Date: 22-08-2025 **Name:** Mithuna S
Experiment: 4 **Roll No:** 3122237001025

Sri Sivasubramaniya Nadar College of Engineering, Chennai
(An autonomous Institution affiliated to Anna University)

Degree & Branch	B.E. Computer Science & Engineering	Semester	V
Subject Code & Name	ICS1512 & Machine Learning Algorithms Laboratory		
Academic year	2025-2026 (Odd)	Batch:2023-2028	**Due date:**

Experiment 4: Ensemble Prediction and Decision Tree Model Evaluation

Aim: To build classifiers such as Decision Tree, AdaBoost, Gradient Boosting, XGBoost, Random Forest, and Stacked Models (using SVM, Na¨ıve Bayes, Decision Tree) and evaluate their performance through 5-Fold Cross-Validation and hyperparameter tuning.

Libraries used:

- pandas - for data handling
- numpy - for numerical operations
- matplotlib.pyplot and seaborn - for visualization
- sklearn - for preprocessing, model building, hyperparameter tuning, and evaluation
- xgboost - for XGBoost model implementation

CODE:

```
#--------------------LOADING THE DATASET--------------------
import pandas as pd

# Define column names
cols = ["ID", "Diagnosis"] + [
    "radius_mean","texture_mean","perimeter_mean","area_mean",
    "smoothness_mean",
    "compactness_mean","concavity_mean","concave_points_mean",
    "symmetry_mean","fractal_dimension_mean",
    "radius_se","texture_se","perimeter_se","area_se","smoothness_se",

    "compactness_se","concavity_se","concave_points_se","symmetry_se","fractal_dimension_se",
    "radius_worst","texture_worst","perimeter_worst","area_worst","smoothness_worst",

    "compactness_worst","concavity_worst","concave_points_worst","symmetry_worst","fractal_dimension_wor
]

# Read your .DATA file
df = pd.read_csv("wdbc.data", names=cols)

print(df.shape)
df.head()
```

OUTPUT:

```
(569, 32)
ID      Diagnosis       radius_mean     texture_mean    perimeter_mean  area_mean
    smoothness_mean compactness_mean        concavity_mean  concave_points_mean
    ...     radius_worst    texture_worst   perimeter_worst area_worst
    smoothness_worst        compactness_worst       concavity_worst
    concave_points_worst    symmetry_worst  fractal_dimension_worst
0       842302  M       17.99   10.38   122.80  1001.0  0.11840 0.27760 0.3001  0.14710
    ...     25.38   17.33   184.60  2019.0  0.1622  0.6656  0.7119  0.2654  0.4601
    0.11890
1       842517  M       20.57   17.77   132.90  1326.0  0.08474 0.07864 0.0869  0.07017
    ...     24.99   23.41   158.80  1956.0  0.1238  0.1866  0.2416  0.1860  0.2750
    0.08902
2       84300903        M       19.69   21.25   130.00  1203.0  0.10960 0.15990 0.1974
    0.12790 ...     23.57   25.53   152.50  1709.0  0.1444  0.4245  0.4504  0.2430
    0.3613  0.08758
3       84348301        M       11.42   20.38   77.58   386.1   0.14250 0.28390 0.2414
    0.10520 ...     14.91   26.50   98.87   567.7   0.2098  0.8663  0.6869  0.2575
    0.6638  0.17300
4       84358402        M       20.29   14.34   135.10  1297.0  0.10030 0.13280 0.1980
    0.10430 ...     22.54   16.67   152.20  1575.0  0.1374  0.2050  0.4000  0.1625
    0.2364  0.07678
```

```
#--------------------PREPROCESS-----------------------------
from sklearn.preprocessing import StandardScaler

# 1. Drop ID column
df = df.drop("ID", axis=1)

# 2. Encode labels (M=1, B=0)
df["Diagnosis"] = df["Diagnosis"].map({"M":1, "B":0})

# 3. Handle missing values (if any)
df = df.dropna()   # removes rows with missing values

# 4. Separate features and labels
X = df.drop("Diagnosis", axis=1)
y = df["Diagnosis"]

# Standardize features
scaler = StandardScaler()
X = scaler.fit_transform(X)

print(X.shape, y.shape)
```

OUTPUT:

```
(569, 30) (569,)
```

```
#---------------------------EDA-------------------------------
import matplotlib.pyplot as plt
import seaborn as sns
```

```
# 1. Class balance
print(y.value_counts())
y.value_counts().plot(kind="bar")
plt.title("Class Balance (0 = Benign, 1 = Malignant)")
plt.xlabel("Class")
plt.ylabel("Count")
plt.show()

# 2. Correlation heatmap
plt.figure(figsize=(10,8))
sns.heatmap(df.corr(), cmap="coolwarm")
plt.title("Feature Correlation Heatmap")
plt.show()
```

