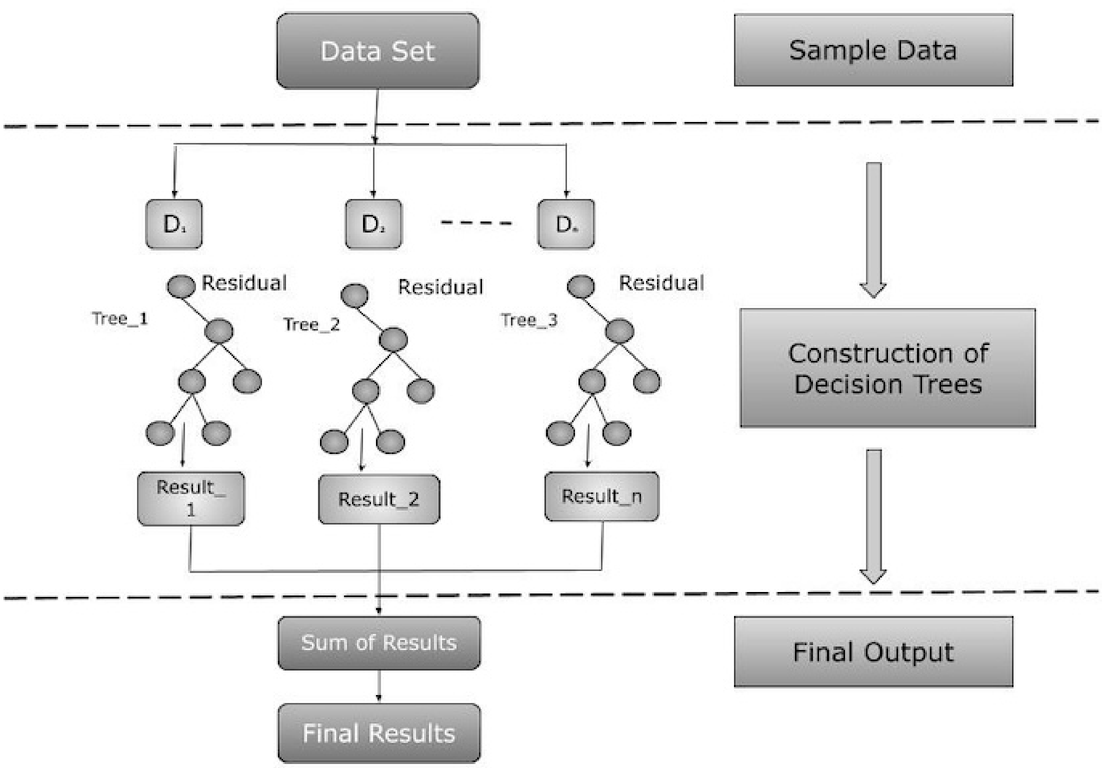
# vignette

December 7, 2025

### 0.1 XGBoost: Extreme Gradient Boosting

XGBoost is a supervised machine learning algorithm based on gradient-boosted decision trees. It builds an ensemble of trees sequentially, where each new tree corrects the errors of the previous one using gradient descent optimization. XGBoost is a powerful tool for several reasons:

- Includes regularization to prevent overfitting
- Handles non-linear feature interactions
- Highly efficient and fast on structured datasets




In this project, XGBoost is used as a multi-class classifier to predict Iris flower species using four numerical features: - Sepal Length - Sepal Width - Petal Length - Petal Width

The categorical species labels are first converted into numeric form (0, 1, 2), and the model is trained using a softmax-based multi-class classification objective.

[ ]:
```python
import xgboost as xgb
from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score
import numpy as np
import pandas as pd
```

[ ]:
```python
data = 'vignette-XGBoost/data/Iris.csv'
df = pd.read_csv(data, index_col=0)

# Display basic information about the dataset
print("Dataset shape:", df.shape)
print("\nFirst few rows:")
print(df.head())
print("\nClass distribution:")
print(df['Species'].value_counts())
```

```
Dataset shape: (150, 5)

First few rows:
    SepalLengthCm  SepalWidthCm  PetalLengthCm  PetalWidthCm      Species
Id
1             5.1           3.5            1.4           0.2  Iris-setosa
2             4.9           3.0            1.4           0.2  Iris-setosa
3             4.7           3.2            1.3           0.2  Iris-setosa
4             4.6           3.1            1.5           0.2  Iris-setosa
5             5.0           3.6            1.4           0.2  Iris-setosa

Class distribution:
Species
Iris-setosa        50
Iris-versicolor    50
Iris-virginica     50
Name: count, dtype: int64
```

