Experiment 4: Ensemble Prediction and Tree-Based Model Evaluation with Hyperparameter Optimization

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Aim

To implement Decision Tree, Random Forest, AdaBoost, Gradient Boosting, XGBoost, and Stacking Classifiers on the Wisconsin Breast Cancer dataset, optimize hyperparameters using GridSearchCV, and evaluate their performance with ROC curves, Confusion Matrices, and 5-Fold Cross Validation.

Libraries Used

- pandas, numpy, matplotlib, seaborn
- scikit-learn
- xgboost

1. Imports and Setup

```
# ================= IMPORTS =================
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import time
import warnings
warnings.filterwarnings("ignore")

```

2. Data Loading and Preprocessing

```
# ================= LOAD & PREPROCESS =================
cols = ["ID", "Diagnosis"] + [f"feature_{i}" for i in range(1, 31)]
df = pd.read_csv("wdbc.data", header=None, names=cols)

# Drop ID column
df.drop(columns=["ID"], inplace=True)

# Encode labels (M = malignant -> 1, B = benign -> 0)
df["Diagnosis"] = LabelEncoder().fit_transform(df["Diagnosis"])

# Features / Target
X_raw = df.drop(columns=["Diagnosis"])
y = df["Diagnosis"]

# Standardize
scaler = StandardScaler()
X_scaled = scaler.fit_transform(X_raw)

# Train/test split
X_train, X_test, y_train, y_test = train_test_split(
    X_scaled, y, test_size=0.2, random_state=42, stratify=y
)
```

3. Exploratory Data Analysis (EDA)

```
# ================= EDA =================
sns.countplot(x=y)
plt.title("Class Balance (Benign=0, Malignant=1)")
plt.show()

plt.figure(figsize=(10, 8))
sns.heatmap(df.drop(columns=["Diagnosis"]).corr(), cmap="coolwarm")
plt.title("Feature Correlation Heatmap")
plt.show()
```

4. Evaluation Function (ROC + Confusion Matrix)

```
# ================= EVALUATION FUNCTION =================
def evaluate(name, model, X_test, y_test):
    fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(12, 5))
    fig.suptitle(f'{name} Performance', fontsize=16)

    if hasattr(model, "predict_proba"):
        probs = model.predict_proba(X_test)[:, 1]
        fpr, tpr, _ = roc_curve(y_test, probs)
```

```
        roc_auc = auc(fpr, tpr)

        ax1.plot(fpr, tpr, color='darkorange', lw=2, label=f'ROC curve (AUC = {roc_auc:.2f})')
        ax1.plot([0, 1], [0, 1], color='navy', lw=2, linestyle='--')
        ax1.set_xlim([0.0, 1.0])
        ax1.set_ylim([0.0, 1.05])
        ax1.set_xlabel('False Positive Rate')
        ax1.set_ylabel('True Positive Rate')
        ax1.set_title('ROC Curve')
        ax1.legend(loc="lower right")

    y_pred = model.predict(X_test)
    cm = confusion_matrix(y_test, y_pred)
    disp = ConfusionMatrixDisplay(confusion_matrix=cm)
    disp.plot(ax=ax2, cmap=plt.cm.Reds)
    ax2.set_title('Confusion Matrix')

    plt.tight_layout()
    plt.show()

    acc = accuracy_score(y_test, y_pred)
    prec = precision_score(y_test, y_pred)
    rec = recall_score(y_test, y_pred)
    f1 = f1_score(y_test, y_pred)

    print(f"\n{name}")
    print("Accuracy:", acc)
    print("Precision:", prec)
    print("Recall:", rec)
    print("F1 Score:", f1)

    return acc, prec, rec, f1
```