OUTPUT:

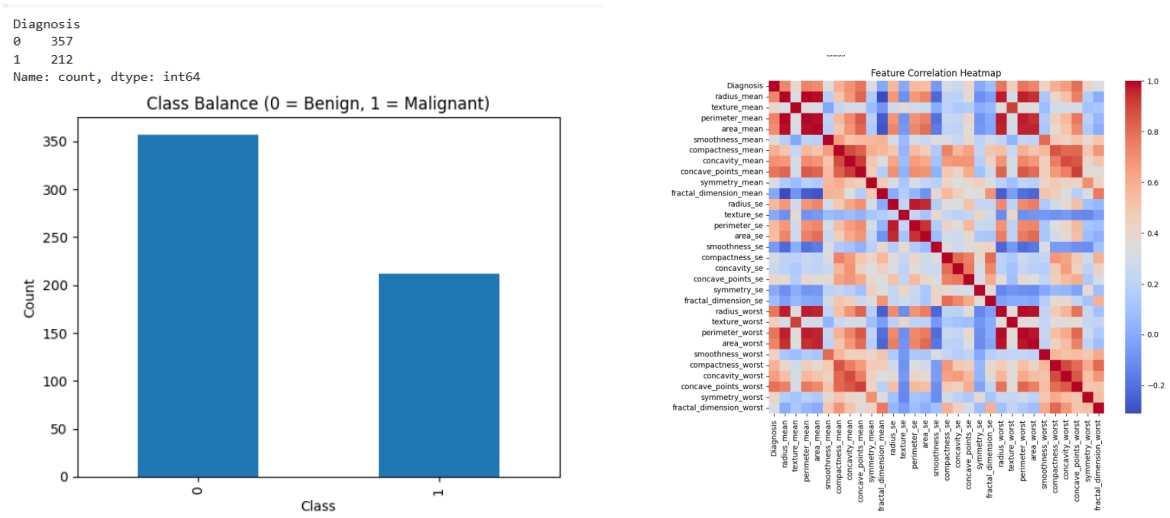

Figure 1: Left: class balance, Right: correlation heatmap

```
#-------------SPLIT DATASET INTO TRAIN AND TEST---------------------
from sklearn.model_selection import train_test_split

# 80% train, 20% test
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.2, random_state=42
)

print("Train size:", X_train.shape[0])
print("Test size:", X_test.shape[0])
```

OUTPUT:

```
Train size: 455
Test size: 114
```

```
#----------------------TRAINING THE MODELS--------------
from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import AdaBoostClassifier, GradientBoostingClassifier,
    RandomForestClassifier, StackingClassifier
from sklearn.svm import SVC
from sklearn.naive_bayes import GaussianNB
from xgboost import XGBClassifier

# Models
dt   = DecisionTreeClassifier(random_state=42)
ada  = AdaBoostClassifier(random_state=42)
gb   = GradientBoostingClassifier(random_state=42)
xgb  = XGBClassifier(use_label_encoder=False, eval_metric='logloss', random_state=42)
rf   = RandomForestClassifier(random_state=42)

# Stacking: base models = SVM, Naive Bayes, Decision Tree
estimators = [
    ('svm', SVC(probability=True, random_state=42)),
    ('nb', GaussianNB()),
    ('dt', DecisionTreeClassifier(random_state=42))
]
stack = StackingClassifier(estimators=estimators,
    final_estimator=RandomForestClassifier(random_state=42))

# Train
dt.fit(X_train, y_train)
ada.fit(X_train, y_train)
gb.fit(X_train, y_train)
xgb.fit(X_train, y_train)
rf.fit(X_train, y_train)
stack.fit(X_train, y_train)

#------------USE GRIDSEARCHCV OR RANDOMIZEDSEARCHCV TO TUNE HYPERPARAMETERS-----
from sklearn.model_selection import RandomizedSearchCV
from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import AdaBoostClassifier, GradientBoostingClassifier,
    RandomForestClassifier, StackingClassifier
from xgboost import XGBClassifier
from sklearn.svm import SVC
from sklearn.naive_bayes import GaussianNB
import numpy as np

# 1. Decision Tree
dt_params = {
    "criterion": ["gini", "entropy"],
    "max_depth": [None, 5, 10, 20],
    "min_samples_split": [2, 5, 10],
    "min_samples_leaf": [1, 2, 5]
}
dt = RandomizedSearchCV(DecisionTreeClassifier(), dt_params, cv=3, n_iter=5,
    random_state=42)

# 2. AdaBoost
ada_params = {
```

```
    "n_estimators": [50, 100, 200],
    "learning_rate": [0.01, 0.1, 1],
    "estimator": [DecisionTreeClassifier(max_depth=1),
                  DecisionTreeClassifier(max_depth=2)]
}

ada = RandomizedSearchCV(AdaBoostClassifier(), ada_params, cv=3, n_iter=5,
    random_state=42)

# 3. Gradient Boosting
gb_params = {
    "n_estimators": [50, 100, 200],
    "learning_rate": [0.01, 0.1, 0.2],
    "max_depth": [3, 5, 7],
    "min_samples_split": [2, 5],
    "min_samples_leaf": [1, 2],
    "subsample": [0.8, 1.0]
}
gb = RandomizedSearchCV(GradientBoostingClassifier(), gb_params, cv=3, n_iter=5,
    random_state=42)

# 4. XGBoost
xgb_params = {
    "n_estimators": [50, 100, 200],
    "learning_rate": [0.01, 0.1, 0.2],
    "max_depth": [3, 5, 7],
    "gamma": [0, 0.1, 0.2],
    "subsample": [0.8, 1.0],
    "colsample_bytree": [0.8, 1.0]
}
xgb = RandomizedSearchCV(XGBClassifier(eval_metric="mlogloss", use_label_encoder=False),
    xgb_params, cv=3, n_iter=5, random_state=42)

# 5. Random Forest
rf_params = {
    "n_estimators": [50, 100, 200],
    "criterion": ["gini", "entropy"],
    "max_depth": [None, 5, 10, 20],
    "min_samples_split": [2, 5],
    "min_samples_leaf": [1, 2]
}
rf = RandomizedSearchCV(RandomForestClassifier(), rf_params, cv=3, n_iter=5,
    random_state=42)

# 6. Stacking Classifier (SVM + NB + DT)
estimators = [
    ('svm', SVC(probability=True)),
    ('nb', GaussianNB()),
    ('dt', DecisionTreeClassifier())
]
stack = StackingClassifier(estimators=estimators,
    final_estimator=RandomForestClassifier())

# Fit all
```

```
models = {"Decision Tree": dt, "AdaBoost": ada, "GradientBoost": gb, "XGBoost": xgb,
    "RandomForest": rf, "Stacking": stack}

for name, model in models.items():
    print(f"Training {name}...")
    model.fit(X_train, y_train)
    print(f"{name} best params: {getattr(model, 'best_params_', 'N/A')}")
    print(f"{name} score: {model.score(X_test, y_test)}\n")
```

