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 6: Dimensionality Reduction and Model Evaluation (With and Without PCA)

1 Aim:

To study the effect of dimensionality reduction using Principal Component Analysis (PCA) on the performance of various machine learning classifiers. The task requires:

a) Training and validating models without PCA (original feature space).

b) Training and validating models with PCA (reduced feature space).

For both cases, students must perform hyperparameter tuning, apply 5-fold cross-validation, and record performance.

2 Libraries used:

- Pandas
- Numpy
- Matplotlib
- Scikit-learn
- XGBoost

3 Objective:

To evaluate how dimensionality reduction using Principal Component Analysis (PCA) influences the accuracy and generalization of different machine learning classifiers, by comparing their performance with and without PCA through hyperparameter tuning and 5-fold cross-validation.

[16]:

```
TARGET_COLUMN = 'class'
df = pd.read_csv('/content/drive/MyDrive/ml-lab/spambase_csv.csv')
print(df.head())
print("Initial shape:", df.shape)
```

```
   word_freq_make  word_freq_address  word_freq_all  word_freq_3d  \
0            0.00               0.64           0.64           0.0   
1            0.21               0.28           0.50           0.0   
2            0.06               0.00           0.71           0.0   
3            0.00               0.00           0.00           0.0   
4            0.00               0.00           0.00           0.0   

   word_freq_our  word_freq_over  word_freq_remove  word_freq_internet  \
0           0.32            0.00              0.00                0.00   
1           0.14            0.28              0.21                0.07   
2           1.23            0.19              0.19                0.12   
3           0.63            0.00              0.31                0.63   
4           0.63            0.00              0.31                0.63   

   word_freq_order  word_freq_mail  ...  char_freq_%3B  char_freq_%28  \
0             0.00            0.00  ...           0.00          0.000   
1             0.00            0.94  ...           0.00          0.132   
2             0.64            0.25  ...           0.01          0.143   
3             0.31            0.63  ...           0.00          0.137   
4             0.31            0.63  ...           0.00          0.135   

   char_freq_%5B  char_freq_%21  char_freq_%24  char_freq_%23  \
0            0.0          0.778          0.000          0.000   
1            0.0          0.372          0.180          0.048   
2            0.0          0.276          0.184          0.010   
3            0.0          0.137          0.000          0.000   
4            0.0          0.135          0.000          0.000   

   capital_run_length_average  capital_run_length_longest  \
0                       3.756                          61   
1                       5.114                         101   
2                       9.821                         485   
3                       3.537                          40   
4                       3.537                          40   

   capital_run_length_total  class  
0                       278      1  
1                      1028      1  
2                      2259      1  
3                       191      1  
4                       191      1  

[5 rows x 58 columns]
Initial shape: (4601, 58)
```

[17]:

```
# HANDLE MISSING VALUES
df = df.dropna(thresh=df.shape[1]//2)  # Drop rows with >50% missing
df.fillna(df.median(numeric_only=True), inplace=True)

# OUTLIER HANDLING (Z-Score)
def remove_outliers(df, threshold=3):
    numeric_cols = df.select_dtypes(include=[np.number]).columns
    z_scores = np.abs((df[numeric_cols] - df[numeric_cols].mean()) / df[numeric_cols].std())
    return df[(z_scores < threshold).all(axis=1)]

df = remove_outliers(df)
# print("After outlier removal:", df.shape)
```

[18]:

```
# FEATURE / TARGET SPLIT
X = df.drop(columns=[TARGET_COLUMN])
y = df[TARGET_COLUMN]

# ENCODE + STANDARDIZE
numeric_cols = X.select_dtypes(include=[np.number]).columns
categorical_cols = X.select_dtypes(exclude=[np.number]).columns
X_encoded = pd.get_dummies(X, columns=categorical_cols)
scaler = StandardScaler()
X_scaled = scaler.fit_transform(X_encoded)

# TRAIN / TEST SPLIT
X_train, X_test, y_train, y_test = train_test_split(
    X_scaled,
    y,
    test_size=0.2,          # 20% test hold-out
    stratify=y,             # keep class balance if classification
    random_state=42
)
```

PCA Variance Explained

[39]:

```
pca = PCA(n_components=0.95)
pca.fit(X_scaled)

print("Chosen components:", pca.n_components_)
print("Total variance explained (%):", pca.explained_variance_ratio_.sum()*100)
```

```
Chosen components: 49
Total variance explained (%): 95.53617010131482
```

