$ | Measures the proportion of variance explained by the model. Higher values indicate a better fit. |
| Mean Absolute Error | Computes the average of the absolute difference between actual and predicted values. Less sensitive to outliers. |
| Mean Squared Error | |
| Root Mean Squared Error | |




Residual

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|$$

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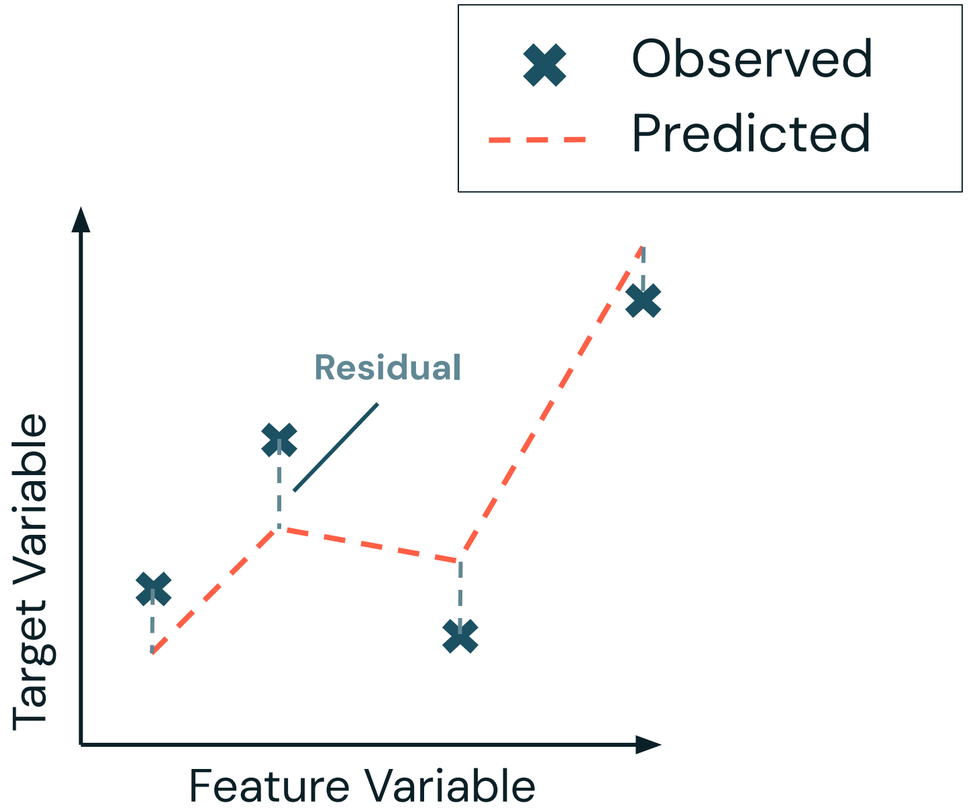
# Review of Some Common Metrics

## Supervised Learning – Regression

| Metric | Description |
|---|---|
| $R^2$ | Measures the proportion of variance explained by the model. Higher values indicate a better fit. |
| Mean Absolute Error | Computes the average of the absolute difference between actual and predicted values. Less sensitive to outliers. |
| Mean Squared Error | Penalizes larger errors more than MAE due to squaring. Common for Optimization. |
| Root Mean Squared Error | |




Residual

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

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# Review of Some Common Metrics

## Supervised Learning – Regression

| Metric | Description |
|---|---|
| $R^2$ | Measures the proportion of variance explained by the model. Higher values indicate a better fit. |
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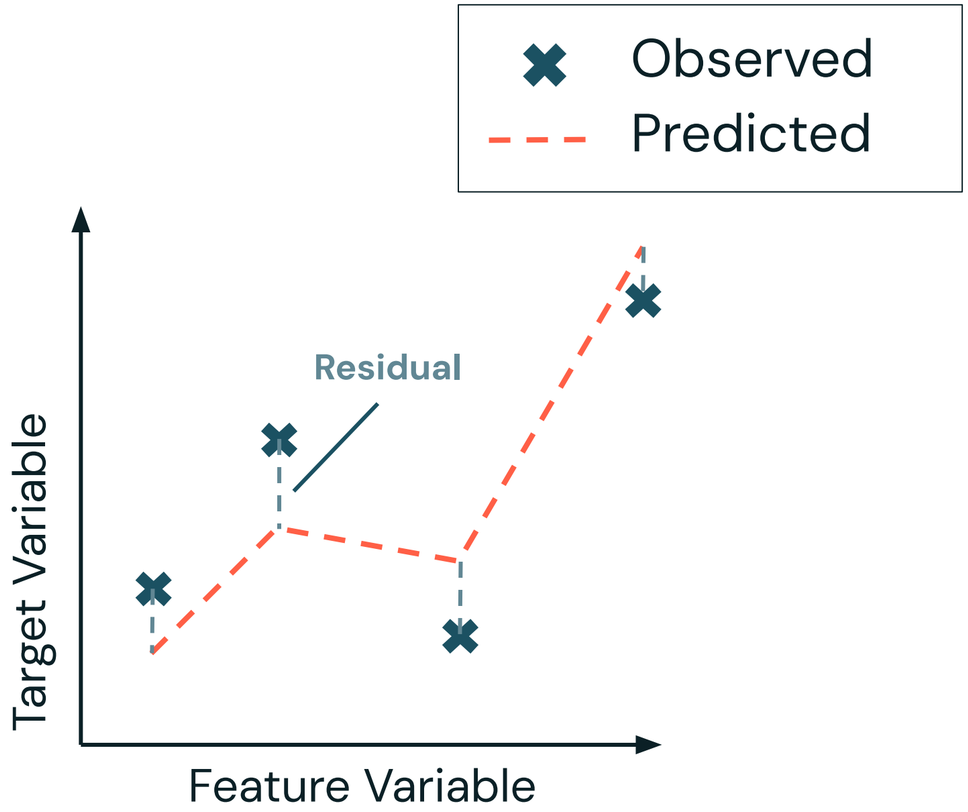
| Mean Squared Error | Penalizes larger errors more than MAE due to squaring. Common for Optimization. |
| Root Mean Squared Error | Similar to MSE but takes the square root, making it more interpretable to the original units. |




$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

Residual

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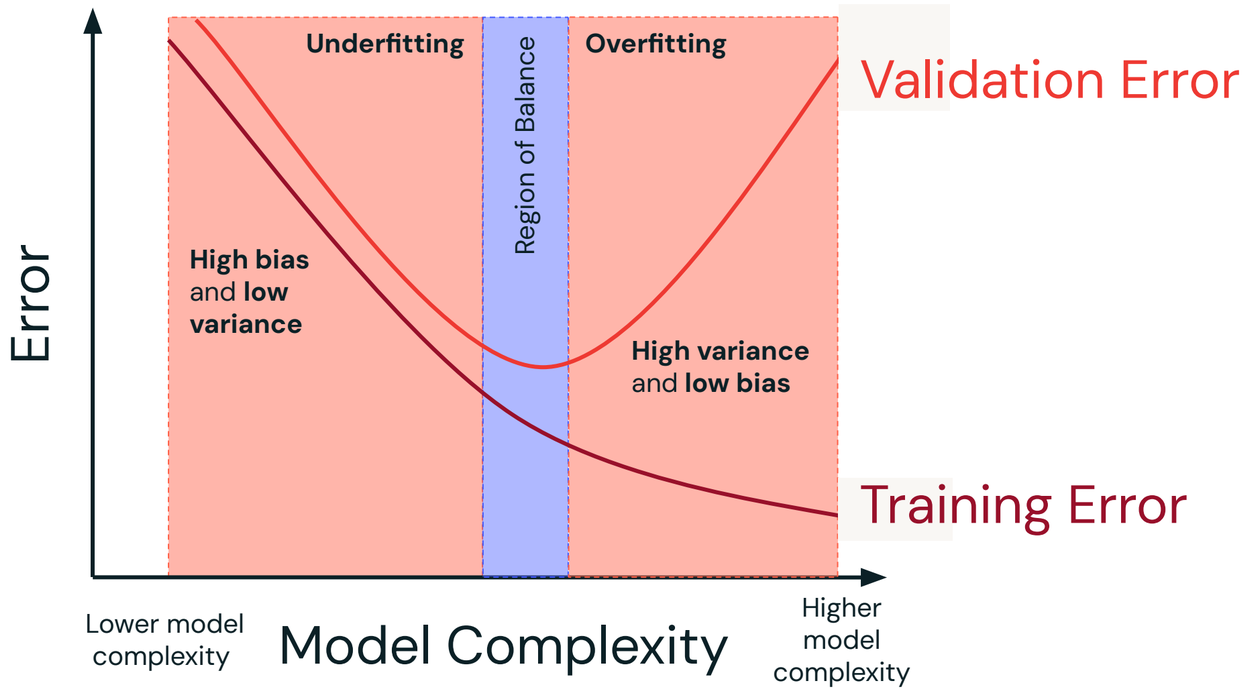
# Bias-Variance Tradeoff

## Underfitting vs Overfitting




| | Description of Error | Mitigation Strategies |
|---|---|---|
| **Bias** | Error due to overly **simplistic assumptions** in the model. | Add more features or increasing model complexity. |
| **Variance** | Error due to **sensitivity to small fluctuations** in the training data. | Add more data to help with generalizability. Add regularization, reduce model complexity, or using cross-validation. |