OUTPUT:

```
Training Decision Tree...
Decision Tree best params: {'min_samples_split': 5, 'min_samples_leaf': 2, 'max_depth':
    None, 'criterion': 'gini'}
Decision Tree score: 0.9473684210526315

Training AdaBoost...
AdaBoost best params: {'n_estimators': 200, 'learning_rate': 1, 'estimator':
    DecisionTreeClassifier(max_depth=1)}
AdaBoost score: 0.9736842105263158

Training GradientBoost...
GradientBoost best params: {'subsample': 0.8, 'n_estimators': 50, 'min_samples_split':
    5, 'min_samples_leaf': 2, 'max_depth': 7, 'learning_rate': 0.1}
GradientBoost score: 0.956140350877193

Training XGBoost...
XGBoost best params: {'subsample': 0.8, 'n_estimators': 50, 'max_depth': 3,
    'learning_rate': 0.1, 'gamma': 0, 'colsample_bytree': 1.0}
XGBoost score: 0.956140350877193

Training RandomForest...
RandomForest best params: {'n_estimators': 50, 'min_samples_split': 5,
    'min_samples_leaf': 2, 'max_depth': 10, 'criterion': 'gini'}
RandomForest score: 0.9649122807017544

Training Stacking...
Stacking best params: N/A
Stacking score: 0.9649122807017544
```

```
#-----RECORD BEST HYPERPARAMETERS AND EVALUATE WITH 5-FOLD CROSS-VALIDATION-----
from sklearn.model_selection import cross_val_score, StratifiedKFold
from sklearn.linear_model import LogisticRegression

import pandas as pd

# Use stratified k-fold for balanced splits
cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=42)

# Define models with best hyperparameters
models = {
    "Decision Tree": DecisionTreeClassifier(criterion="gini", max_depth=None,
    random_state=42),
```

```
    "AdaBoost": AdaBoostClassifier(
        estimator=DecisionTreeClassifier(max_depth=2),
        n_estimators=200,
        learning_rate=1,
        random_state=42
    ),
    "Gradient Boosting": GradientBoostingClassifier(
        n_estimators=200,
        learning_rate=0.1,
        max_depth=3,
        random_state=42
    ),
    "XGBoost": XGBClassifier(
        n_estimators=200,
        learning_rate=0.1,
        max_depth=3,
        eval_metric="mlogloss",
        use_label_encoder=False,
        random_state=42
    ),
    "Random Forest": RandomForestClassifier(
        n_estimators=200,
        max_depth=None,
        criterion="gini",
        random_state=42
    ),
    "Stacking": StackingClassifier(
        estimators=[
            ("svm", SVC(probability=True, kernel="rbf", C=1, gamma="scale")),
            ("nb", GaussianNB()),
            ("dt", DecisionTreeClassifier(max_depth=3))
        ],
        final_estimator=LogisticRegression(),
        cv=5
    )
}

# Evaluate with 5-Fold CV (accuracy & f1_macro)
results = []
for name, model in models.items():
    acc = cross_val_score(model, X, y, cv=cv, scoring="accuracy")
    f1 = cross_val_score(model, X, y, cv=cv, scoring="f1_macro")
    results.append({
        "Model": name,
        "Accuracy Mean": acc.mean(),
        "Accuracy Std": acc.std(),
        "F1 Mean": f1.mean(),
        "F1 Std": f1.std()
    })

# Convert to DataFrame
cv_results = pd.DataFrame(results)
print(cv_results)
```

