xgboost

August 29, 2025

[3]:
```
import pandas as pd
import numpy as np
from sklearn.model_selection import train_test_split, GridSearchCV,␣
↪StratifiedKFold
from sklearn.preprocessing import StandardScaler
from sklearn.pipeline import Pipeline
from sklearn.compose import ColumnTransformer
from sklearn.tree import DecisionTreeClassifier
from sklearn.metrics import (
    accuracy_score, precision_score, recall_score, f1_score, roc_auc_score,␣
↪roc_curve,auc
)
import matplotlib.pyplot as plt
from xgboost import XGBClassifier
import seaborn as sns
```

[4]:
```
# 1. Load dataset
# wdbc.data does not have headers, so we define them
columns = ["ID", "Diagnosis"] + [f"feature_{i}" for i in range(1, 31)]
data = pd.read_csv("wdbc.data", header=None, names=columns)
```

[5]:
```
# 2. Prepare features and target
X = data.drop(["ID", "Diagnosis"], axis=1)
y = data["Diagnosis"].map({"M": 1, "B": 0})  # Malignant=1, Benign=0
```

[6]:
```
# 4. Preprocessor (scaling not needed for trees, but kept for pipeline␣
↪consistency)
num_features = X.columns.tolist()
preprocessor = ColumnTransformer(
    transformers=[("scale", StandardScaler(), num_features)],
    remainder="drop"
)
```

[7]:
```
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.2, random_state=42, stratify=y
)
```

[15]:
```python
pipe = Pipeline([
    ("scaler", StandardScaler()),
    ("clf", XGBClassifier(
        eval_metric="logloss",    # keep this
        random_state=42
    ))
])
```

[16]:
```python
# 6. Hyperparameter grid
param_grid = {
    "clf__n_estimators": [50, 100, 200],
    "clf__learning_rate": [0.01, 0.1, 0.2],
    "clf__max_depth": [3, 5, 7],
    "clf__gamma": [0, 0.1, 0.5],
    "clf__subsample": [0.8, 1.0],
    "clf__colsample_bytree": [0.8, 1.0],
}
```

[18]:
```python
grid = GridSearchCV(
    estimator=pipe,
    param_grid=param_grid,
    cv=5,
    scoring={"accuracy": "accuracy", "f1": "f1_macro"},  # track both
    refit="accuracy",    # choose best by accuracy
    n_jobs=-1,
    verbose=1
)

grid.fit(X_train, y_train)
```

```
Fitting 5 folds for each of 324 candidates, totalling 1620 fits
```

[18]:
```
GridSearchCV(cv=5,
             estimator=Pipeline(steps=[('scaler', StandardScaler()),
                                       ('clf',
                                        XGBClassifier(base_score=None,
                                                      booster=None,
                                                      callbacks=None,
                                                      colsample_bylevel=None,
                                                      colsample_bynode=None,
                                                      colsample_bytree=None,
                                                      device=None,
early_stopping_rounds=None,
                                                      enable_categorical=False,
                                                      eval_metric='logloss',
                                                      feature_types=None,
                                                      feature_weights=None,
                                                      gamma=None,
```

```
                                                          grow_poli…
                                                          multi_strategy=None,
                                                          n_estimators=None,
                                                          n_jobs=None,
                                                          num_parallel_tree=None,
…))]),
             n_jobs=-1,
             param_grid={'clf__colsample_bytree': [0.8, 1.0],
                         'clf__gamma': [0, 0.1, 0.5],
                         'clf__learning_rate': [0.01, 0.1, 0.2],
                         'clf__max_depth': [3, 5, 7],
                         'clf__n_estimators': [50, 100, 200],
                         'clf__subsample': [0.8, 1.0]},
             refit='accuracy',
             scoring={'accuracy': 'accuracy', 'f1': 'f1_macro'}, verbose=1)
```

[19]:

```
# 5. Extract results into DataFrame
xgb_results = pd.DataFrame(grid.cv_results_)

# 6. Select only required columns
xgb_table = xgb_results[[
    "param_clf__n_estimators",
    "param_clf__learning_rate",
    "param_clf__max_depth",
    "param_clf__gamma",
    "mean_test_accuracy",
    "mean_test_f1"
]]

# 7. Rename for clarity
xgb_table = xgb_table.rename(columns={
    "param_clf__n_estimators": "n_estimators",
    "param_clf__learning_rate": "learning_rate",
    "param_clf__max_depth": "max_depth",
    "param_clf__gamma": "gamma",
    "mean_test_accuracy": "Accuracy",
    "mean_test_f1": "F1 Score"
})

top10 = xgb_table.sort_values(by="Accuracy", ascending=False).head(10)

print("XGBoost Model")
print("Hyperparameter Trials")
print("Table 4: XGBoost - Hyperparameter Tuning (Top 10)")
print(top10[["n_estimators", "learning_rate", "max_depth", "gamma", "Accuracy",␣
↪"F1 Score"]])
```

```
XGBoost Model
```