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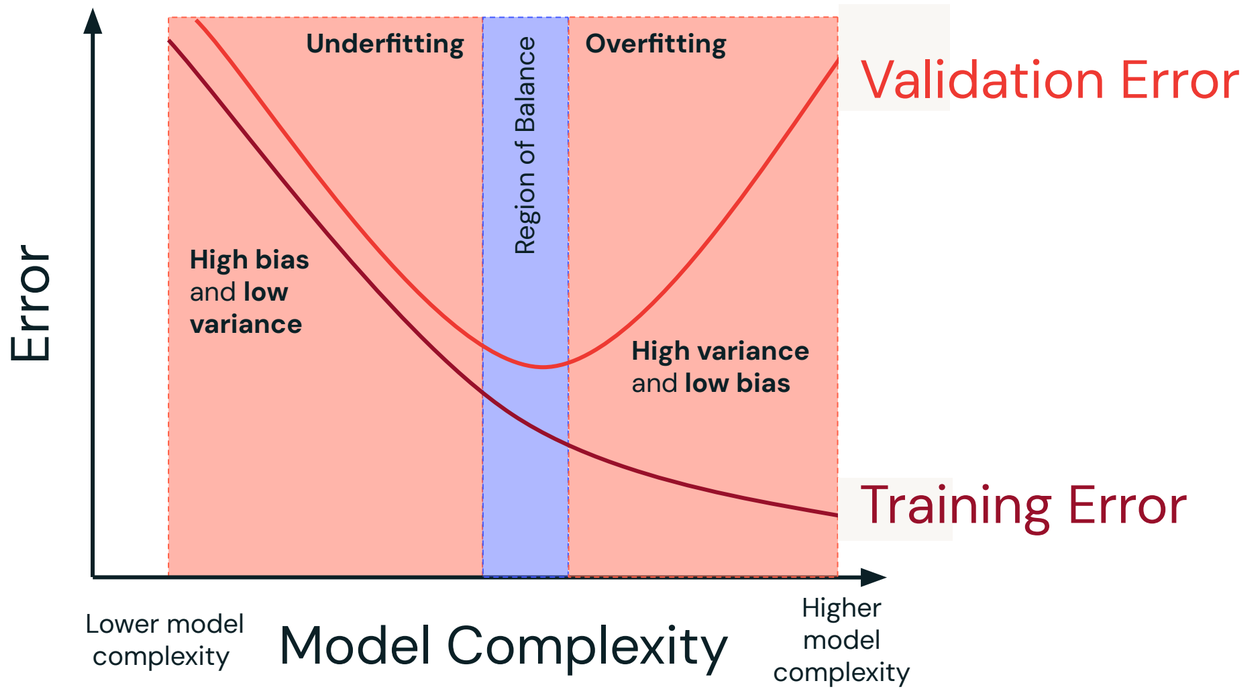
# Bias-Variance Tradeoff

## Underfitting vs Overfitting




| | Reason | Increase/ Decrease |
|---|---|---|
| **High Bias** | Model is too simple. | ▲FP & ▲FN |
| **High Variance** | Model does not generalize well, leading to precision-recall tradeoffs. | ▲FP & ▼ FN<br>or<br>▼ FP & ▲FN |

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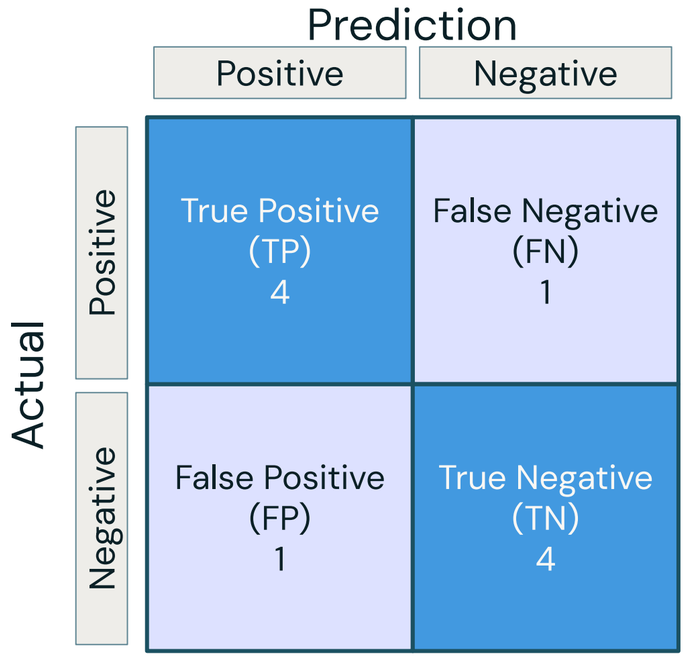
# Review of Some Common Metrics

## Supervised Learning - Classification

| Metric | Description |
|---|---|
| Accuracy | Measures the proportion of correctly classified instances. It can be misleading for imbalance datasets. |
| Precision | |
| Recall (Sensitivity) | |
| F1 Score | |




$$\frac{TP+TN}{TP+TN+FP+FN} = \frac{4}{5}$$

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# Review of Some Common Metrics

## Supervised Learning – Classification

| Metric | Description |
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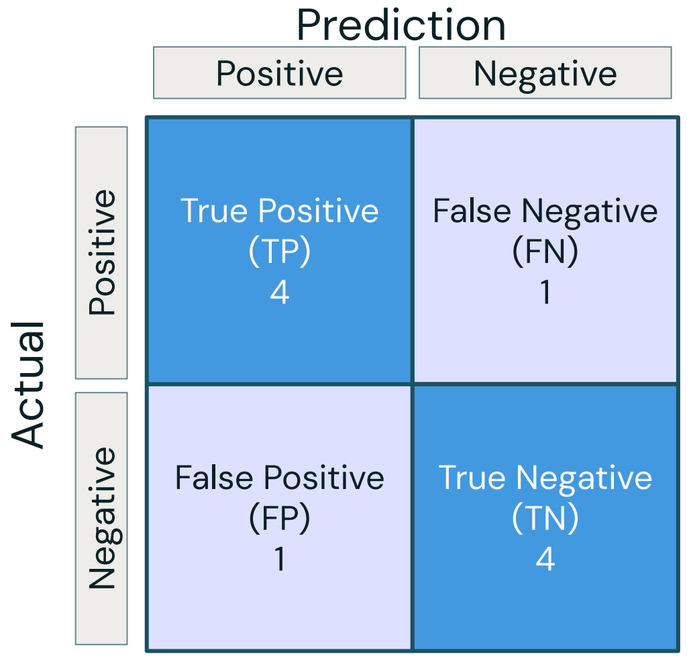
| Accuracy | Measures the proportion of correctly classified instances. It can be misleading for imbalance datasets. |
| Precision | Measures how many predicted positives are actually correct. Important when false positives are costly. |
| Recall (Sensitivity) | |
| F1 Score | |




$$\frac{TP}{TP+FP} = \frac{4}{5}$$

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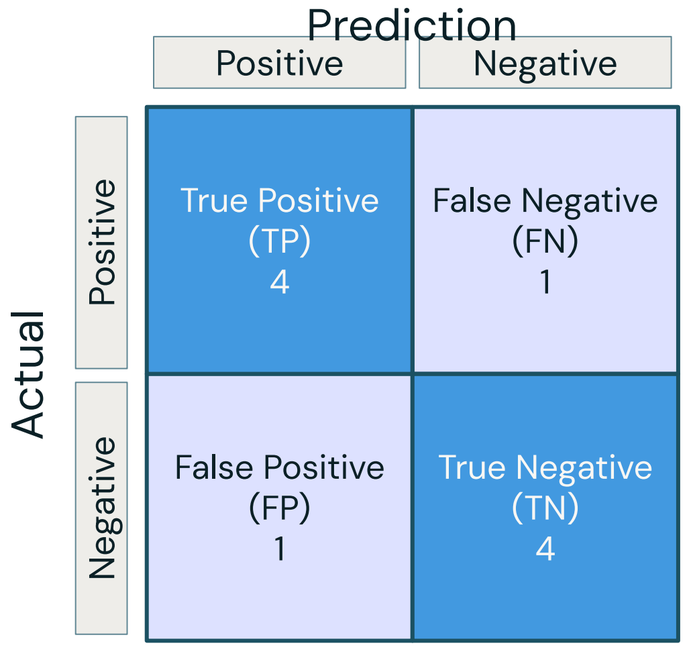
# Review of Some Common Metrics

## Supervised Learning – Classification

| Metric | Description |
|---|---|
| Accuracy | Measures the proportion of correctly classified instances. It can be misleading for imbalance datasets. |
| Precision | Measures how many predicted positives are actually correct. Important when false positives are costly. |
| Recall (Sensitivity) | Measures how many actual positives were correctly identified. Important when false negatives are costly. |
| F1 Score | |




$$\frac{TP}{TP+FN} = \frac{4}{5}$$

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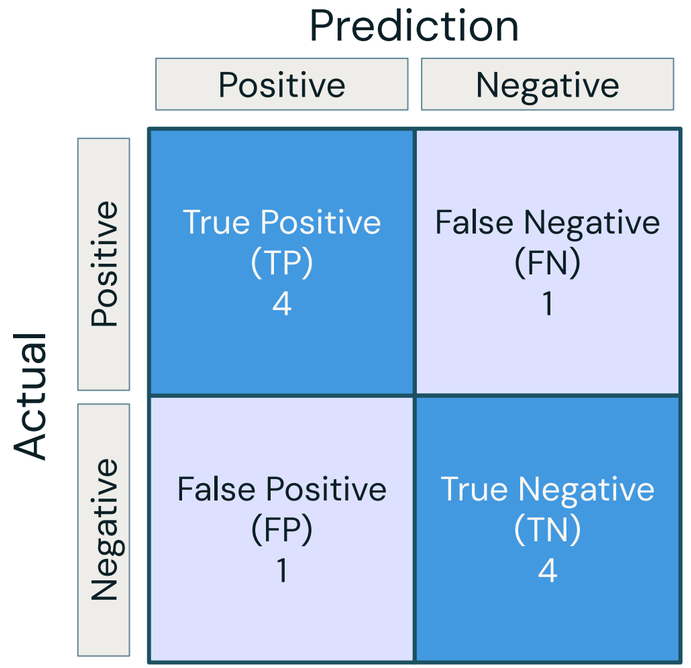
# Review of Some Common Metrics