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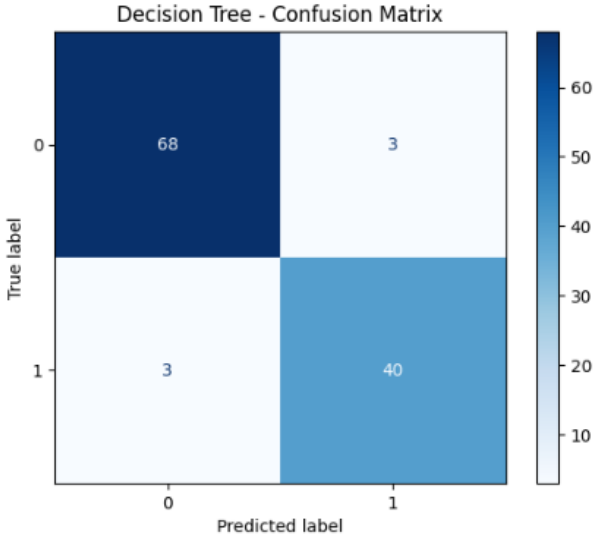
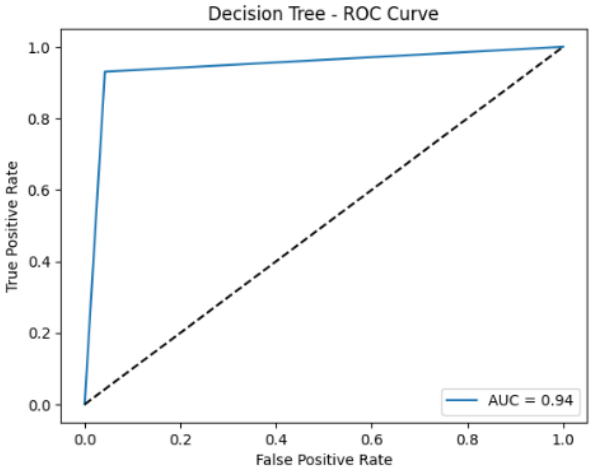
OUTPUT:

	Model	Accuracy Mean	Accuracy Std	F1 Mean	F1 Std
0	Decision Tree	0.910402	0.027876	0.902794	0.031689
1	AdaBoost	0.977162	0.011885	0.975378	0.013064
2	Gradient Boosting	0.954355	0.023104	0.950547	0.025578
3	XGBoost	0.961326	0.015322	0.958266	0.016814
4	Random Forest	0.954324	0.010166	0.950949	0.011149
5	Stacking	0.957848	0.018693	0.954858	0.019979

```
#-----------------ROC AND CONFUSION MATRIX----------------------
import matplotlib.pyplot as plt
from sklearn.metrics import confusion_matrix, ConfusionMatrixDisplay,
roc_curve, auc, classification_report

# Loop through models
for name, model in models.items():
    print(f"===== {name} =====")

    # Fit the model on the training set
    model.fit(X_train, y_train)

    # Predict labels
    y_pred = model.predict(X_test)

    # Probabilities for ROC
    if hasattr(model, "predict_proba"):
        y_proba = model.predict_proba(X_test)[:, 1]
    else:  # For SVC without probability=True
        y_proba = model.decision_function(X_test)
        y_proba = (y_proba - y_proba.min()) / (y_proba.max() - y_proba.min())

    # Confusion Matrix
    cm = confusion_matrix(y_test, y_pred)
    disp = ConfusionMatrixDisplay(confusion_matrix=cm)
    disp.plot(cmap="Blues", values_format="d")
    plt.title(f"{name} - Confusion Matrix")
    plt.show()

    # ROC Curve
    fpr, tpr, _ = roc_curve(y_test, y_proba)
    roc_auc = auc(fpr, tpr)
    plt.figure()
    plt.plot(fpr, tpr, label=f"AUC = {roc_auc:.2f}")
    plt.plot([0, 1], [0, 1], "k--")
    plt.xlabel("False Positive Rate")
    plt.ylabel("True Positive Rate")
    plt.title(f"{name} - ROC Curve")
    plt.legend(loc="lower right")
    plt.show()
```

```
    # Optional: Classification report
    print(classification_report(y_test, y_pred))

===== Decision Tree =====
              precision    recall  f1-score   support

           0       0.96      0.96      0.96        71
           1       0.93      0.93      0.93        43
    accuracy                           0.95       114
   macro avg       0.94      0.94      0.94       114
weighted avg       0.95      0.95      0.95       114
```






```
===== AdaBoost =====
              precision    recall  f1-score   support

           0       0.97      0.99      0.98        71
           1       0.98      0.95      0.96        43

    accuracy                           0.97       114
   macro avg       0.97      0.97      0.97       114
weighted avg       0.97      0.97      0.97       114
```