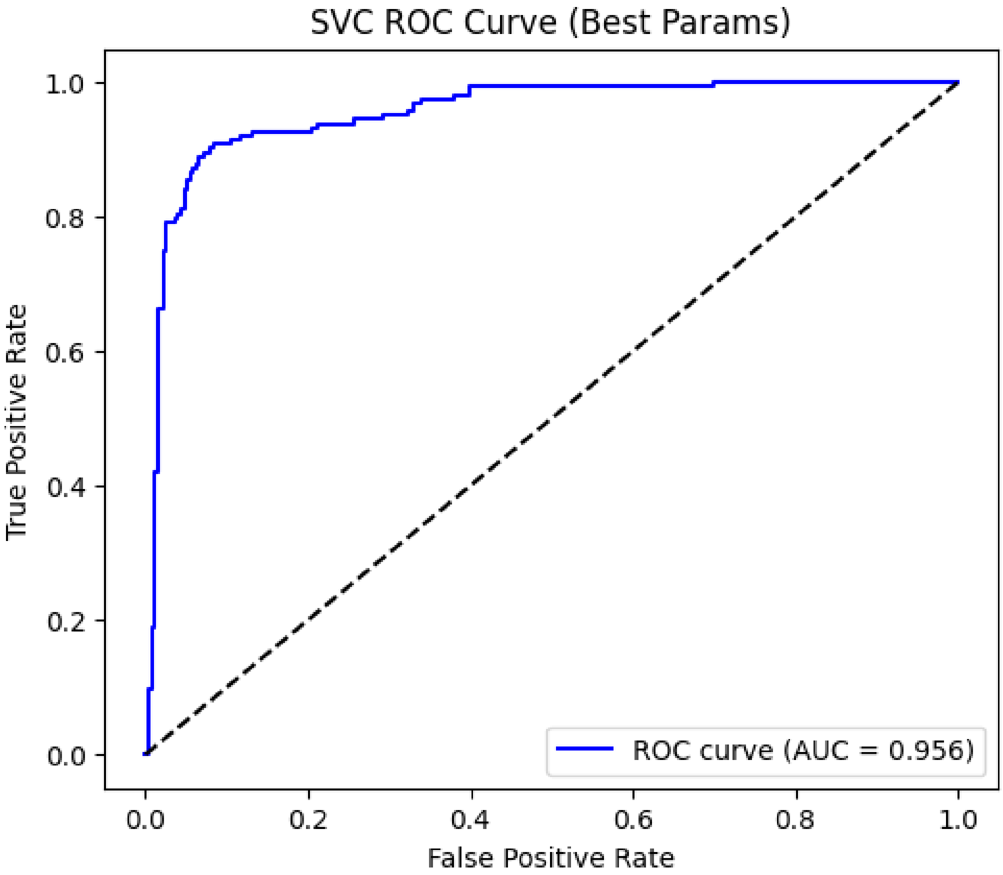
Support Vector Machine (SVM)