## Supervised Learning - Classification

| Metric | Description |
|---|---|
| Accuracy | Measures the proportion of correctly classified instances. It can be misleading for imbalance datasets. |
| Precision | Measures how many predicted positives are actually correct. Important when false positives are costly. |
| Recall (Sensitivity) | Measures how many actual positives were correctly identified. Important when false negatives are costly. |
| F1 Score | Measures the proportion of correctly classified instances. It can be misleading for imbalance datasets. |




$$2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}} = \frac{4}{5}$$

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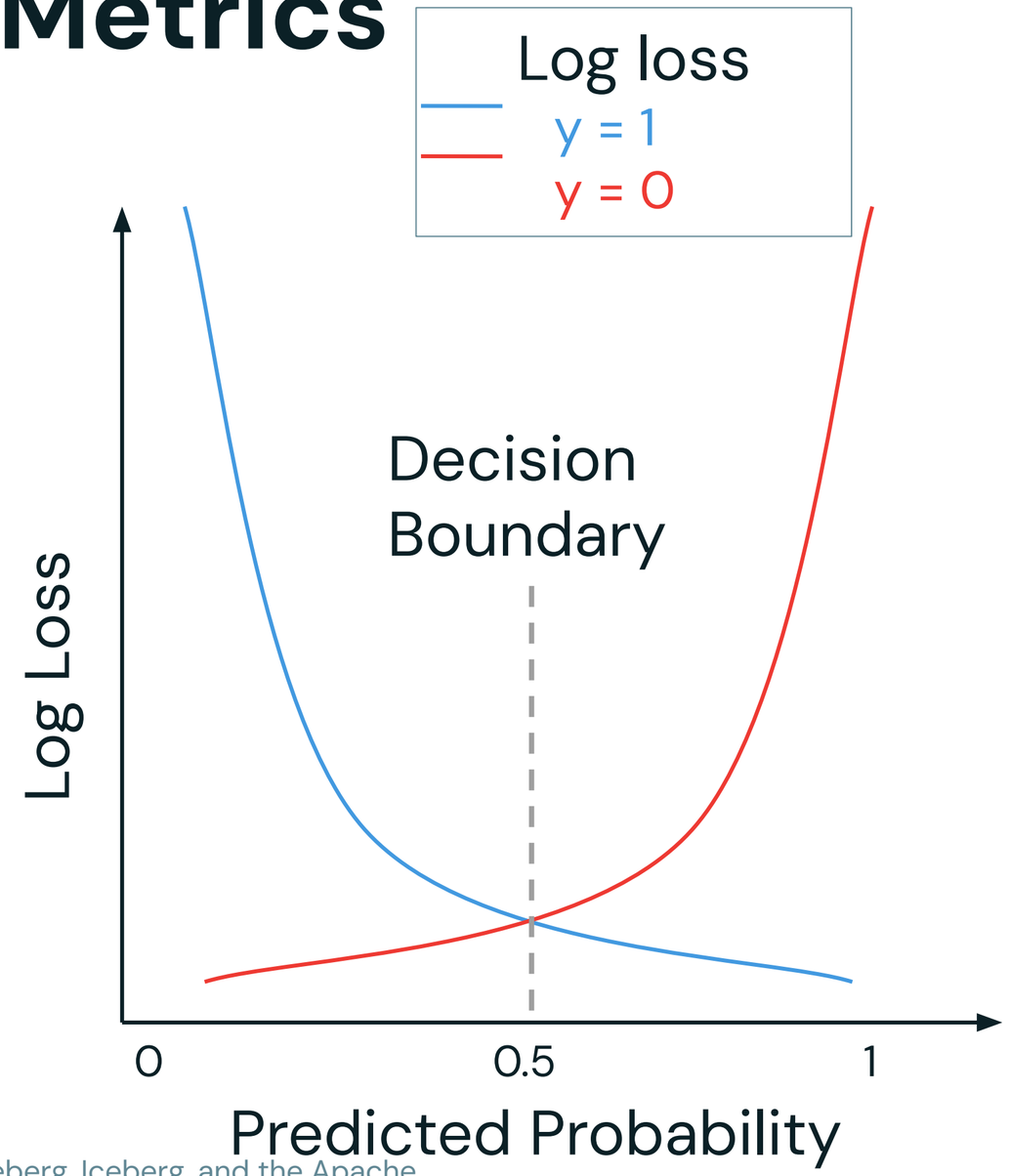
# Review of Some Common Metrics

## Supervised Learning – Classification

| Metric | Description |
|---|---|
| Log loss (Cross-Entropy Loss) | Measures how many predicted positives are actually correct. Important when false positives are costly. |
| ROC/AUC | |

$$-\frac{1}{n}\sum_{i=1}^{n}\left[y_i \log(\hat{y}_i) + (1-y_i)\log(1-\hat{y}_i)\right]$$

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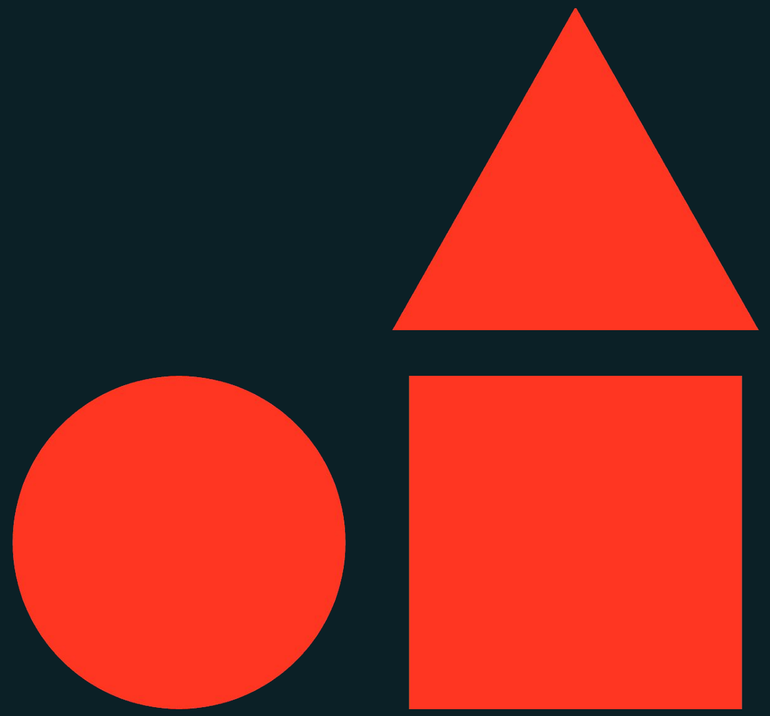
# Hyperparameter Tuning



## Machine Learning Model Development

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# Learning objectives

Things you'll be able to do after completing this module

- Define a hyperparameters
- Describe, compare, and contrast grid, random, and Bayesian search methods for hyperparameter tuning
- Describe cross-validation as a method for robust performance estimation
- Describe Optuna as an open-source hyperparameter optimization (HPO) framework

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Hyperparameter Tuning

LECTURE

# Hyperparameter Tuning Fundamentals

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# What is a Hyperparameter

## Definitions

- **Hyperparameter** is a parameter whose value is used to **control** the training process.

- **Hyperparameter Tuning** (model tuning) is the process of adjusting the hyperparameters of a model **to find the best configuration** that **maximizes its performance** on a given dataset.

**Example Hyperparameters:**

- Random Forest:
  - `Maximum depth of trees`
  - `Number of trees`
  - `Number of features`
- Linear regression
  - `Normalize features or not`
- Neural Networks
  - `Activation function`
  - `Number of neurons in each hidden layer`

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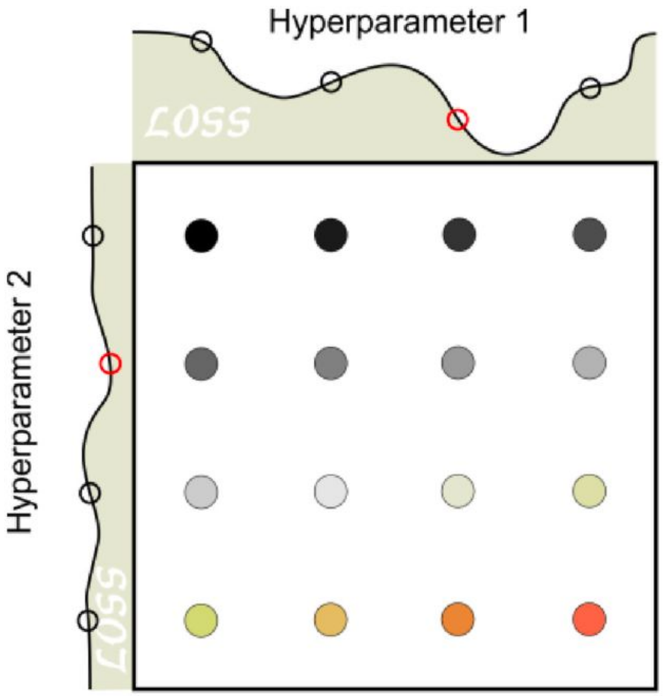
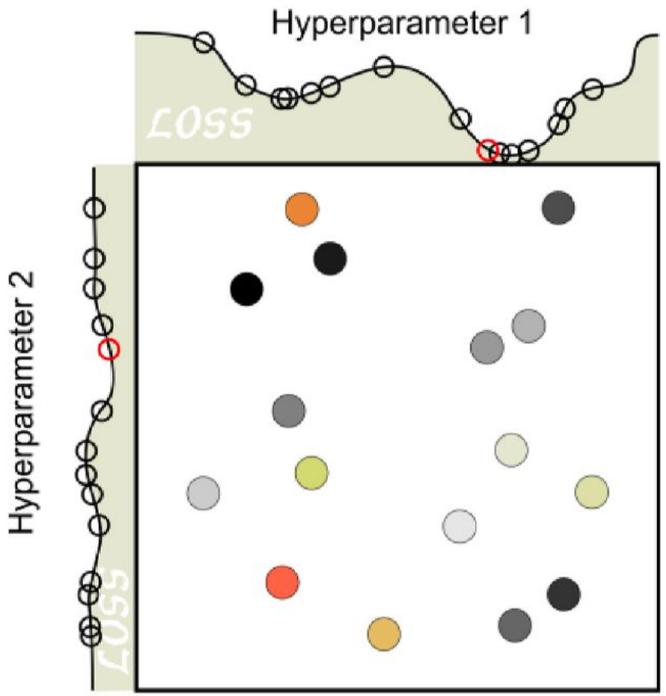
# Hyperparameter Search Methods