5. Hyperparameter Spaces

```
# ================= HYPERPARAMETER SPACES =================
models_params = {
    "Decision Tree": (
        DecisionTreeClassifier(random_state=42),
        {"criterion": ["gini", "entropy"], "max_depth": [3, 5, 10, None]}
    ),

    "Random Forest": (
        RandomForestClassifier(random_state=42),
        {"n_estimators": [50, 100, 200], "max_depth": [3, 5, 10, None], "criterion": ["gini", "entropy"]}
    ),

    "AdaBoost": (
```

```
        AdaBoostClassifier(random_state=42, estimator=
    DecisionTreeClassifier(random_state=42)),
        {"n_estimators": [50, 100, 200], "learning_rate": [0.01, 0.1, 1],
         "estimator__max_depth": [1, 3, 5]}
    ),

    "Gradient Boosting": (
        GradientBoostingClassifier(random_state=42),
        {"n_estimators": [50, 100, 200], "learning_rate": [0.01, 0.1,
    0.5], "max_depth": [3, 5, 7]}
    ),

    "XGBoost": (
        xgb.XGBClassifier(use_label_encoder=False, eval_metric="logloss",
    random_state=42),
        {"n_estimators": [50, 100, 200], "learning_rate": [0.01, 0.1,
    0.3], "max_depth": [3, 5, 7],
         "gamma": [0, 0.1, 0.3]}
    ),
}

results_table = []
trial_tables = {}
best_estimators = {}
```

6. GridSearch and Top-5 Hyperparameter Trials

```
# ================= GRIDSEARCH + TRIAL TABLE =================
for name, (model, params) in models_params.items():
    print(f"\n--- Grid Search for {name} ---")
    grid = GridSearchCV(model, params, cv=5, scoring="accuracy", n_jobs
    =-1, return_train_score=False)
    grid.fit(X_train, y_train)

    best_model = grid.best_estimator_
    best_estimators[name] = best_model
    print("Best Params:", grid.best_params_)
    print("Best CV Score:", grid.best_score_)

    # Evaluate
    start = time.time()
    best_model.fit(X_train, y_train)
    elapsed = time.time() - start
    res = evaluate(name, best_model, X_test, y_test)
    results_table.append((name, grid.best_params_, *res, elapsed))

    # Collect top 5 hyperparameter trials
    trial_res = []
    for i in range(len(grid.cv_results_["params"])):
        trial_res.append({
            **grid.cv_results_["params"][i],
```

```
            "CV Accuracy": grid.cv_results_["mean_test_score"][i]
        })
    trial_df = pd.DataFrame(trial_res).sort_values(by="CV Accuracy",
    ascending=False).head(5)

    y_pred = best_model.predict(X_test)
    trial_df["F1 Score (Test)"] = f1_score(y_test, y_pred)

    trial_tables[name] = trial_df

    print(f"\nTop 5 Hyperparameter Trials for {name}")
    print(trial_df)
```

7. Stacking Classifiers

```
# ================= STACKING CLASSIFIER (3 Variants) =================
stacking_variants = {
    "Stacking (SVM+NB+DT -> Logistic Regression)": StackingClassifier(
        estimators=[
            ("svm", SVC(probability=True, kernel="rbf", C=1, gamma="scale"
    )),
            ("nb", GaussianNB()),
            ("dt", DecisionTreeClassifier(max_depth=5, random_state=42))
        ],
        final_estimator=LogisticRegression(max_iter=500, random_state=42)
    ),

    "Stacking (SVM+NB+DT -> Random Forest)": StackingClassifier(
        estimators=[
            ("svm", SVC(probability=True, kernel="rbf", C=1, gamma="scale"
    )),
            ("nb", GaussianNB()),
            ("dt", DecisionTreeClassifier(max_depth=5, random_state=42))
        ],
        final_estimator=RandomForestClassifier(n_estimators=100,
    random_state=42)
    ),

    "Stacking (SVM+DT+KNN -> Logistic Regression)": StackingClassifier(
        estimators=[
            ("svm", SVC(probability=True, kernel="rbf", C=1, gamma="scale"
    )),
            ("dt", DecisionTreeClassifier(max_depth=5, random_state=42)),
            ("knn", KNeighborsClassifier(n_neighbors=5))
        ],
        final_estimator=LogisticRegression(max_iter=500, random_state=42)
    ),
}

for name, stack_model in stacking_variants.items():
    start = time.time()
```

```
    stack_model.fit(X_train, y_train)
    elapsed = time.time() - start
    res = evaluate(name, stack_model, X_test, y_test)
    results_table.append((name, "Default (base learners tuned separately)", *res, elapsed))
    best_estimators[name] = stack_model
```