[23]:

```
# ========== HYPERPARAM GRID ==========
param_grid = {
    'kernel': ['linear', 'rbf'],
    'C': [0.1, 10],
    'gamma': ['scale']
}

# ========== HELPER FUNCTION ==========
def evaluate_svc(X_train, X_test, y_train, y_test, use_pca=False, pca_variance=0.
↪95):
    if use_pca:
        pca = PCA(n_components=pca_variance)
        X_train_proc = pca.fit_transform(X_train)
        X_test_proc = pca.transform(X_test)
    else:
        X_train_proc = X_train
        X_test_proc = X_test

    svc = SVC(probability=True)
    grid = GridSearchCV(svc, param_grid, cv=5, scoring='accuracy')  # you can␣
↪switch scoring
    grid.fit(X_train_proc, y_train)

    best_model = grid.best_estimator_
    y_pred = best_model.predict(X_test_proc)
    y_proba = best_model.predict_proba(X_test_proc)[:,1]

    acc = accuracy_score(y_test, y_pred)
    auc = roc_auc_score(y_test, y_proba)

    return grid.best_params_, acc, auc, y_test, y_proba


# ========== EVALUATE ALL COMBOS ==========
results = []
for kernel in param_grid['kernel']:
    for C in param_grid['C']:
        for gamma in param_grid['gamma']:
            params = {'kernel': kernel, 'C': C, 'gamma': gamma}

            # No PCA
            _, acc_no_pca, auc_no_pca, y_test_val, y_proba_no_pca = evaluate_svc(
                X_train, X_test, y_train, y_test, use_pca=False
            )

            # With PCA
            _, acc_pca, auc_pca, _, y_proba_pca = evaluate_svc(
                X_train, X_test, y_train, y_test, use_pca=True, pca_variance=0.95
            )

            results.append({
                'kernel': kernel,
                'C': C,
                'gamma': gamma,
                'Accuracy_no_PCA': acc_no_pca,
                'Accuracy_PCA': acc_pca
            })

# ========== RESULTS TABLE ==========
results_df = pd.DataFrame(results)
print("SVC Performance Table")
print(results_df)

# ========== BEST MODEL ==========
best_idx = results_df['Accuracy_no_PCA'].idxmax()  # you can also pick max of PCA
best_params = results_df.iloc[best_idx]
print("\nBest Params (No PCA)")
print(best_params)


# ========== ROC CURVE FOR BEST MODEL ==========
# Using No PCA best model
best_kernel = best_params['kernel']
best_C = best_params['C']
best_gamma = best_params['gamma']

svc_best = SVC(kernel=best_kernel, C=best_C, gamma=best_gamma, probability=True)
svc_best.fit(X_train, y_train)
y_proba_best = svc_best.predict_proba(X_test)[:,1]
fpr, tpr, _ = roc_curve(y_test, y_proba_best)
roc_auc = roc_auc_score(y_test, y_proba_best)

plt.figure(figsize=(6,5))
plt.plot(fpr, tpr, label=f'ROC curve (AUC = {roc_auc:.3f})', color='blue')
plt.plot([0,1], [0,1], 'k--')
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('SVC ROC Curve (Best Params)')
plt.legend(loc='lower right')
plt.show()
```

OUTPUT:

```
SVC Performance Table

   kernel     C  gamma  Accuracy_no_PCA  Accuracy_PCA
0  linear   0.1  scale          0.93135      0.924485
1  linear  10.0  scale          0.93135      0.924485
2     rbf   0.1  scale          0.93135      0.924485
3     rbf  10.0  scale          0.93135      0.924485

Best Params (No PCA)

kernel                linear
C                        0.1
gamma                  scale
Accuracy_no_PCA      0.93135
Accuracy_PCA        0.924485
Name: 0, dtype: object
```