## How to pick a hyperparameter?

### Grid Search




### Random Search




### Bayesian Optimization

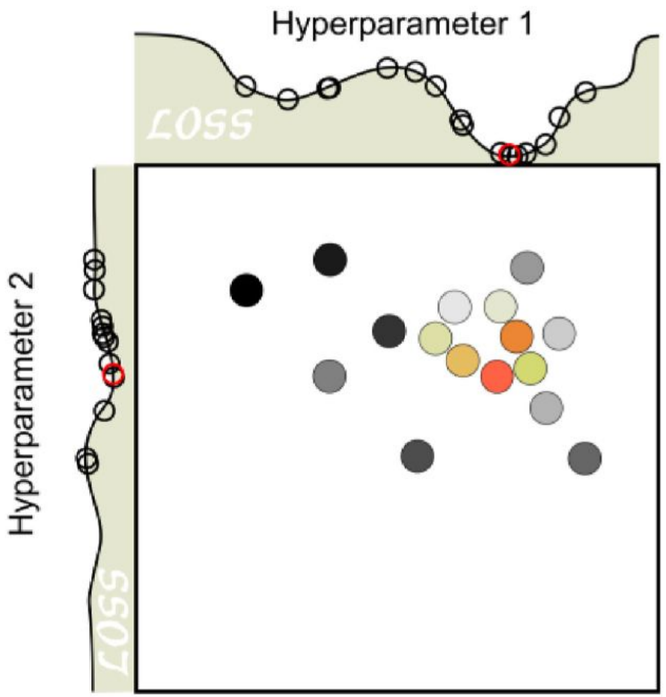



Image Source

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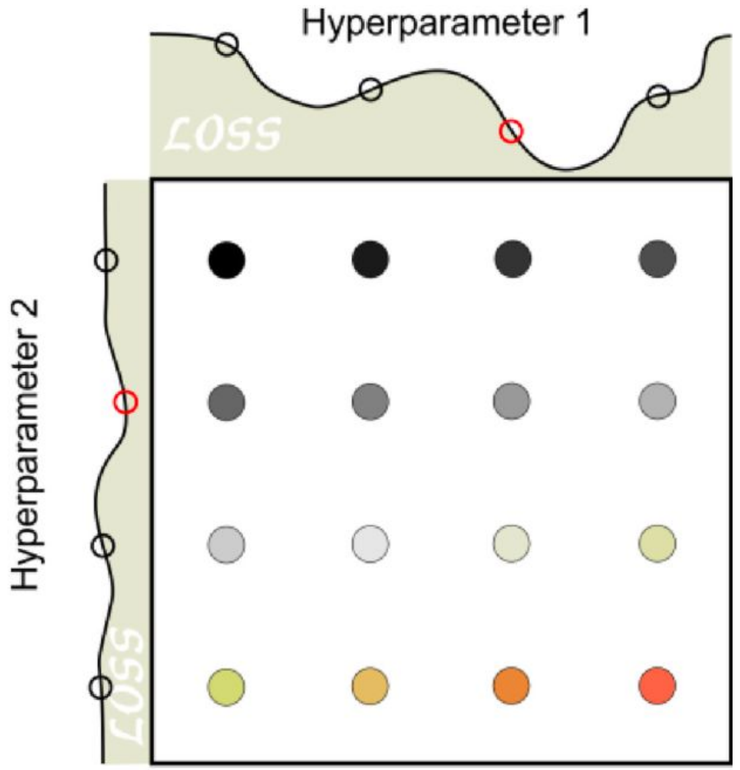
# Grid Search

## Systematic parameter selection

- Define a grid of hyperparameter values and exhaustively searching through all possible combinations.
- Evaluate each combination using cross-validation and selects the best set of hyperparameters.
- Can be computationally expensive, especially when the number of hyperparameters and their possible values is large




Grid Search will always find the best parameter, but is computational expensive.

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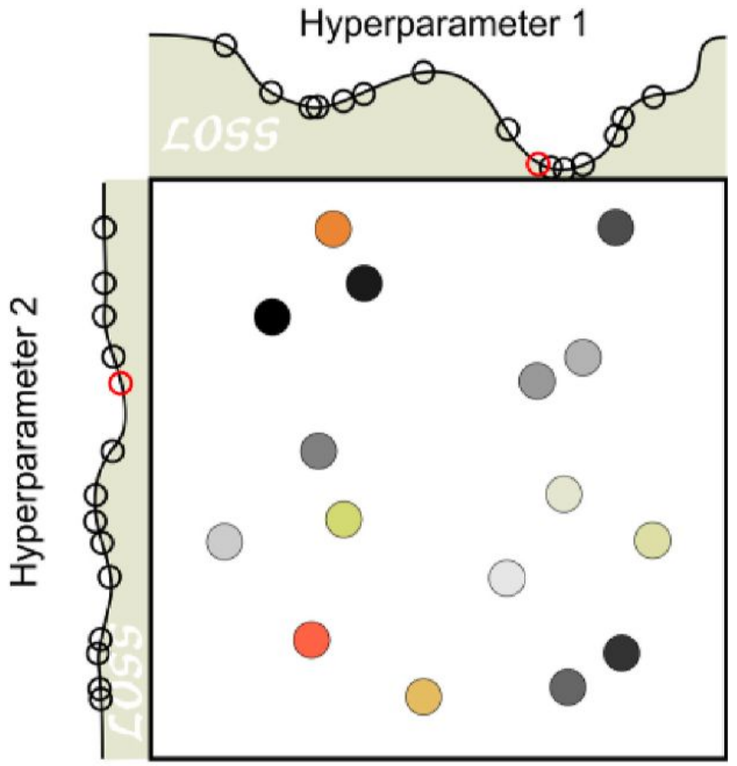
# Random Search

## Stochastic parameter selection

- Randomly samples hyperparameter values from specified distributions.
- Random search is more efficient than grid search, especially when dealing with large datasets or hyperparameters.
- It doesn't guarantee the best combination.




Random Search generally outperforms grid search, but does not systematically cover all possible values.

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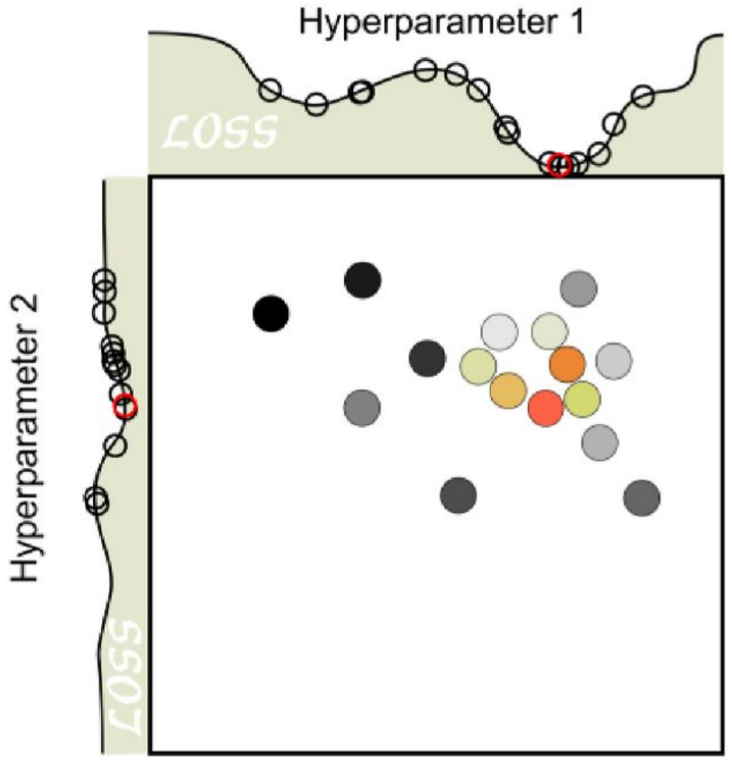
# Bayesian Optimization

## Probabilistic parameter selection

- Aiming to **minimize validation error** by constructing a **probability model** of the objective function.
- Guides the search based on **previous evaluations** to focus on promising regions of the hyperparameter space.
- **The Tree of Parzen Estimators (TPE)** algorithm is a popular Bayesian method.




Bayesian approaches generally outperform grid search and random search, but more complex to implement.

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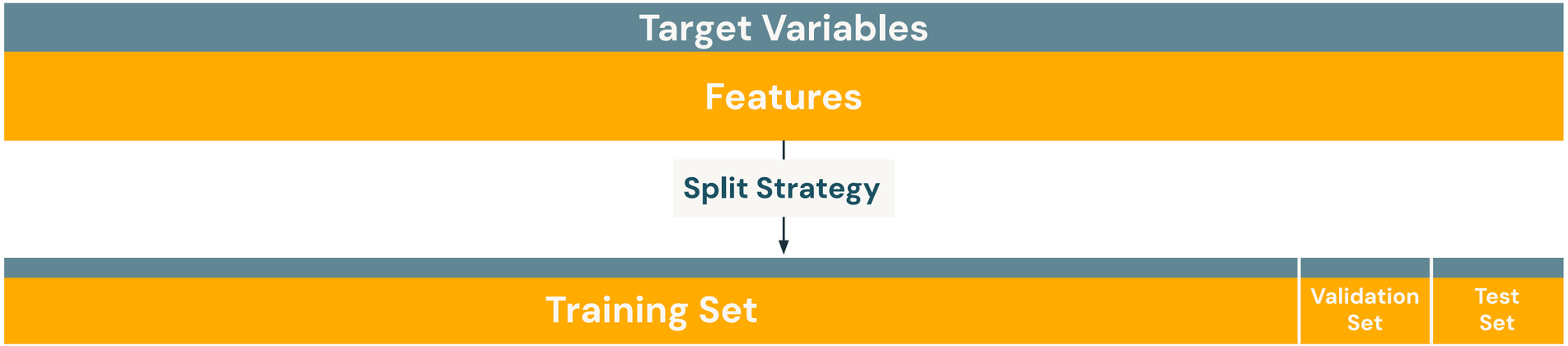
# Validation

- The validation set is one of our holdout datasets
- Build a model for each set of hyperparameter values
- Evaluate each model to identify the optimal hyperparameter values
- What dataset should we use to train and evaluate?