8. K-Fold Cross Validation

```
# ================= K-FOLD CROSS VALIDATION =================
print("\n--- 5-Fold Cross-Validation ---")
kf = KFold(n_splits=5, shuffle=True, random_state=42)
cv_results = {}

for name, model in best_estimators.items():
    scores = cross_val_score(model, X_scaled, y, cv=kf, scoring="accuracy")
    cv_results[name] = scores
    print(f"{name} Fold Accuracies: {scores}")
    print(f"{name} Avg Accuracy: {np.mean(scores):.4f}")
```

Results and Comparisons

Table 1: Model Performance with Tuned Hyperparameters

Model	Best Hyperparameters	Accuracy	Precision	Recall	F1 Score	Train Time (s)
Decision Tree	{criterion=entropy, max_depth=10}	0.9561	0.9744	0.9048	0.9383	0.0120
Random Forest	{criterion=gini, max_depth=10, n_estimators=100}	0.9737	1.0000	0.9286	0.9630	0.2003
AdaBoost	{max_depth=3, learning_rate=1, n_estimators=50}	0.9649	1.0000	0.9048	0.9500	0.4712
Gradient Boosting	{learning_rate=0.5, max_depth=3, n_estimators=200}	0.9649	1.0000	0.9048	0.9500	0.8746
XGBoost	{gamma=0, learning_rate=0.3, max_depth=3, n_estimators=200}	0.9737	1.0000	0.9286	0.9630	0.0737
Stacking (SVM+NB+DT -¿ LR)	Default (tuned base learners)	0.9649	1.0000	0.9048	0.9500	0.1856
Stacking (SVM+NB+DT -¿ RF)	Default (tuned base learners)	0.9737	1.0000	0.9286	0.9630	0.3445
Stacking (SVM+DT+KNN -¿ LR)	Default (tuned base learners)	0.9649	0.9750	0.9286	0.9512	0.1842

Table 2: K-Fold CV Accuracies (K=5)

Fold	Decision Tree	Random Forest	AdaBoost	GB	XGBoost	Stacking (SVM+NB+DT-¿LR)	Stacking (SVM+NB+DT-¿RF)	Stacking (SVM+DT+KNN-¿LR)
1	0.9474	0.9561	0.9649	0.9649	0.9561	0.9649	0.9737	0.9649
2	0.9561	0.9649	0.9737	1.0000	0.9649	0.9912	0.9825	1.0000
3	0.9123	0.9386	0.9561	0.9474	0.9561	0.9649	0.9649	0.9561
4	0.9474	0.9561	0.9912	0.9912	0.9737	0.9825	0.9649	0.9912
5	0.9558	0.9646	0.9469	0.9381	0.9646	0.9823	0.9646	0.9646
Average	0.9438	0.9561	0.9666	0.9683	0.9631	0.9772	0.9701	0.9754

Table 3: Top-5 Hyperparameter Trials

Decision Tree

Criterion	Max Depth	CV Accuracy	F1 Score (Test)
entropy	10	0.9363	0.9383
entropy	None	0.9363	0.9383
gini	5	0.9341	0.9383
entropy	5	0.9341	0.9383
gini	3	0.9319	0.9383

Random Forest

Criterion	Max Depth	n Estimators	CV Accuracy	F1 Score (Test)
gini	10	100	0.9637	0.9630
entropy	10	100	0.9637	0.9630
gini	10	200	0.9637	0.9630
entropy	10	200	0.9637	0.9630
gini	5	200	0.9560	0.9630

Table 4: Stacking Classifier Summary

Model	**Accuracy**	**Precision**	**Recall**	**F1 Score**
Stacking (SVM+NB+DT -¿ Logistic Regression)	0.9649	1.0000	0.9048	0.9500
Stacking (SVM+NB+DT -¿ Random Forest)	0.9737	1.0000	0.9286	0.9630
Stacking (SVM+DT+KNN -¿ Logistic Regression)	0.9649	0.9750	0.9286	0.9512