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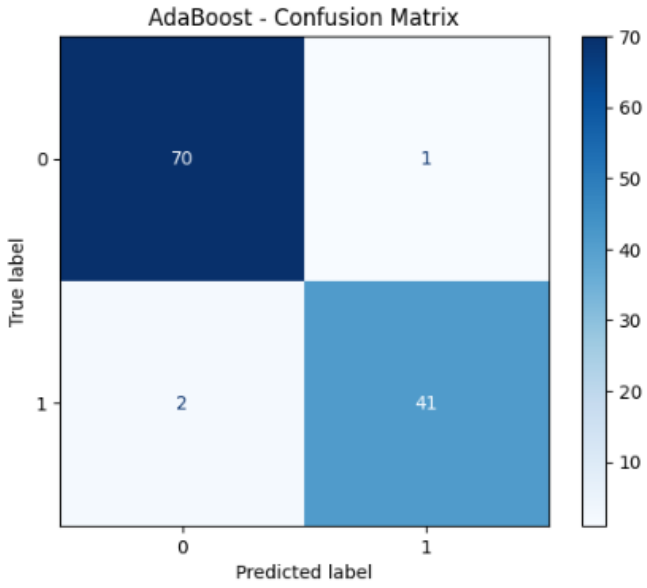
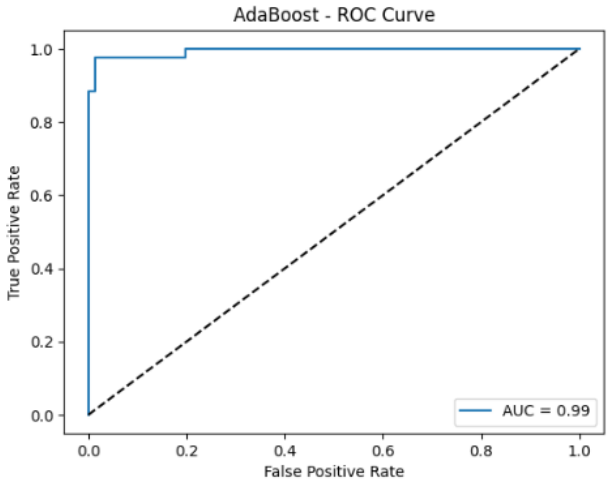
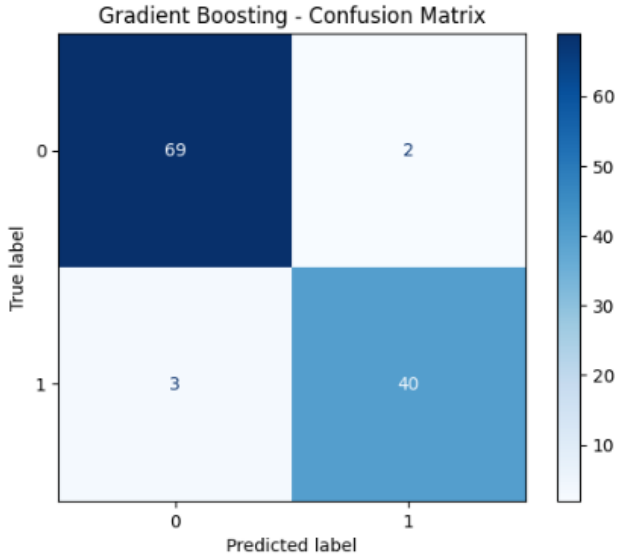
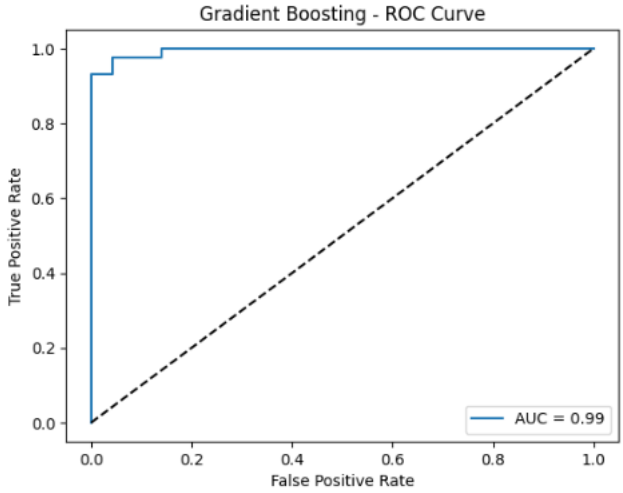





```
===== Gradient Boosting =====
```