**What if there isn't enough data to split into three separate sets?**
**Risk of overfitting due to non-random initial split?**

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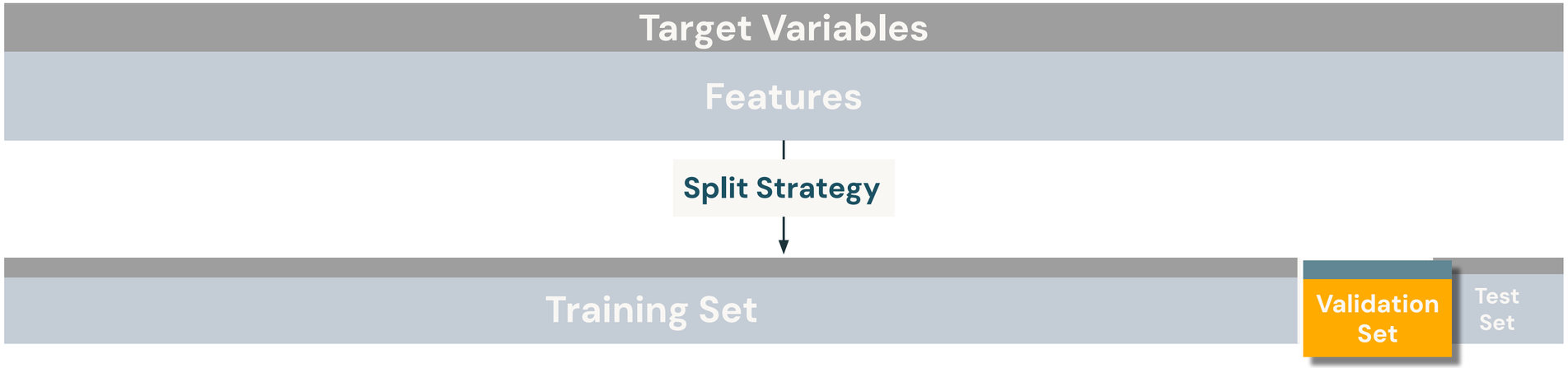


**What if there isn't enough data to split into three separate sets?**
**Risk of overfitting due to non-random initial split?**

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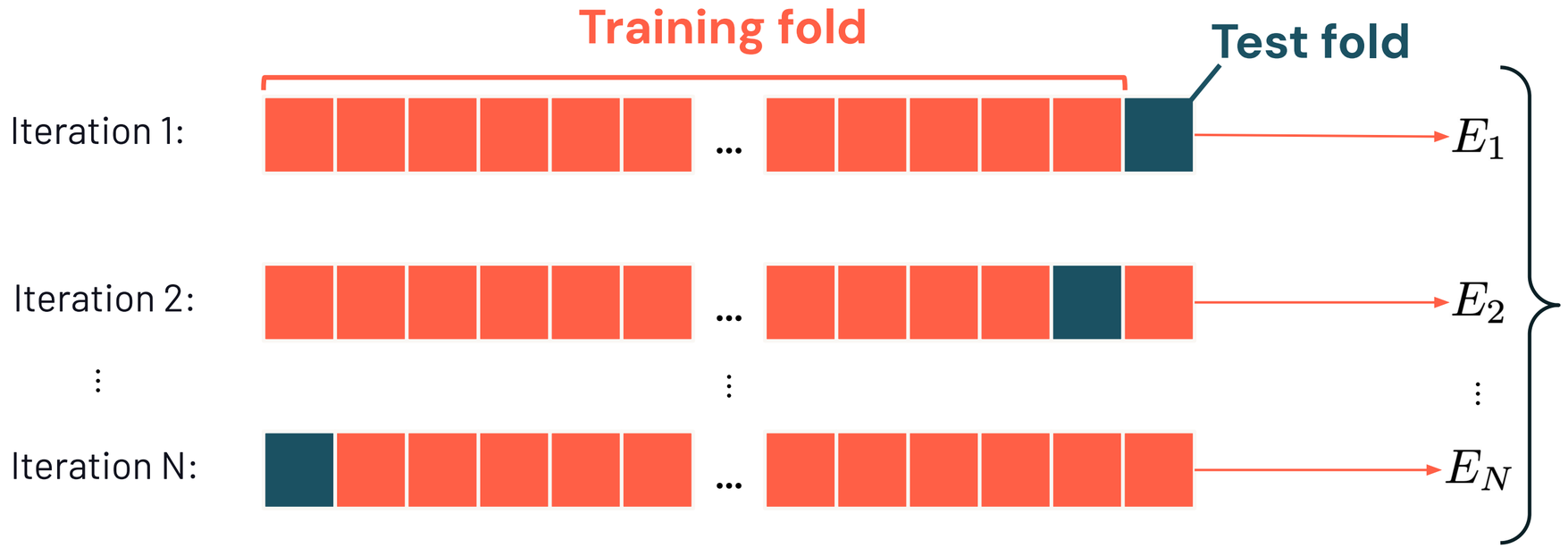
# K-Fold Cross Validation

## A method for robust performance estimation




Average the errors:

$$\frac{1}{N}\sum_{i=1}^{N} E_i$$

Final Pass: **Training with Optimal Hyperparameters** | **Test**

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# Tuning Can be Expensive!

## A **Grid Search** example

Train and validate **every unique combination** of hyperparameters

| Tree Depth | Number of Trees |
|---|---|
| 5 | 2 |
| 8 | 4 |

| Tree Depth | Number of Trees |
|---|---|
| 5 | 2 |
| 5 | 4 |
| 8 | 2 |
| 8 | 4 |

**K (folds)**

**Best model**

**Question:** With 3-fold cross validation, how many models will this build?

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# Optuna

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# Popular Tools for Hyperparameter Opt.





- **Scikit-learn's** `GridSearchCV` and `RandomizedSearchCV`: Offer grid search and random search for hyperparameter tuning.
- **Hyperopt**: A popular library for performing hyperparameter optimization using Bayesian methods. **Hyperopt will be removed with DBR ML version 17.0+.**
- **Ray**: Ray Tune provides a scalable library for hyperparameter tuning, offering both grid and advanced search algorithms.
- **Optuna**: **An open source hyperparameter optimization framework to automate hyperparameter search.**

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# Optuna: Lightweight, Versatile, and Platform Agnostic

## Simple installation and minimal requirements

- Optuna is written entirely in Python with few dependencies.
- Intuitive API:
  - Define parameters within your code.
  - No need for framework-specific syntax.
- Platform and Framework Agnostic
  - e.g. PyTorch, TensorFlow, Keras, Scikit-Learn, XGBoost, LightGBM, etc.


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# Optuna Terminology

## Definitions

- A **trial** is a single call of the objective function.
- A **study** is an optimization session, which is a collection of trials.
- A **parameter** is a variable whose value is to be optimized, which is typically the loss or accuracy of the model.

Optuna is a framework designed for the *automation* and the *acceleration* of the *optimization* studies.

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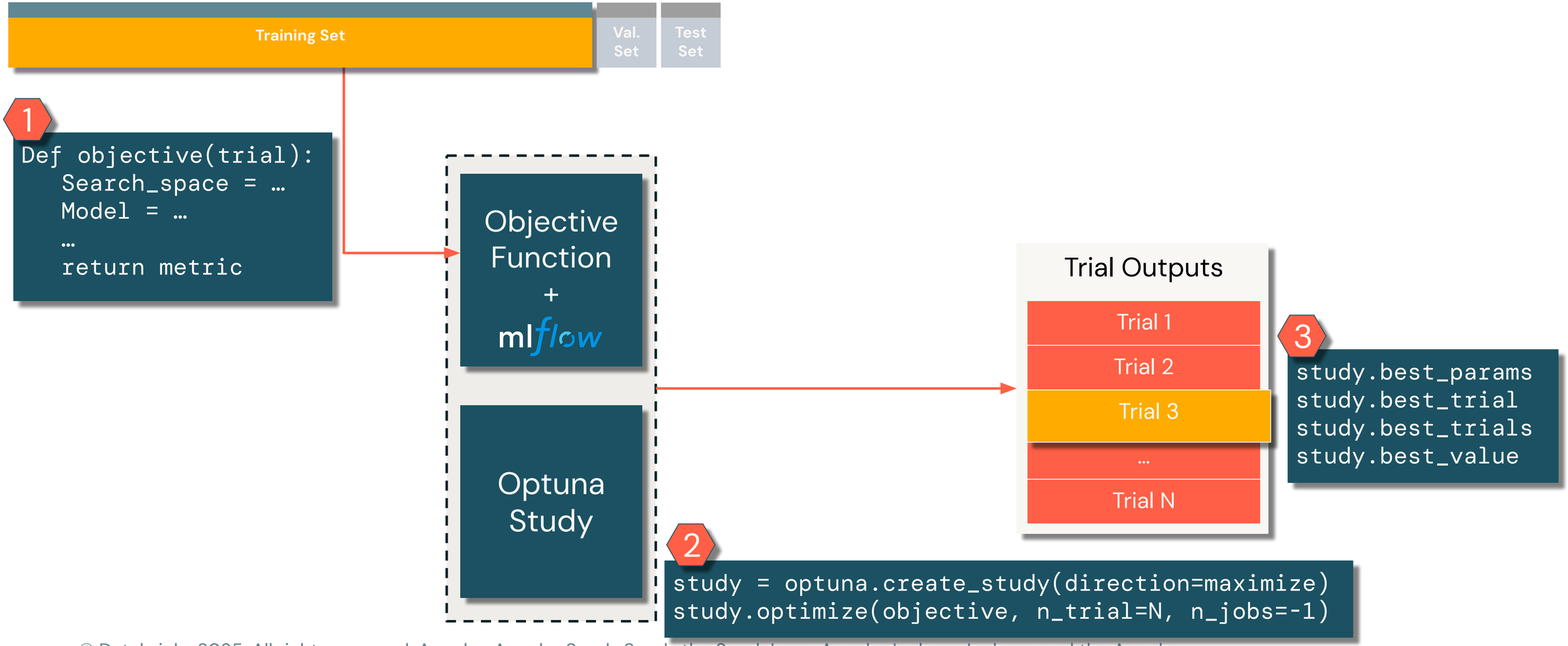
# Hyperparameter Optimization Framework

## Automating Hyperparameter Search

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# Key Concepts

## Search space and algorithms

### Search Space Definition with Python Syntax

- Hyperparameter search space can be defined using functions such as;
  - `suggest_discrete_uniform`
  - `suggest_categorical`
  - `suggest_float`
  - `suggest_int`
  - `suggest_uniform`

### Sampling Strategy

- Sampling strategy determines how to decide the next hyperparameter.
- Continuously refine the search space using past evaluation results to focus on promising areas.
- Some of the supported strategies; Grid Search, Random Search, **Tree-structured Parzen Estimator algorithm (default)**

### Pruning Strategy*

- Early stopping halts unpromising trials early based on intermediate results.
- Call report() and should_prune() after each step to activate pruning.

*Not covered in this course.

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# Optuna – MLflow Integration

## Track hyperparameters and metrics of all the Optuna trials

**MLflowCallback**: This callback **enables automatic logging** of hyperparameters and metrics for each trial into MLflow, streamlining experiment tracking.