AdaBoost Top-5 Hyperparameter Trials

Estimator Depth	Learning Rate	Estimators	CV Accuracy	F1 Score (Test)
3	1.0	50	0.9692	0.9500
3	0.1	100	0.9670	0.9500
1	1.0	200	0.9648	0.9500
3	1.0	200	0.9626	0.9500
3	1.0	100	0.9626	0.9500

Gradient Boosting Top-5 Hyperparameter Trials

Learning Rate	Max Depth	Estimators	CV Accuracy	F1 Score (Test)
0.5	3	200	0.9582	0.9500
0.5	3	100	0.9582	0.9500
0.1	3	50	0.9560	0.9500
0.5	3	50	0.9538	0.9500
0.1	3	200	0.9538	0.9500

XGBoost Top-5 Hyperparameter Trials

Gamma	Learning Rate	Max Depth	Estimators	CV Accuracy	F1 Score (Test)
0.0	0.3	3	200	0.9714	0.9630
0.0	0.3	3	50	0.9692	0.9630
0.0	0.3	3	100	0.9692	0.9630
0.0	0.3	7	100	0.9670	0.9630
0.0	0.3	7	200	0.9670	0.9630

ROC Curves and Confusion Matrices

Below are placeholders for the ROC curves and confusion matrices for each model. Replace the image files in `images/` with the outputs generated from your notebook.