[13]:
```python
# Transform species labels to numeric values for XGBoost classifier
# XGBoost requires numeric labels for multi-class classification
# Iris-setosa -> 0, Iris-versicolor -> 1, Iris-virginica -> 2
def transform(val):
    if val == "Iris-setosa":
        return 0
    elif val == "Iris-versicolor":
        return 1
    else:
        return 2

df["Species"] = df["Species"].apply(transform)
print("Transformed labels:", df["Species"].unique())
```

Transformed labels: [0 1 2]

[ ]:
```
# Prepare features (X) and target variable (y)
# Features: sepal and petal measurements
# Target: species class (0, 1, or 2)
X = df[["SepalLengthCm", "SepalWidthCm", "PetalLengthCm", "PetalWidthCm"]]
y = df["Species"]

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,␣
↪random_state=42)

print(f"Training set size: {len(X_train)}")
print(f"Test set size: {len(X_test)}")
```

```
Training set size: 120
Test set size: 30
```

[15]:
```
# Initialize XGBoost classifier
# objective='multi:softmax' - for multi-class classification with class␣
↪predictions
# eval_metric='merror' - multi-class classification error rate
model = xgb.XGBClassifier(objective='multi:softmax', eval_metric='merror',␣
↪random_state=42)

# Train the model on training data
model.fit(X_train, y_train)
print("Model training complete!")
```

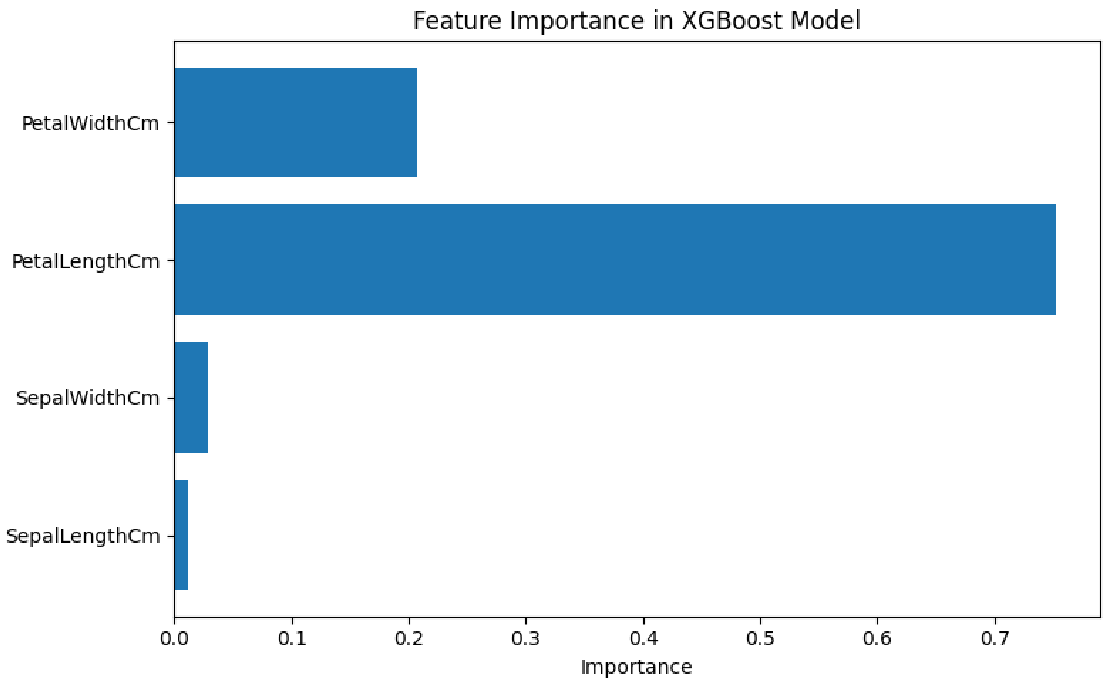
```
Model training complete!
```

[16]:
```
# Make predictions on test set
predictions = model.predict(X_test)

# Evaluate model performance
# Calculate accuracy on both training and test sets
test_accuracy = accuracy_score(y_test, predictions)
train_predictions = model.predict(X_train)
train_accuracy = accuracy_score(y_train, train_predictions)

print(f"Training Accuracy: {train_accuracy:.4f}")
print(f"Test Accuracy: {test_accuracy:.4f}")
```