**Parent-Child Run Organization**: MLflow's support for hierarchical run structures allows grouping of all Optuna trials under a single parent run.

```
from optuna.integration.mlflow import MLflowCallback
mlflow_callback = MLflowCallback(
    tracking_uri = “databricks”,
    create_experiment= False,
    mlflow_kwargs = {
        “experiment_id”: <experiment_id>,
        “Nested”: True
    }
}

study.optimize(
    objective,
    n_trials = N,
    callbacks = [mlflow_callback])
```

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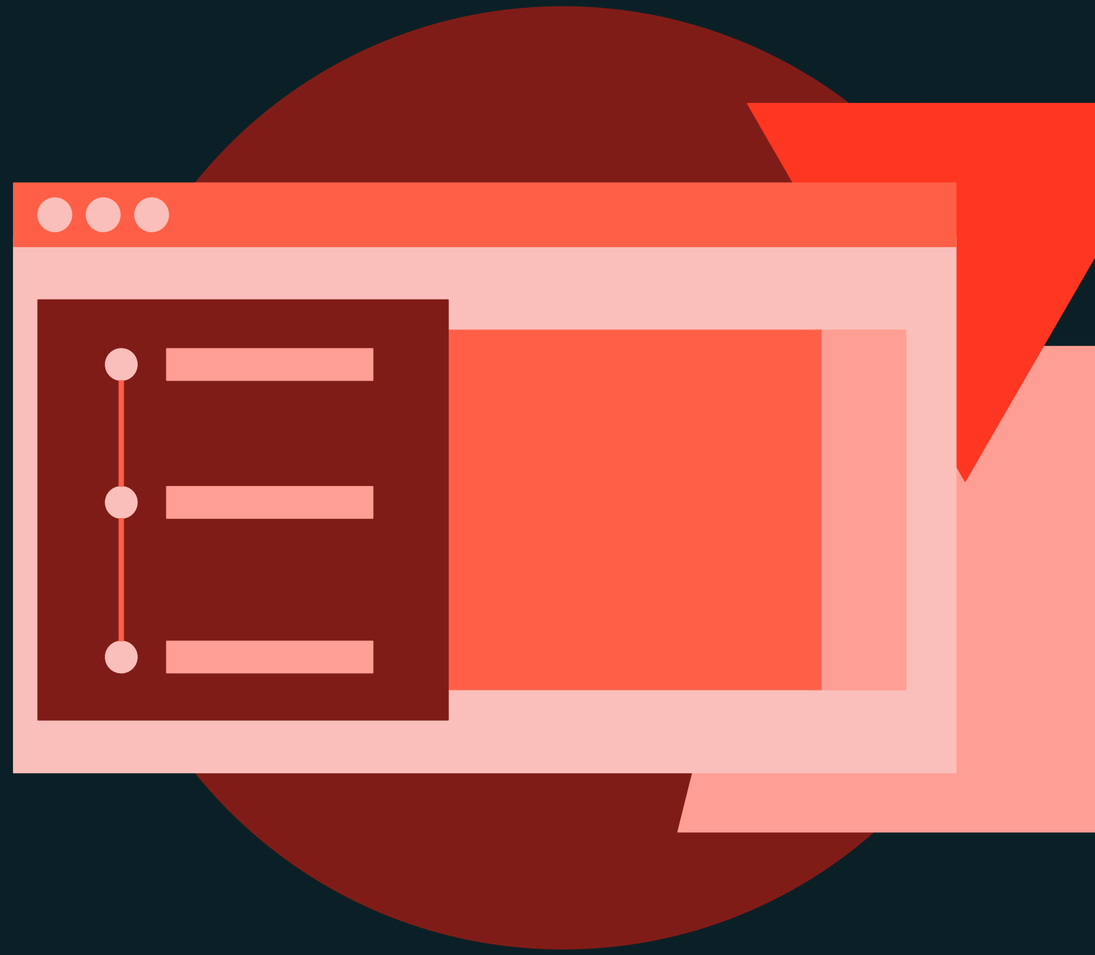
Hyperparameter Tuning

DEMONSTRATION

# Hyperparameter Tuning with Optuna



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Hyperparameter Tuning

LAB EXERCISE

# Hyperparameter Tuning with Optuna

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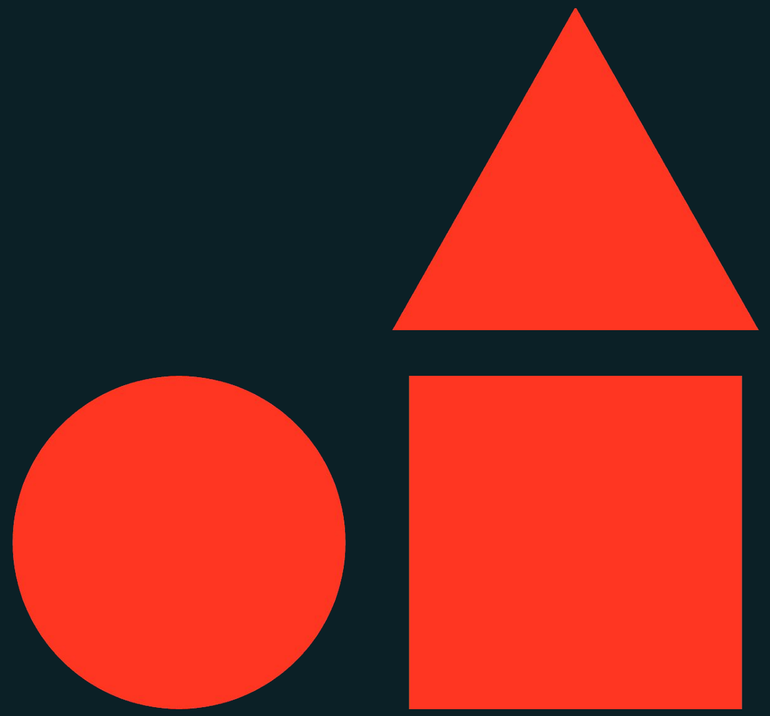
# AutoML



## Machine Learning Model Development

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# Learning objectives

Things you'll be able to do after completing this module

- Describe the benefits of using AutoML to generate machine learning models.
- Describe the glass box nature of AutoML.
- Start an AutoML experiment via the UI and the API.
- Open and edit a notebook generated by AutoML.
- Identify the best model generated by AutoML based on a given metric.
- Modify the best model generated by AutoML.

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AutoML

LECTURE

# Introduction to AutoML

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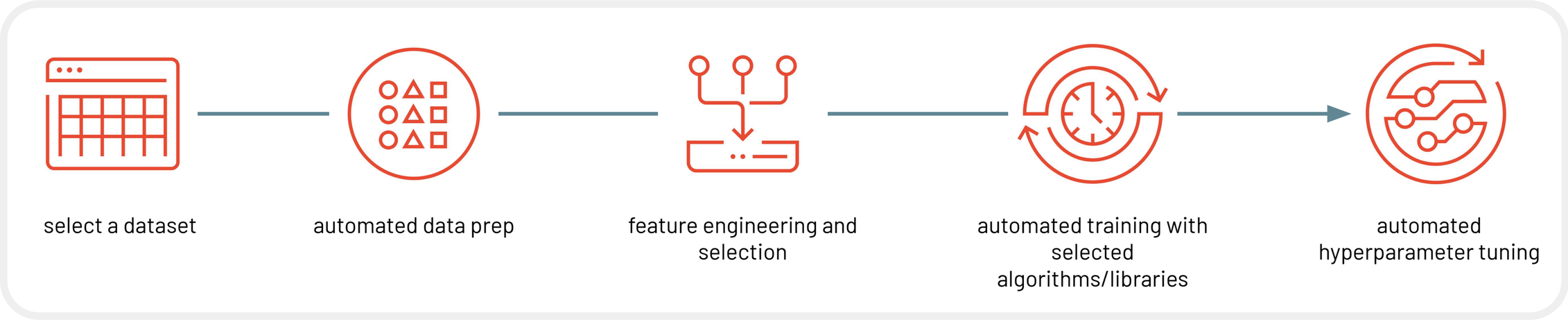
# What is AutoML?

**Automated machine learning** (**AutoML**) is a fully-automated model development solution seeking to "democratize" machine learning. While the scope of the automation varies, AutoML technologies usually **automate the ML process from data to model selection**.

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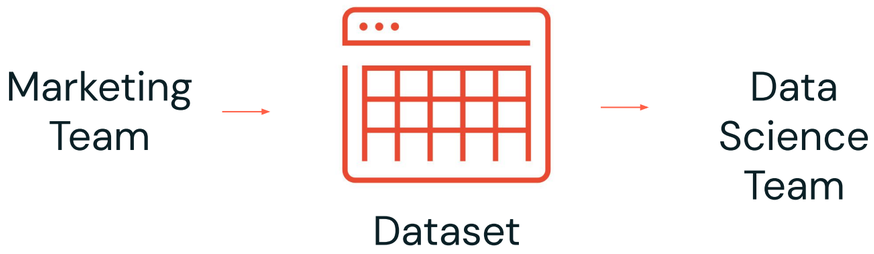
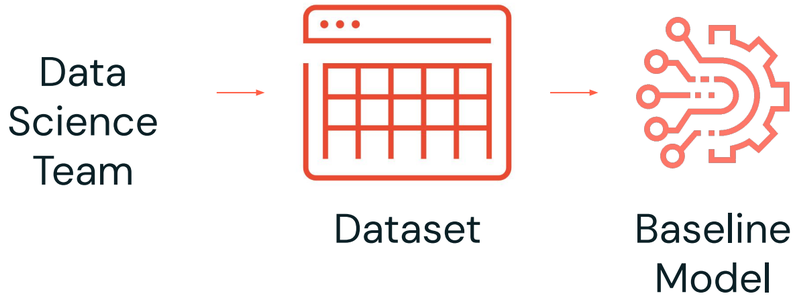
# Two Key Pain Points Solved with AutoML

## Quickly Verify the Predictive Power of a Dataset




*"Can this dataset be used to predict customer churn?"*

## Get a Baseline Model to Guide Project Direction




*"What direction should I go in for this ML project and what benchmark should I aim to beat?"*