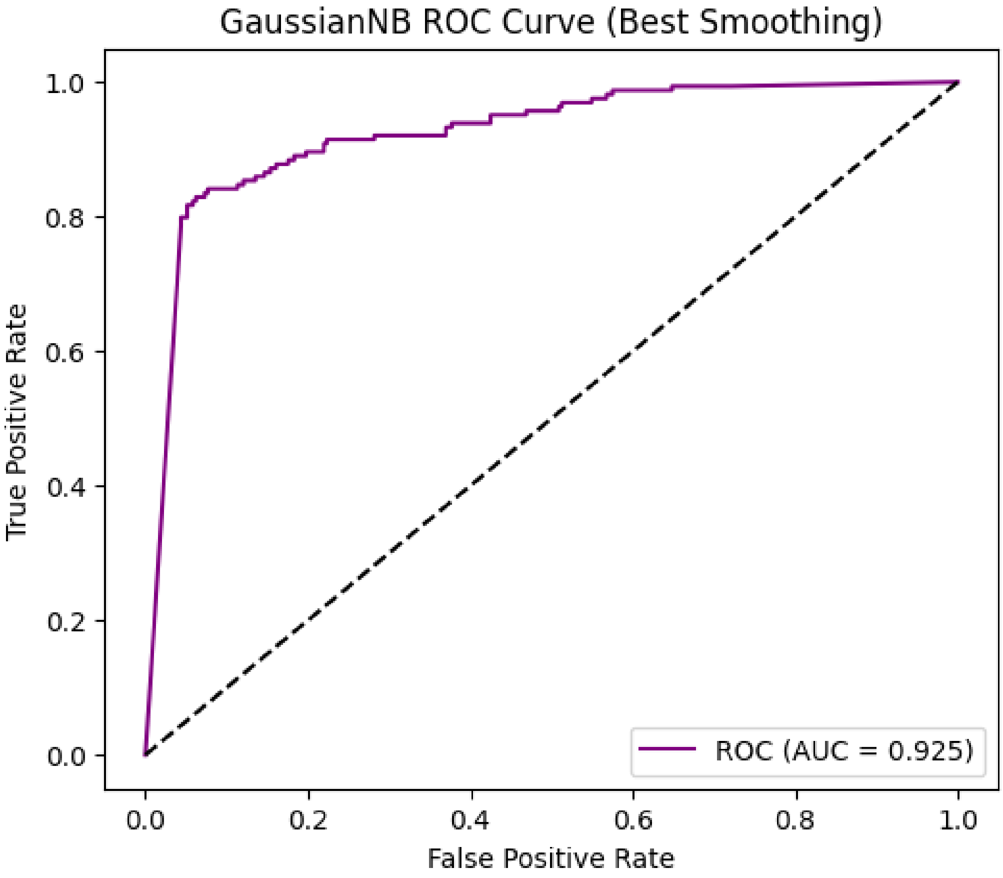
Naive Bayes

[22]:

```
smoothing_values = [1e-9, 1e-8, 1e-7, 1e-6]

def evaluate_nb(X_train, X_test, y_train, y_test, smoothing, use_pca=False):
    if use_pca:
        pca = PCA(n_components=0.95)
        X_train_proc = pca.fit_transform(X_train)
        X_test_proc = pca.transform(X_test)
    else:
        X_train_proc = X_train
        X_test_proc = X_test
    model = GaussianNB(var_smoothing=smoothing)
    model.fit(X_train_proc, y_train)
    y_pred = model.predict(X_test_proc)
    y_prob = model.predict_proba(X_test_proc)[:, 1]
    acc = accuracy_score(y_test, y_pred)
    auc = roc_auc_score(y_test, y_prob)
    return acc, auc, y_prob

results = []
for s in smoothing_values:
    acc_no_pca, auc_no_pca, prob_no_pca = evaluate_nb(
        X_train, X_test, y_train, y_test, s, use_pca=False)
    acc_pca, auc_pca, prob_pca = evaluate_nb(
        X_train, X_test, y_train, y_test, s, use_pca=True
    )
    results.append({
        "smoothing": s,
        "Accuracy_no_PCA": acc_no_pca,
        "Accuracy_PCA": acc_pca
    })

results_df = pd.DataFrame(results)
print("Naive Bayes Performance Table")
print(results_df)

best_idx = results_df['Accuracy_no_PCA'].idxmax()
best_params = results_df.iloc[best_idx]
print("\nBest Smoothing (No PCA)")
print(best_params)

best_s = best_params['smoothing']
nb_best = GaussianNB(var_smoothing=best_s)
nb_best.fit(X_train, y_train)
y_proba_best = nb_best.predict_proba(X_test)[:, 1]
fpr, tpr, _ = roc_curve(y_test, y_proba_best)
```

```
roc_auc = roc_auc_score(y_test, y_proba_best)

plt.figure(figsize=(6,5))
plt.plot(fpr, tpr, label=f'ROC (AUC = {roc_auc:.3f})', color='purple')
plt.plot([0,1],[0,1],'k--')
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('GaussianNB ROC Curve (Best Smoothing)')
plt.legend(loc='lower right')
plt.show()
```

```
Naive Bayes Performance Table
      smoothing  Accuracy_no_PCA  Accuracy_PCA
0  1.000000e-09         0.720824      0.832952
1  1.000000e-08         0.723112      0.832952
2  1.000000e-07         0.725400      0.832952
3  1.000000e-06         0.725400      0.832952

Best Smoothing (No PCA)
smoothing          1.000000e-07
Accuracy_no_PCA    7.254005e-01
Accuracy_PCA       8.329519e-01
```