Hyperparameter Trials
Table 4: XGBoost - Hyperparameter Tuning (Top 10)

	n_estimators	learning_rate	max_depth	gamma	Accuracy	F1 Score
53	200	0.2	7	0.0	0.975824	0.974103
38	100	0.2	3	0.0	0.971429	0.969321
238	200	0.1	3	0.1	0.971429	0.969288
51	100	0.2	7	0.0	0.971429	0.969347
47	200	0.2	5	0.0	0.971429	0.969406
214	200	0.2	7	0.0	0.971429	0.969202
208	200	0.2	5	0.0	0.971429	0.969202
184	200	0.1	3	0.0	0.971429	0.969288
194	100	0.1	7	0.0	0.969231	0.967212
29	200	0.1	5	0.0	0.969231	0.967184

[21]:
```python
print("Best Parameters:", grid.best_params_)
print("Best CV Accuracy:", grid.best_score_)
```

```
Best Parameters: {'clf__colsample_bytree': 0.8, 'clf__gamma': 0,
'clf__learning_rate': 0.2, 'clf__max_depth': 7, 'clf__n_estimators': 200,
'clf__subsample': 1.0}
Best CV Accuracy: 0.9758241758241759
```

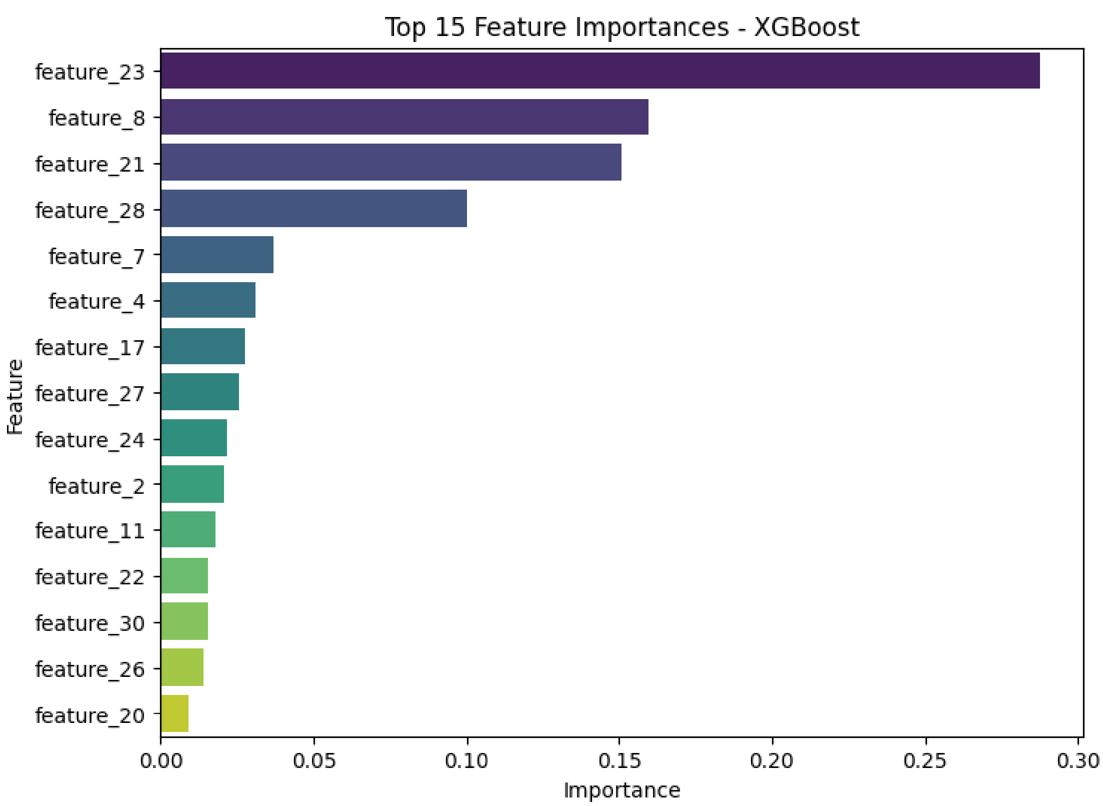
[22]:
```python
best_xgb = grid.best_estimator_
y_pred = best_xgb.predict(X_test)

print("\nTest Accuracy:", accuracy_score(y_test, y_pred))
print("Test F1 Score:", f1_score(y_test, y_pred))
print("Test Precision:", precision_score(y_test, y_pred))
print("Test Recall:", recall_score(y_test, y_pred))
print("Test ROC AUC:", roc_auc_score(y_test, y_pred))
```