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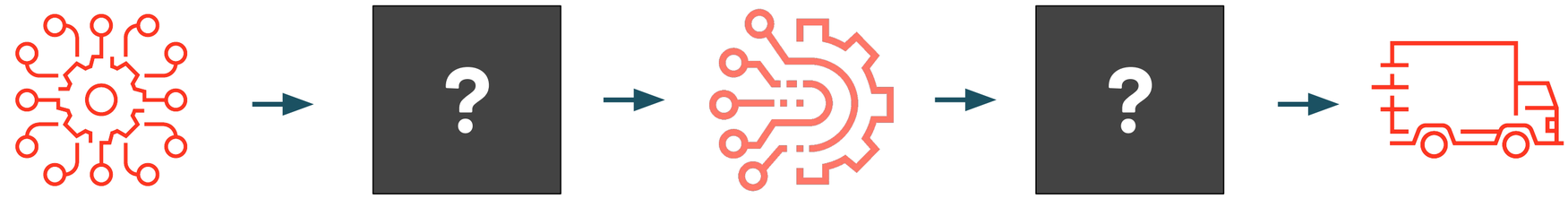
# Problems with Existing AutoML Solutions

**Opaque-Box and Production Cliff Problems in AutoML**




| Problem | Result / Pain Points |
| --- | --- |
| 🚨 Data scientists need to be able to explain how they trained a model for regulatory purposes (e.g., FDA, GDPR, etc.) - "opaque box" models do not help. | ⚠️ Time and energy required to reverse engineering these "opaque-box" returned models to modify and/or explain them. |
| 🚨 A "production cliff" exists where data scientists need to modify the returned "best" model using their domain expertise. | ⚠️ The "best" model returned is often not good enough to deploy |

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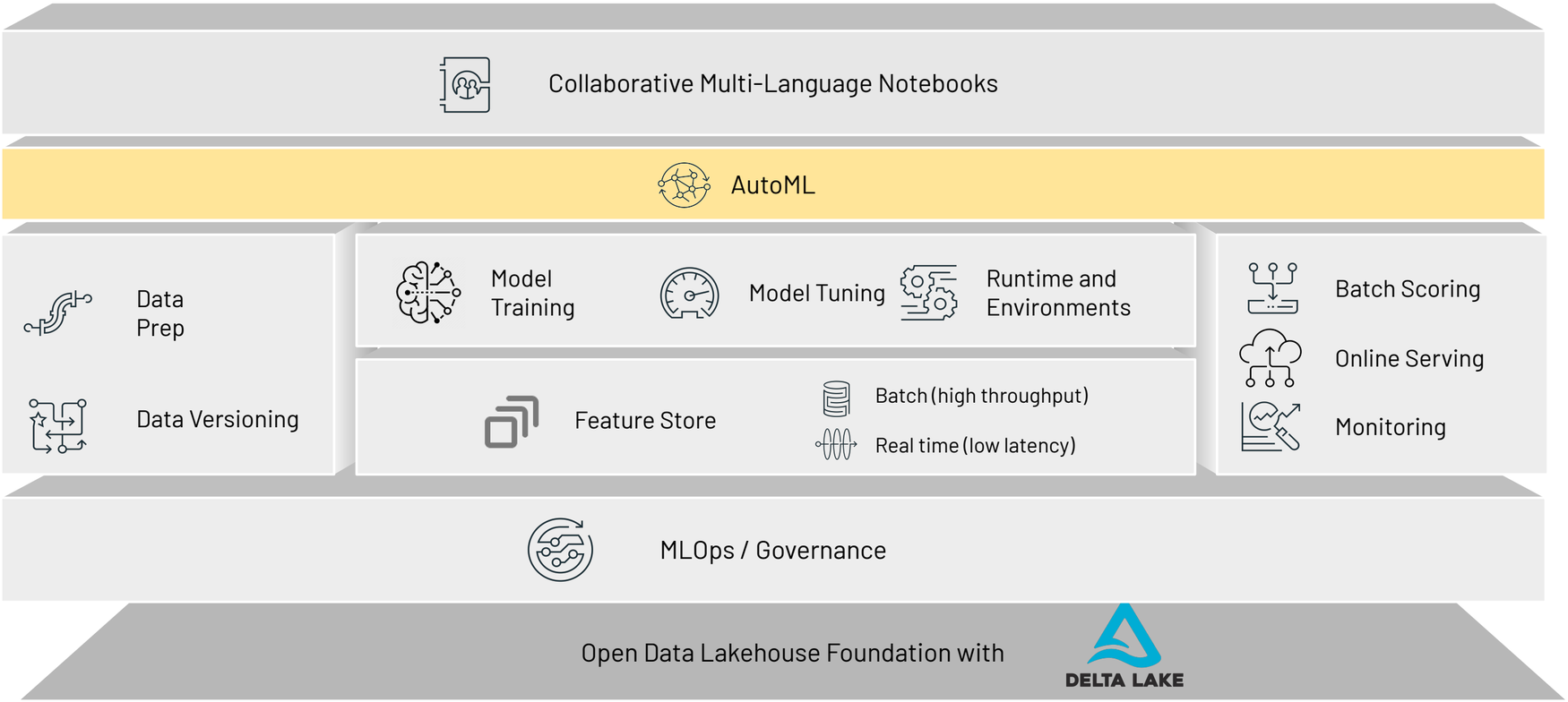
# Solution: Databricks AutoML

## Rapid, simplified machine learning built on the Lakehouse Architecture

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# Solution: Databricks AutoML

## Rapid, simplified machine learning **for everyone**

### Quick-start ML initiatives

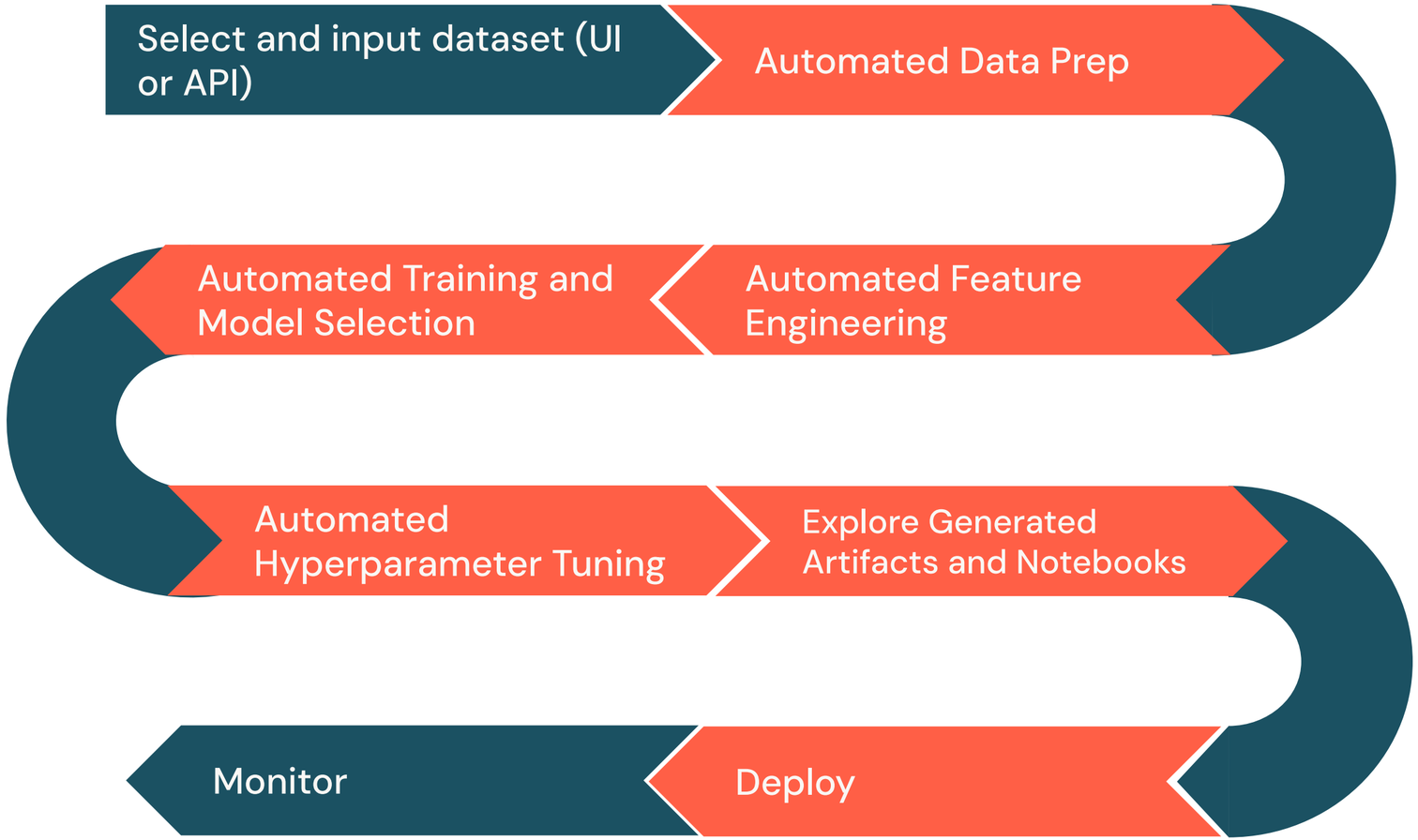
Accelerate your time to production,
Save weeks on ML projects

### Auto-generated notebooks

Ensure best practices.
Customize baseline models with your domain expertise

### Wide range of problems

Solve classification, regression, and forecasting problems from a variety of ML libraries

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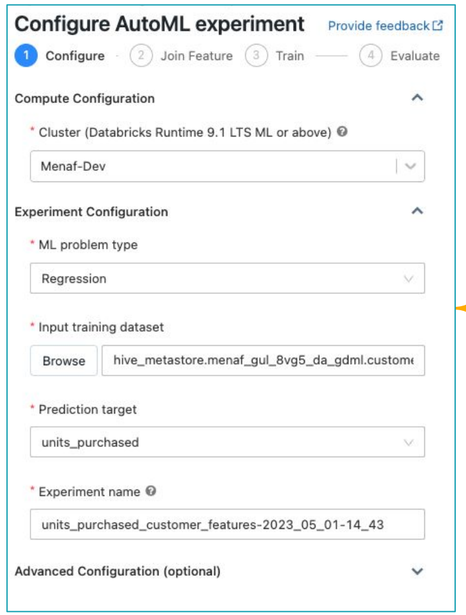
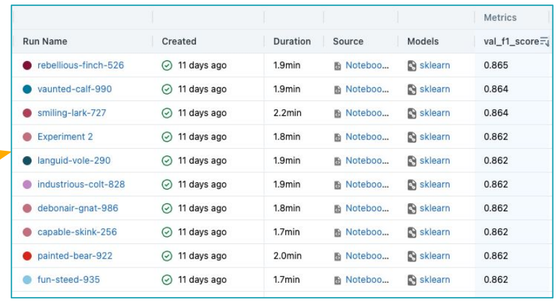
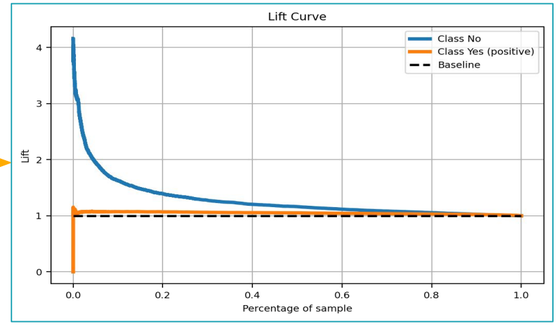
# Databricks AutoML