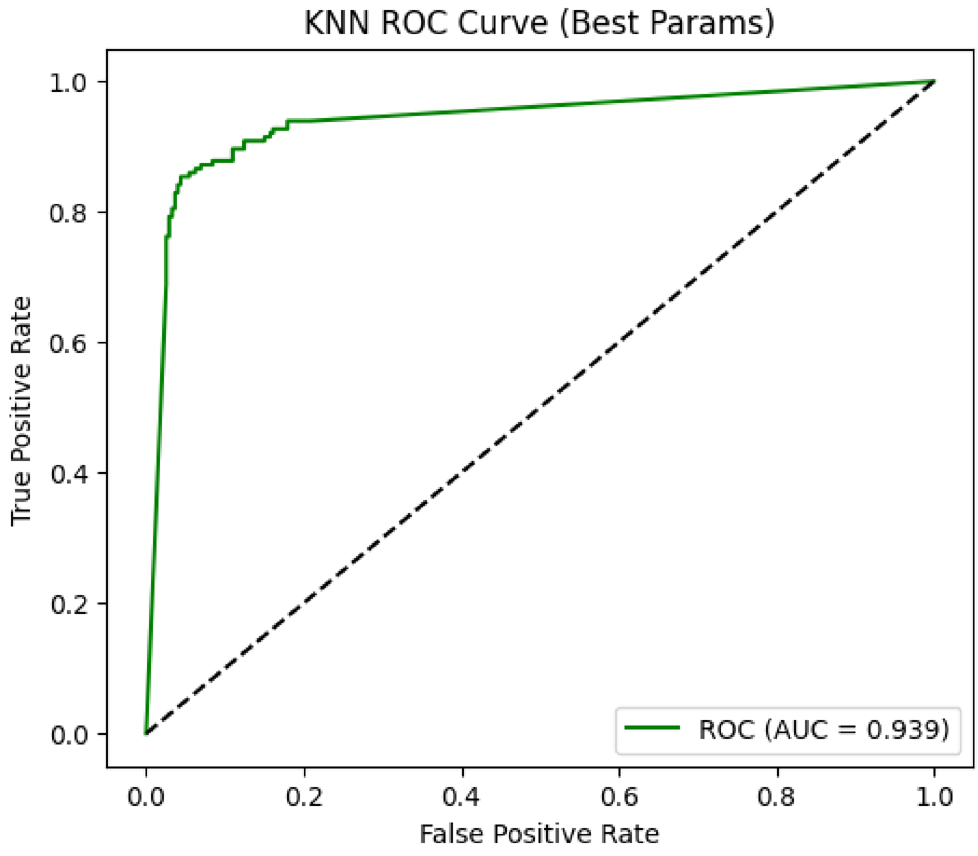
K-Nearest Neighbours

[24]:

```
k_values = [3, 5]
weights_options = ['uniform', 'distance']
metrics_options = ['euclidean', 'manhattan']

def evaluate_knn(X_train, X_test, y_train, y_test,
                 k, weight, metric, use_pca=False):
        X_train_proc, X_test_proc = X_train, X_test

    model = KNeighborsClassifier(n_neighbors=k,
                                 weights=weight,
                                 metric=metric)
    model.fit(X_train_proc, y_train)
    y_pred = model.predict(X_test_proc)
    y_prob = model.predict_proba(X_test_proc)[:, 1]
    acc = accuracy_score(y_test, y_pred)
    auc = roc_auc_score(y_test, y_prob)
    return acc, auc, y_prob

results = []
for k in k_values:
    for w in weights_options:
        for m in metrics_options:
            acc_no_pca, auc_no_pca, _ = evaluate_knn(
                X_train, X_test, y_train, y_test,
                k, w, m, use_pca=False
            )
            acc_pca, auc_pca, _ = evaluate_knn(
                X_train, X_test, y_train, y_test,
                k, w, m, use_pca=True
            )
            results.append({
                "k": k,
                "weights": w,
                "metric": m,
                "Accuracy_no_PCA": acc_no_pca,
                "Accuracy_PCA": acc_pca
            })

print(results_df)
print(best_params)
knn_best.fit(X_train, y_train)
y_proba_best = knn_best.predict_proba(X_test)[:, 1]
fpr, tpr, _ = roc_curve(y_test, y_proba_best)
roc_auc = roc_auc_score(y_test, y_proba_best)
```

```
plt.plot(fpr, tpr, label=f'ROC (AUC = {roc_auc:.3f})', color='green')
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('KNN ROC Curve (Best Params)')
plt.show()
```

```
KNN Performance Table
   k   weights     metric  Accuracy_no_PCA  Accuracy_PCA
0  3   uniform  euclidean         0.899314      0.901602
1  3   uniform  manhattan         0.899314      0.897025
2  3  distance  euclidean         0.910755      0.908467
3  3  distance  manhattan         0.903890      0.906178
4  5   uniform  euclidean         0.892449      0.899314
5  5   uniform  manhattan         0.897025      0.894737
6  5  distance  euclidean         0.908467      0.910755
7  5  distance  manhattan         0.906178      0.906178

Best KNN Params (No PCA)
k                          3
weights             distance
metric             euclidean
Accuracy_no_PCA     0.910755
Accuracy_PCA        0.908467
```