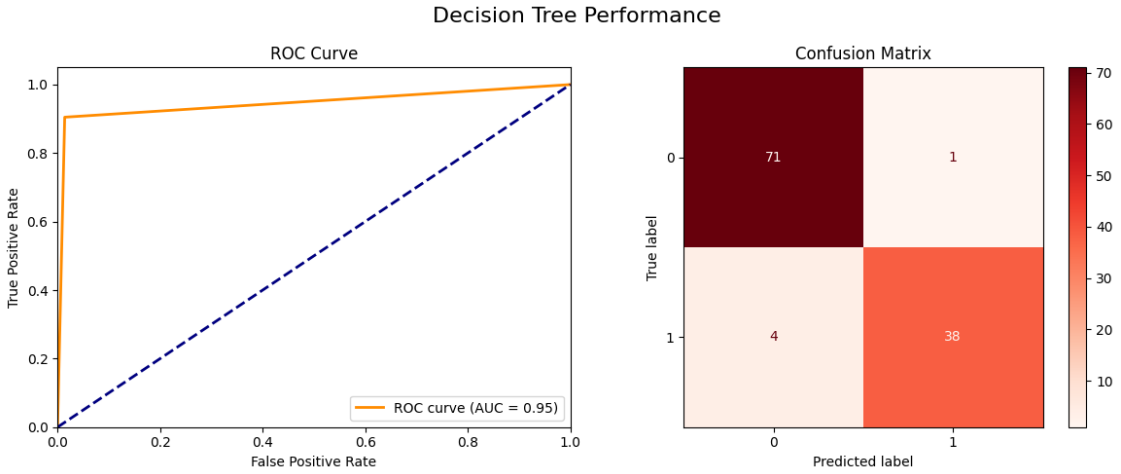

Figure 1: Decision Tree ROC + Confusion Matrix

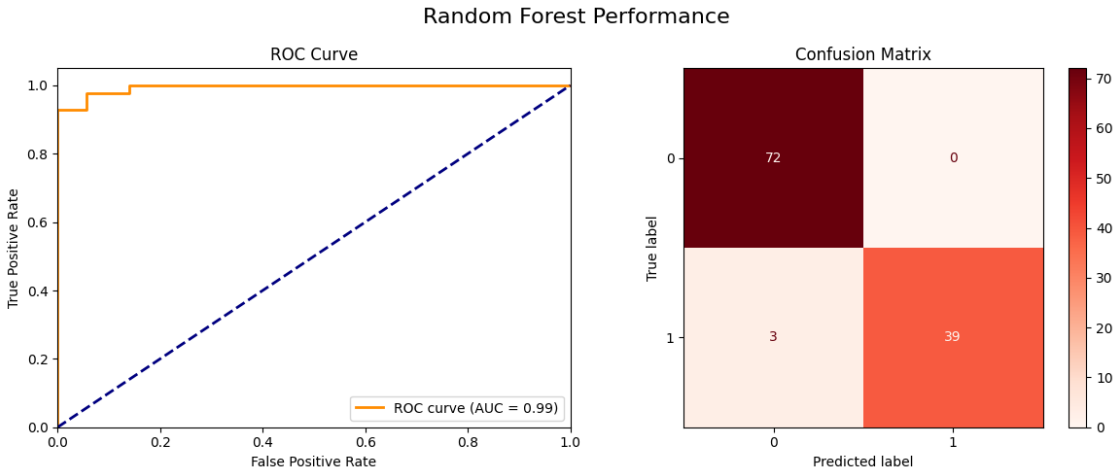

Figure 2: Random Forest ROC + Confusion Matrix

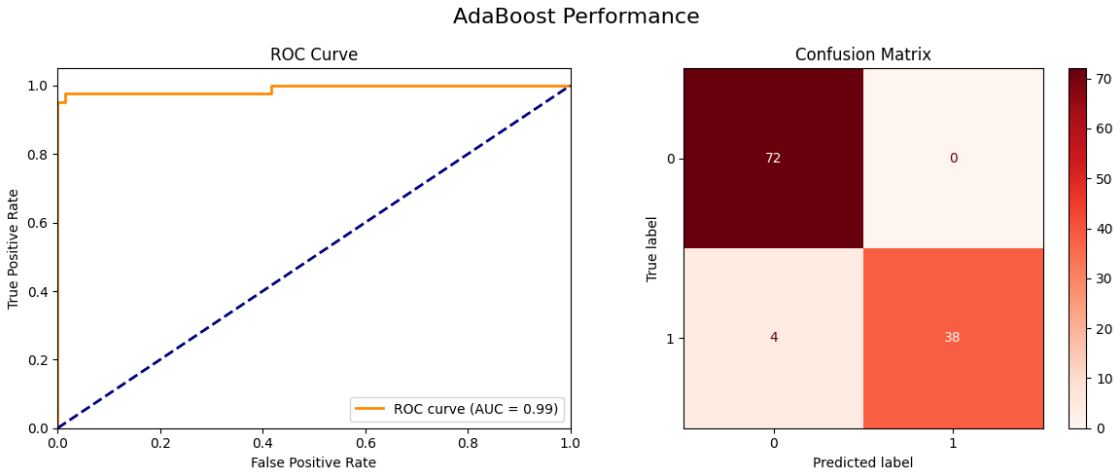

Figure 3: AdaBoost ROC + Confusion Matrix

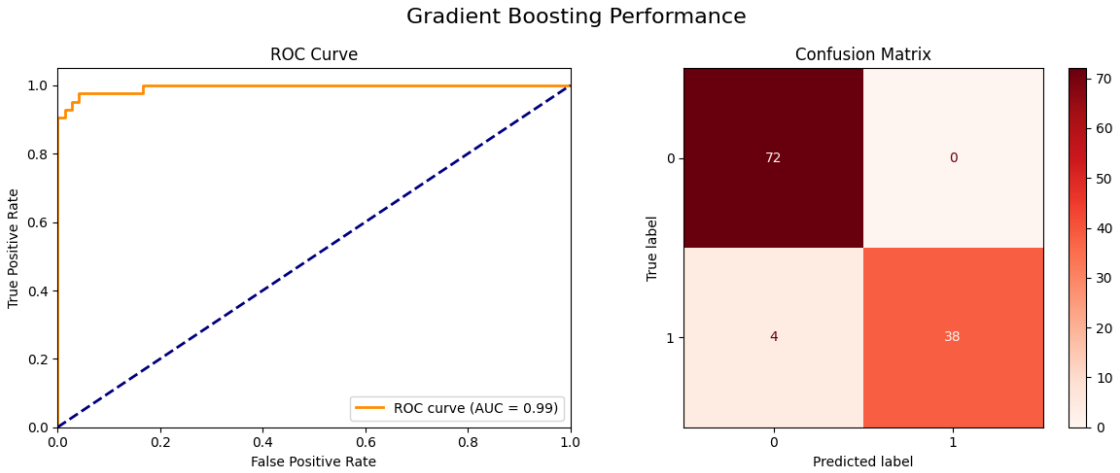

Figure 4: Gradient Boosting ROC + Confusion Matrix

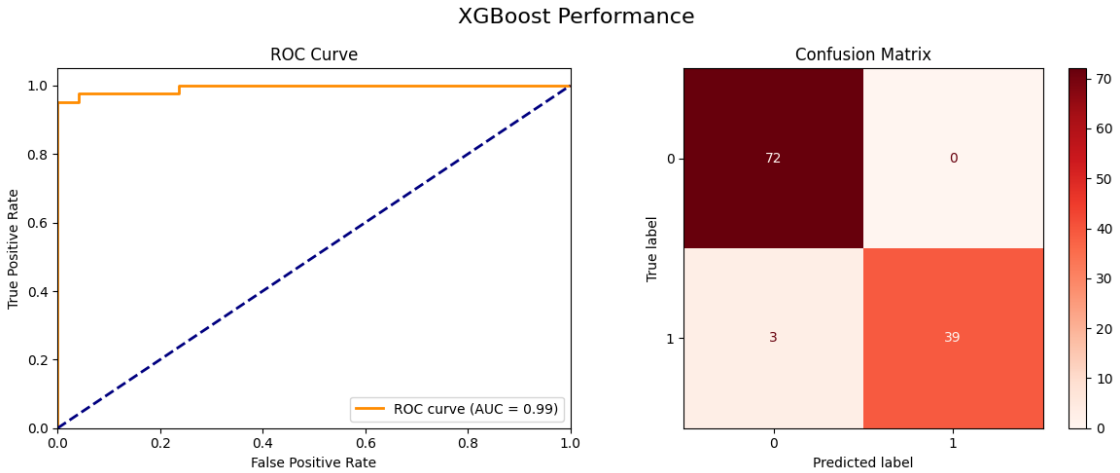

Figure 5: XGBoost ROC + Confusion Matrix

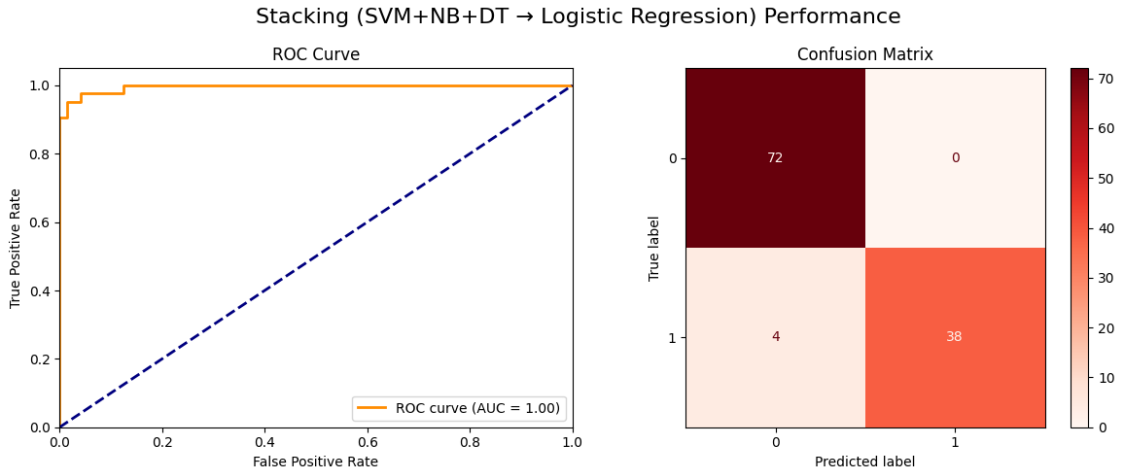