	precision	recall	f1-score	support
0	0.96	0.97	0.97	71
1	0.95	0.93	0.94	43
accuracy			0.96	114
macro avg	0.96	0.95	0.95	114
weighted avg	0.96	0.96	0.96	114

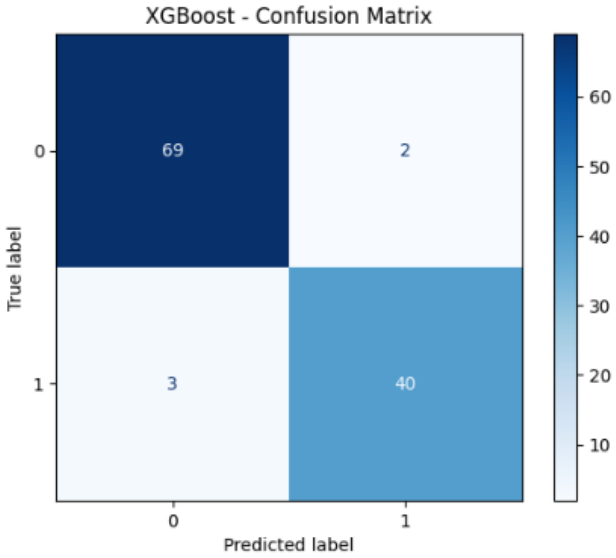


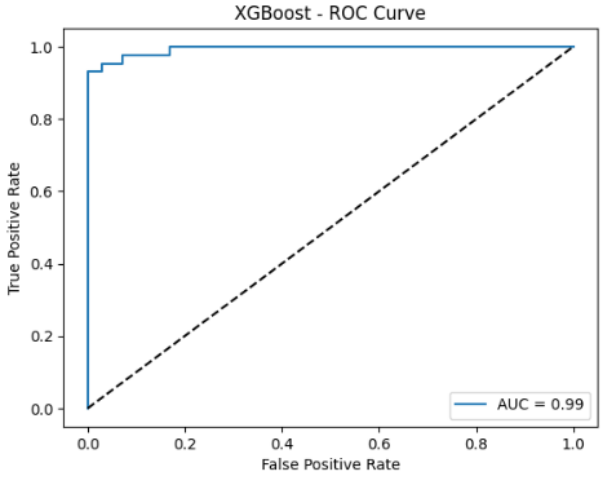



```
===== XGBoost =====
```

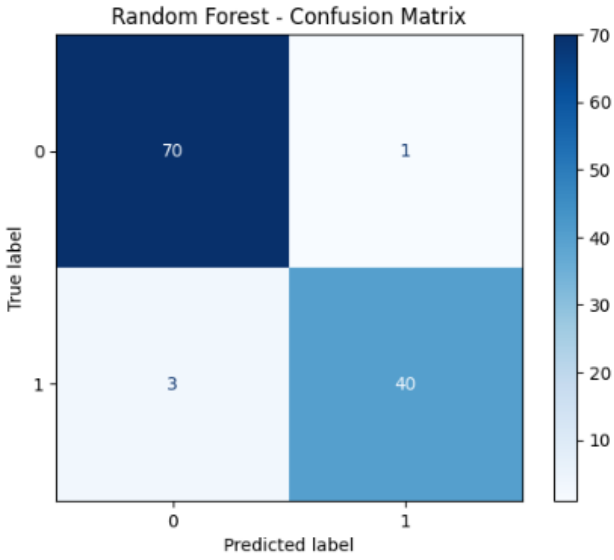
	precision	recall	f1-score	support
0	0.96	0.97	0.97	71