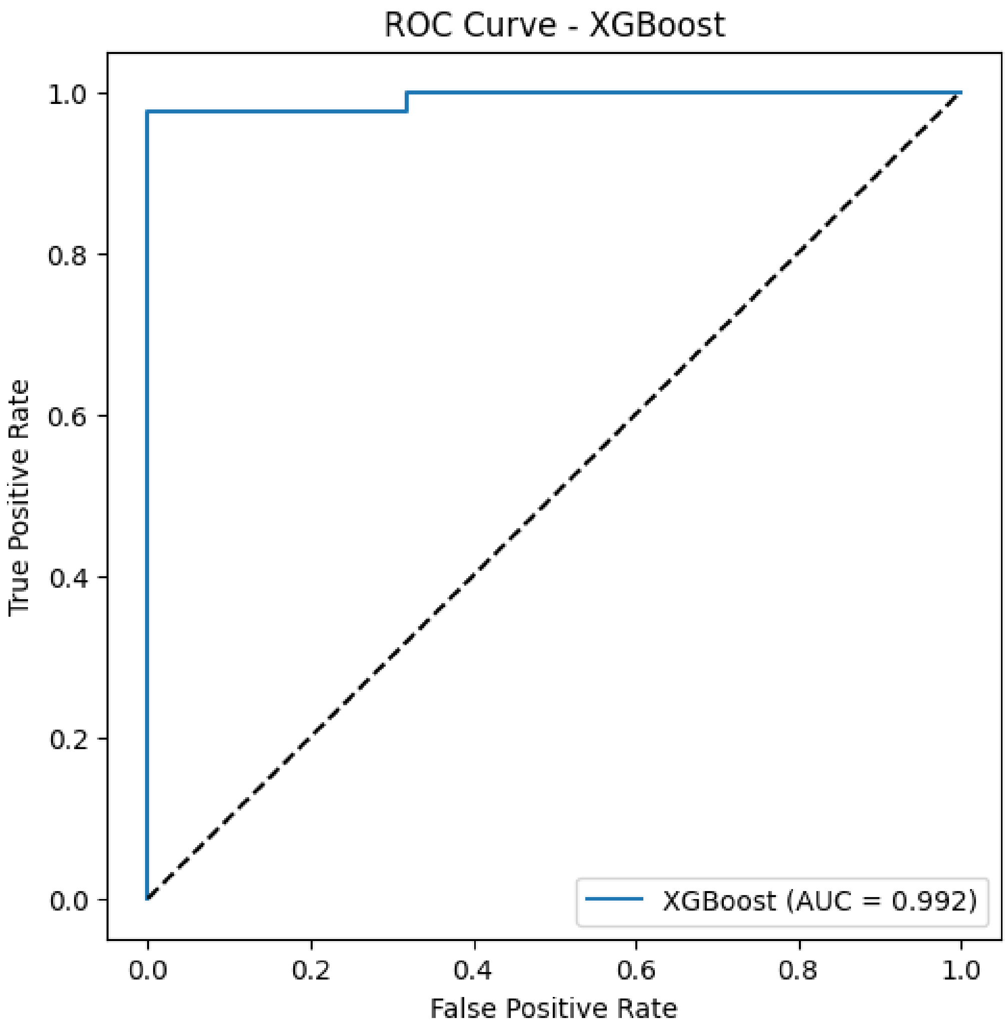
```
Test Accuracy: 0.9824561403508771
Test F1 Score: 0.975609756097561
Test Precision: 1.0
Test Recall: 0.9523809523809523
Test ROC AUC: 0.9761904761904762
```

[23]:
```python
# --- 7. Feature Importances ---
importances = best_xgb.named_steps["clf"].feature_importances_
feat_imp = pd.Series(importances, index=X.columns).
 ↪sort_values(ascending=False)[:15]

plt.figure(figsize=(8,6))
sns.barplot(x=feat_imp, y=feat_imp.index, palette="viridis")
plt.title("Top 15 Feature Importances - XGBoost")
plt.xlabel("Importance")
plt.ylabel("Feature")
```

```
plt.show()

# --- 8. ROC Curve & AUC ---
y_prob = best_xgb.predict_proba(X_test)[:, 1]
fpr, tpr, _ = roc_curve(y_test, y_prob)
roc_auc = auc(fpr, tpr)

plt.figure(figsize=(6,6))
plt.plot(fpr, tpr, label=f"XGBoost (AUC = {roc_auc:.3f})")
plt.plot([0,1], [0,1], "k--")
plt.xlabel("False Positive Rate")
plt.ylabel("True Positive Rate")
plt.title("ROC Curve - XGBoost")
plt.legend()
plt.show()
```

```
/tmp/ipykernel_9875/472011034.py:6: FutureWarning:

Passing `palette` without assigning `hue` is deprecated and will be removed in
v0.14.0. Assign the `y` variable to `hue` and set `legend=False` for the same
effect.

  sns.barplot(x=feat_imp, y=feat_imp.index, palette="viridis")
```




ROC Curve - XGBoost
1.0
0.8
0.6
0.4
0.2
0.0
True Positive Rate
XGBoost (AUC = 0.992)
0.0
0.2
0.4
0.6
0.8
1.0
False Positive Rate