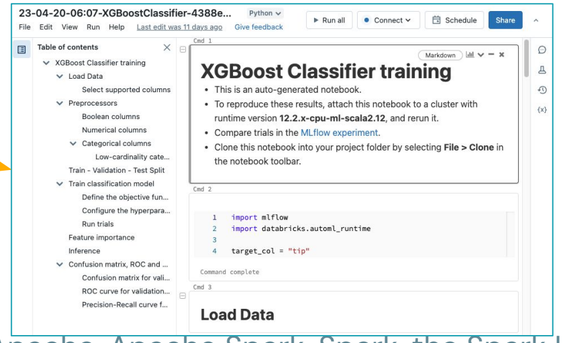
## A glass-box solution empowering data teams without taking away control

**UI and API** to start AutoML training




**Auto-created MLflow Experiment to track models and metrics** → Easily deploy to Model Registry

**Auto-generated *Data Exploration* notebook** → Understand and debug data quality and preprocessing

**Auto-generated notebooks with source code** → Iterate further on models from AutoML, adding your expertise

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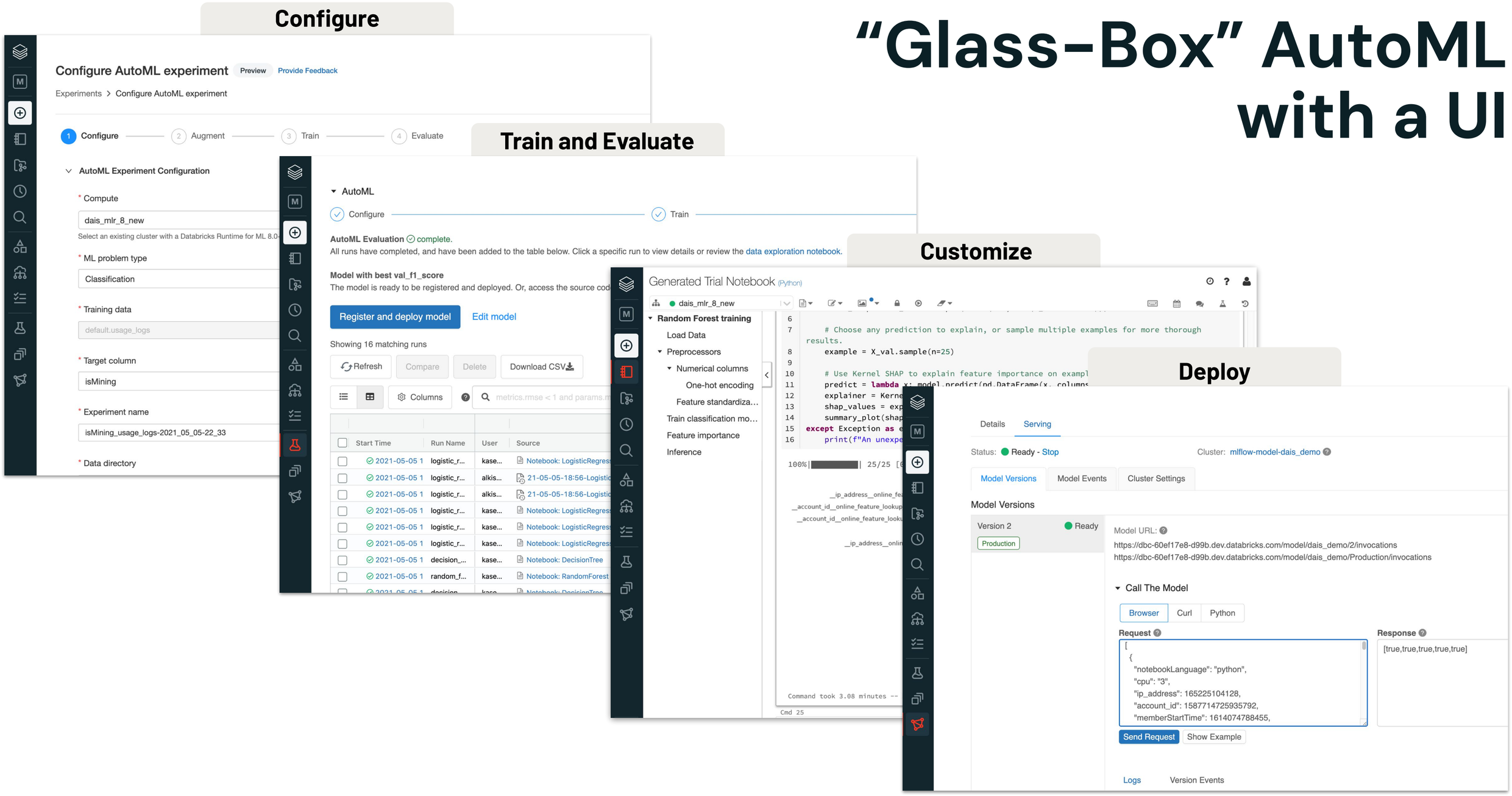
# “Glass-Box” AutoML with a UI

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# AutoML Supports Common Problem Types

## Support for problem, model, feature types

### Problem Types

Classification

Regression

Time Series Forecasting (~~Serverless~~)

### Models / Tuning

scikit learn

XGBoost

HYPEROPT

LightGBM

PROPHET

### Features

Numerical

Categorical

Timestamp

Text

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# Complete Integration

## AutoML integrated with other products

**AutoML integrates with;**

- **Feature Store**: You can expand the input training dataset using existing feature tables.
- **Model Tracking**:  All trial run metrics and parameters are tracked.
- **Model Registry**: You can register generated models to Unity Catalog.
- **Model Serving**: You can deploy generated models with Model Serving for real-time inference.

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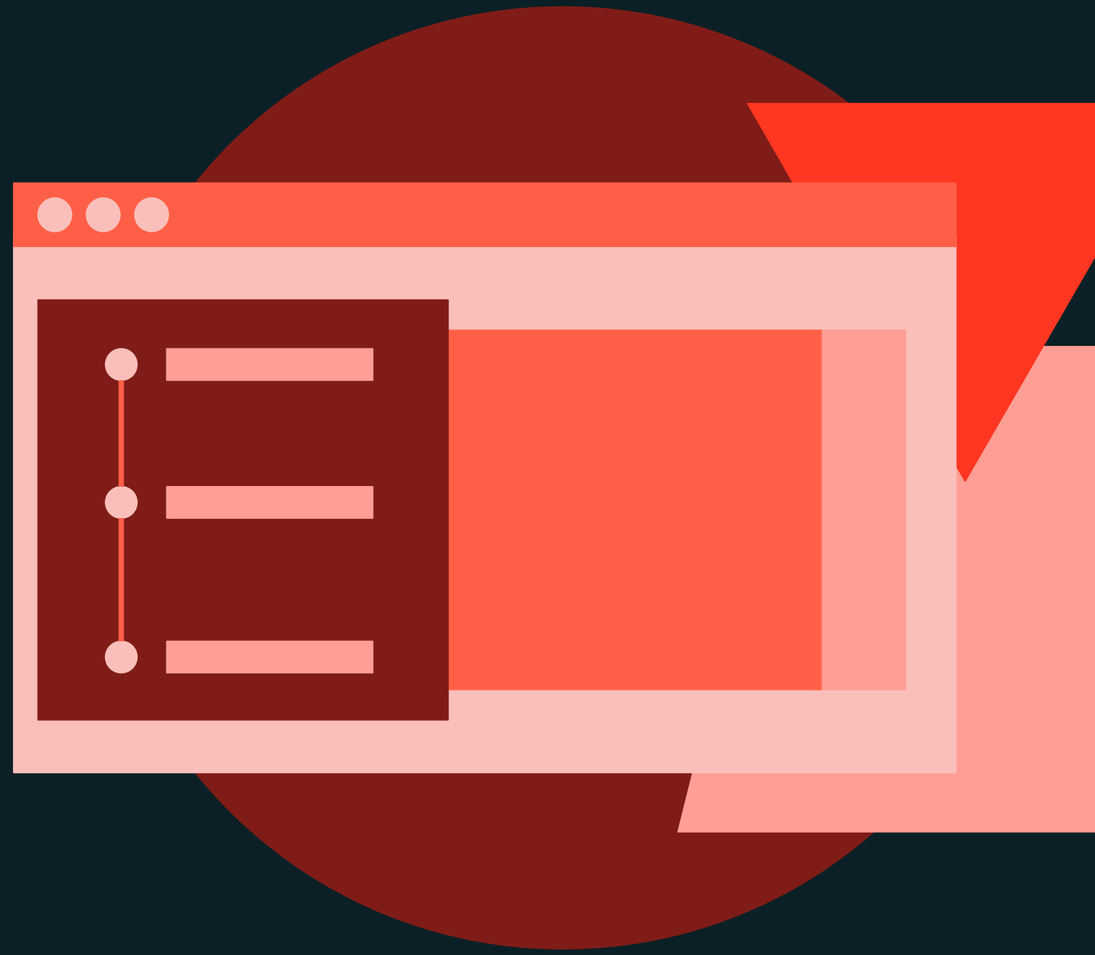
AutoML

DEMONSTRATION

# Automated Model Development with AutoML



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# Demo

## Outline

**What we'll cover:**

- Prepare data
- AutoML Experiment with the UI
  - Create an experiment
  - View the best run
- AutoML Experiment with the API
  - Start an experiment
  - Search for best run
  - Import notebooks for other experiments

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AutoML

LAB EXERCISE

# AutoML

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# Lab

## Outline

**What you'll do:**

- Load dataset
- Create a classification experiment using the AutoML UI
- Create a classification experiment with the AutoML API
- Retrieve the best run and show the model URI
- Import the notebook for a run

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# Summary and Next Steps

Machine Learning Model Development

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