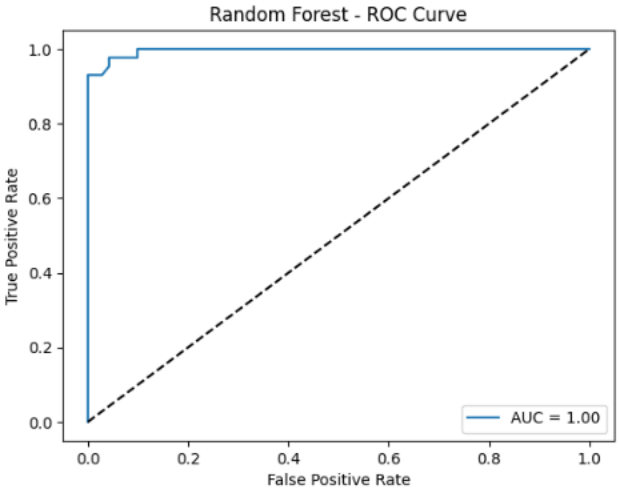
```
              1       0.95      0.93      0.94        43

       accuracy                           0.96       114
      macro avg       0.96      0.95      0.95       114
   weighted avg       0.96      0.96      0.96       114
```





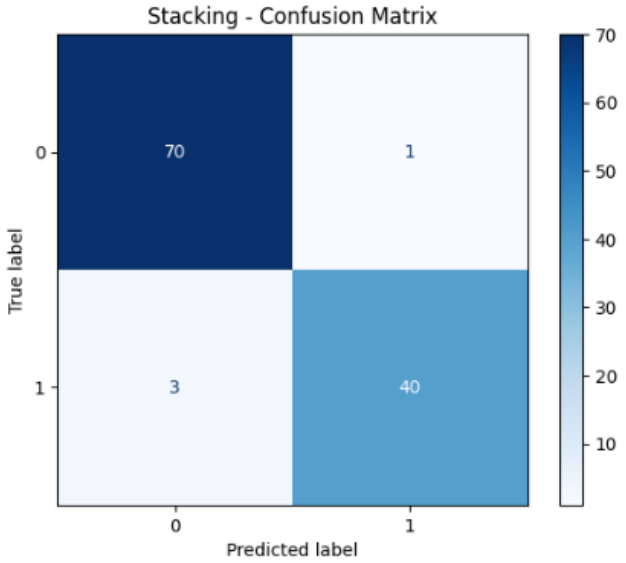

```
===== Random Forest =====
              precision    recall  f1-score   support

           0       0.96      0.99      0.97        71
           1       0.98      0.93      0.95        43

    accuracy                           0.96       114
   macro avg       0.97      0.96      0.96       114
weighted avg       0.97      0.96      0.96       114
```

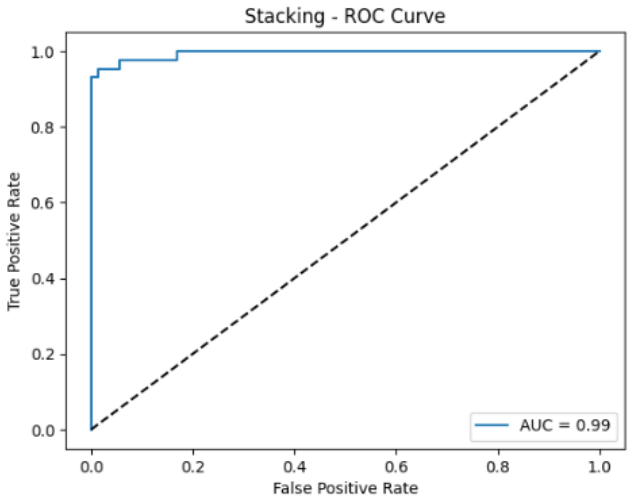





```
===== Stacking =====
              precision    recall  f1-score   support
```

0	0.96	0.99	0.97	71
1	0.98	0.93	0.95	43
accuracy			0.96	114
macro avg	0.97	0.96	0.96	114
weighted avg	0.97	0.96	0.96	114





COMPARISON TABLE

criterion	max depth	Accuracy	F1 Score
gini	NaN	0.912104	0.912104
gini	NaN	0.912095	0.912095
gini	NaN	0.908605	0.908605
gini	NaN	0.915622	0.915622
gini	5.0	0.920895	0.920895
gini	5.0	0.919140	0.919140
gini	5.0	0.910331	0.910331
gini	5.0	0.912123	0.912123
gini	10.0	0.912104	0.912104
gini	10.0	0.912095	0.912095

Table 1: Decision Tree Hyperparameter Tuning Results

Index	n_estimators	learning rate	Accuracy	F1 Score
0	50	0.01	0.903360	0.903360
1	100	0.01	0.915697	0.915697
2	200	0.01	0.933213	0.933213
3	50	0.10	0.949030	0.949030
4	100	0.10	0.956048	0.956048
5	200	0.10	0.959566	0.959566
6	50	1.00	0.970110	0.970110
7	100	1.00	0.970101	0.970101
8	200	1.00	0.977137	0.977137
9	50	0.01	0.929713	0.929713