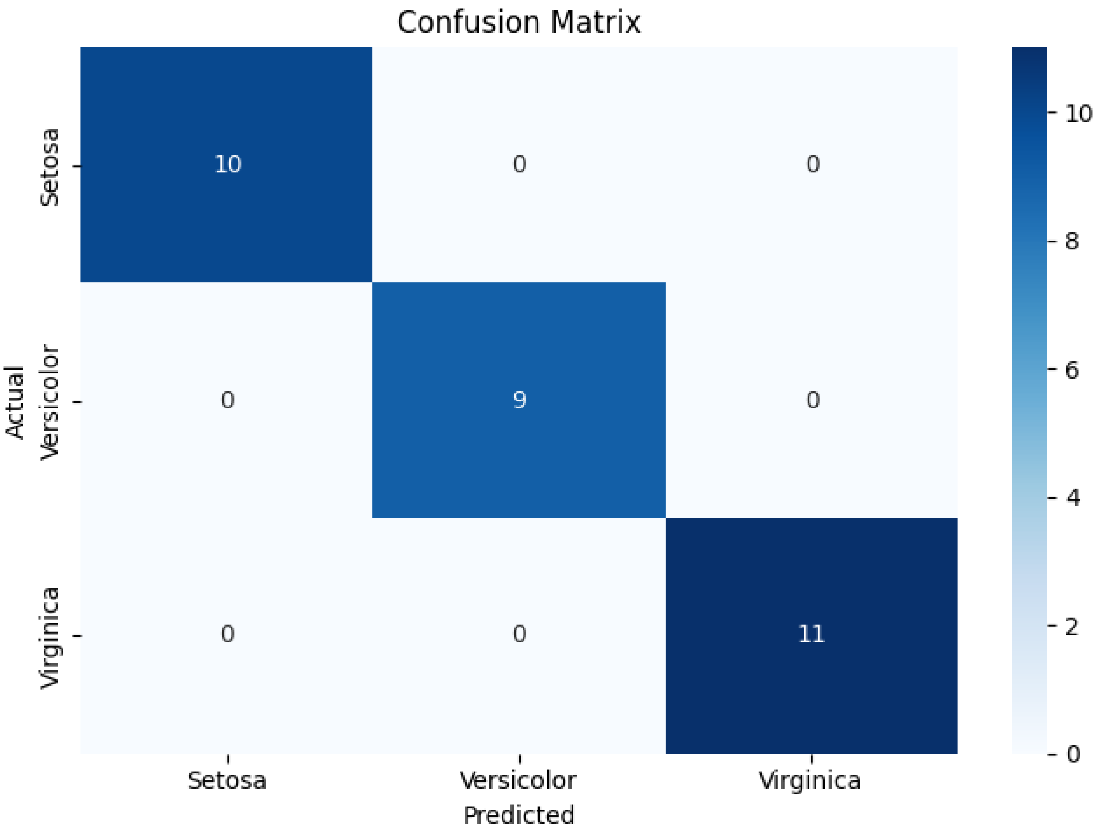
```
Training Accuracy: 1.0000
Test Accuracy: 1.0000
```

[ ]:
```
# Visualize feature importance
import matplotlib.pyplot as plt
```

```python
feature_importance = model.feature_importances_
features = X.columns

plt.figure(figsize=(8, 5))
plt.barh(features, feature_importance)
plt.xlabel('Importance')
plt.title('Feature Importance in XGBoost Model')
plt.tight_layout()
plt.show()
```




[18]:
```python
# Confusion matrix to see prediction performance by class
from sklearn.metrics import confusion_matrix
import seaborn as sns

cm = confusion_matrix(y_test, predictions)

plt.figure(figsize=(7, 5))
sns.heatmap(cm, annot=True, fmt='d', cmap='Blues',
            xticklabels=['Setosa', 'Versicolor', 'Virginica'],
            yticklabels=['Setosa', 'Versicolor', 'Virginica'])
plt.xlabel('Predicted')
plt.ylabel('Actual')
plt.title('Confusion Matrix')
plt.tight_layout()
plt.show()
```


Confusion Matrix
Setosa
Versicolor
Virginica
Actual
10
0
0
0
9
0
0
0
11
Setosa
Versicolor
Virginica
Predicted
10
8
6
4
2
0