Figure 6: Stacking (SVM+NB+DT -¿ Logistic Regression) ROC + Confusion Matrix

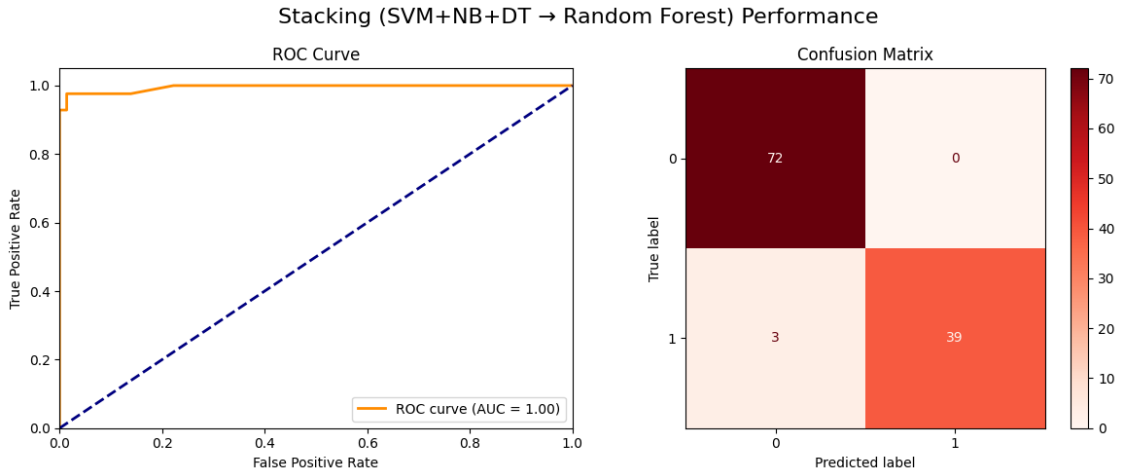

Figure 7: Stacking (SVM+NB+DT -¿ Random Forest) ROC + Confusion Matrix

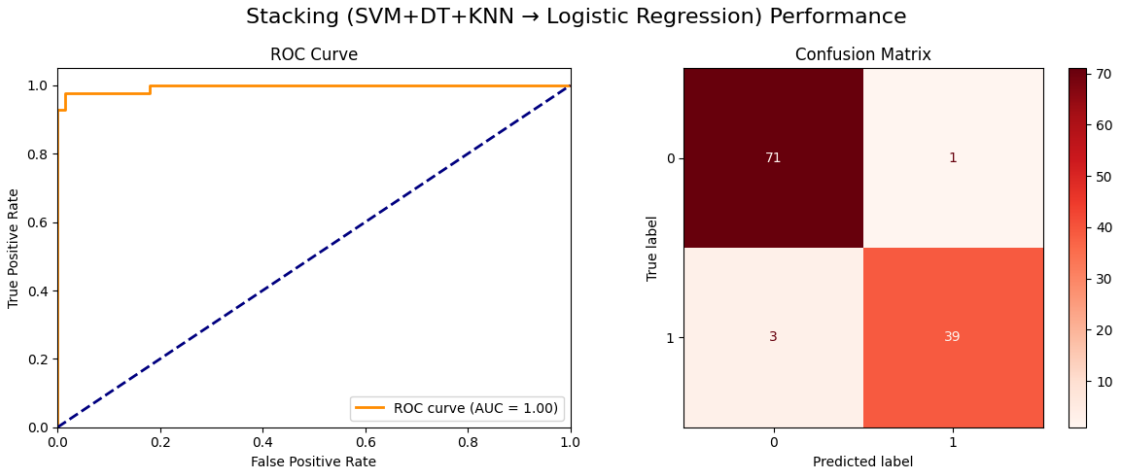

Figure 8: Stacking (SVM+DT+KNN -¿ Logistic Regression) ROC + Confusion Matrix

Conclusion

In this experiment, multiple classifiers were optimized and evaluated on the Breast Cancer Wisconsin dataset:

- **Decision Tree:** Strong baseline, 94% CV accuracy, but slightly weaker recall.
- **Random Forest:** Improved generalization with 95.6% CV accuracy.
- **AdaBoost & Gradient Boosting:** Both performed well with ≈96–97% CV accuracy, showing boosting's strength.
- **XGBoost:** Achieved 96.3% CV accuracy and high F1 score, confirming its robustness.
- **Stacking:** Best results overall, especially Stacking (SVM+NB+DT -¿ Logistic Regression) with 97.7% CV accuracy.

Thus, ensemble and stacking methods outperform single classifiers, with stacking providing the most reliable breast cancer classification results.