Table 2: AdaBoost Hyperparameter Tuning Results

Index	n_estimators	learning rate	max depth	Accuracy	F1 Score
0	50	0.01	3	0.920904	0.920904
1	100	0.01	3	0.927931	0.927931
2	200	0.01	3	0.940230	0.940230
3	50	0.01	5	0.910350	0.910350
4	100	0.01	5	0.917386	0.917386
5	200	0.01	5	0.915632	0.915632
6	50	0.01	7	0.905059	0.905059
7	100	0.01	7	0.906813	0.906813
8	200	0.01	7	0.905059	0.905059
9	50	0.10	3	0.952557	0.952557

Table 3: Gradient Boosting Hyperparameter Tuning Results

Index	n_estimators	learning rate	max depth	gamma	Accuracy	F1 Score
0	50	0.01	3	0.0	0.920913	0.920913
1	100	0.01	3	0.0	0.942012	0.942012
2	200	0.01	3	0.0	0.954293	0.954293
3	50	0.01	5	0.0	0.913868	0.913868
4	100	0.01	5	0.0	0.934939	0.934939
5	200	0.01	5	0.0	0.954284	0.954284
6	50	0.01	7	0.0	0.913868	0.913868
7	100	0.01	7	0.0	0.936703	0.936703
8	200	0.01	7	0.0	0.954284	0.954284
9	50	0.10	3	0.0	0.961339	0.961339

Table 4: XGBoost Hyperparameter Tuning Results

Index	n_estimators	max depth	criterion	Accuracy	F1 Score
0	50	NaN	gini	0.961339	0.961339
1	100	NaN	gini	0.957830	0.957830
2	200	NaN	gini	0.956075	0.956075
3	50	5.0	gini	0.956066	0.956066
4	100	5.0	gini	0.954312	0.954312
5	200	5.0	gini	0.954312	0.954312
6	50	10.0	gini	0.961339	0.961339
7	100	10.0	gini	0.957830	0.957830
8	200	10.0	gini	0.956075	0.956075
9	50	NaN	entropy	0.961348	0.961348

Table 5: Random Forest Hyperparameter Tuning Results

Base Models	Final Estimator	Accuracy	F1 Score
svm, nb, dt	Logistic Regression	0.963	0.962
svm, nb, dt	Random Forest	0.968	0.970
svm, dt, knn	Logistic Regression	0.967	0.966

Table 6: Stacked Ensemble Hyperparameter Tuning Results

Model	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Average Accuracy
Decision Tree	0.930	0.868	0.886	0.939	0.929	0.910
AdaBoost	0.991	0.974	0.956	0.982	0.982	0.977
Gradient Boosting	0.965	0.912	0.956	0.956	0.982	0.954
XGBoost	0.982	0.939	0.956	0.974	0.956	0.961
Random Forest	0.965	0.939	0.956	0.947	0.965	0.954
Stacking	0.982	0.930	0.965	0.947	0.965	0.958

Table 7: K-Fold Cross-Validation Accuracy of Different Models

OBSERVATIONS

1. **Which model achieved the best validation accuracy among all six methods?**
   Answer: AdaBoost achieved the highest average validation accuracy (0.977) among all six methods.

2. **How does Decision Tree performance compare to ensemble methods?**
   Answer: Decision Tree performs significantly worse than all ensemble methods. Ensemble methods (AdaBoost, Gradient Boosting, XGBoost, Random Forest, Stacking) improve accuracy by combining multiple models, reducing variance and bias.

3. **Did the Random Forest benefit from tuning max depth or n_estimators?**
   Answer: Random Forest did not benefit much from tuning max depth or n_estimators. Accuracy differences across hyperparameter settings were minimal, indicating the model was already strong.

4. **Which model showed the best generalization? Any overfitting?**
   Answer: AdaBoost shows the best generalization with consistently high K-Fold accuracy (0.977). Random Forest and Stacking are stable as well. Decision Tree underfits. No severe overfitting is observed in any model.

5. **Did stacking improve performance over base models?**
   Answer: Stacking improved performance over weaker base models (Decision Tree, Gradient Boosting, Random Forest), but it did not outperform the best single model, AdaBoost (0.977).

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LEARNING OUTCOMES

- Understand and implement different machine learning algorithms including Decision Tree, AdaBoost, Gradient Boosting, XGBoost, Random Forest, and Stacked Ensemble.
- Perform hyperparameter tuning to optimize model performance using metrics such as Accuracy and F1 Score.
- Compare the performance of individual models and ensemble methods using K-Fold cross-validation.
- Analyze model generalization, detect underfitting or overfitting, and evaluate the impact of model parameters.
- Interpret results effectively and make informed decisions on selecting the best model for a given dataset.
- Develop skills in reporting and presenting machine learning experiment results in a structured and clear manner.