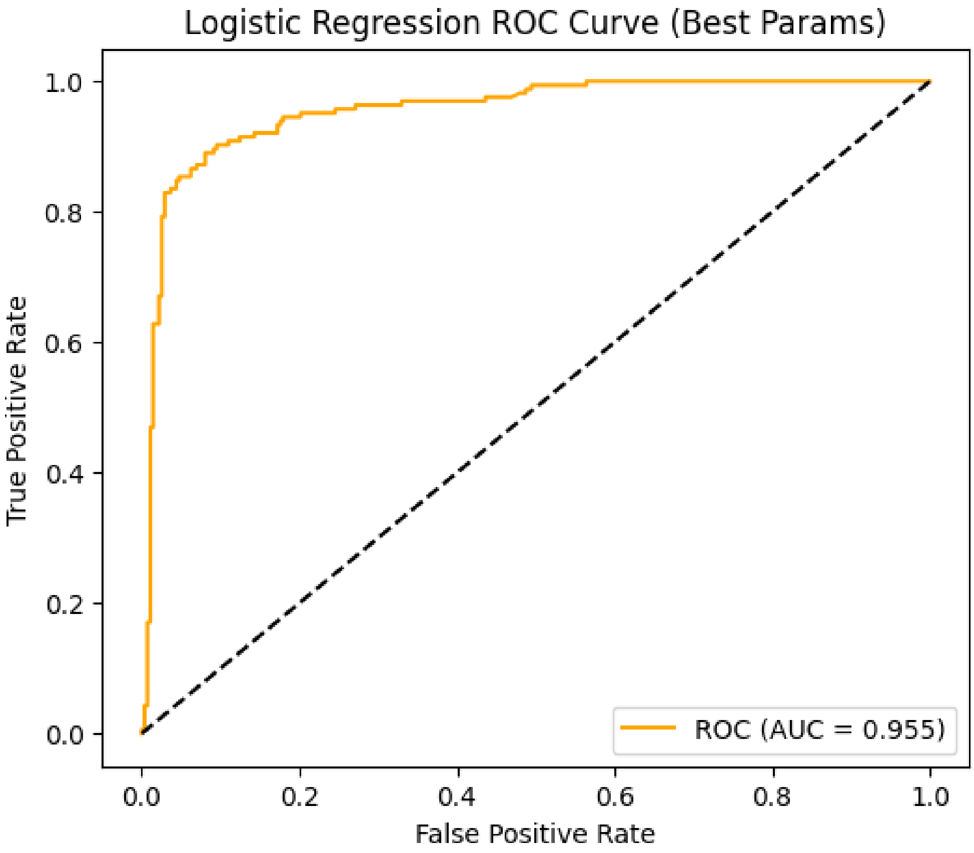
Logistic Regression

[25]:

```
c_values = [0.01, 0.1, 1]
penalties = ['l2', 'l1']

def evaluate_logreg(X_train, X_test, y_train, y_test,
                    c_val, penalty, use_pca=False):
        X_train_proc, X_test_proc = X_train, X_test

    solver = 'saga' if penalty == 'l1' else 'lbfgs'
    model = LogisticRegression(C=c_val,
                               penalty=penalty,
                               solver=solver,
                               max_iter=5000)
    model.fit(X_train_proc, y_train)
    y_pred = model.predict(X_test_proc)
    y_prob = model.predict_proba(X_test_proc)[:, 1]
    acc = accuracy_score(y_test, y_pred)
    auc = roc_auc_score(y_test, y_prob)
    return acc, auc, y_prob

results = []
for c in c_values:
    for p in penalties:
        acc_no_pca, auc_no_pca, _ = evaluate_logreg(
            X_train, X_test, y_train, y_test,
            c, p, use_pca=False
        )
        acc_pca, auc_pca, _ = evaluate_logreg(
            X_train, X_test, y_train, y_test,
            c, p, use_pca=True
        )
        results.append({
            "C": c,
            "penalty": p,
            "Accuracy_no_PCA": acc_no_pca,
            "Accuracy_PCA": acc_pca
        })

print(results_df)
print(best_params)
log_best = LogisticRegression(C=best_c,
                              penalty=best_p,
                              solver=solver,
                              max_iter=5000)
log_best.fit(X_train, y_train)
y_proba_best = log_best.predict_proba(X_test)[:, 1]
```

```
fpr, tpr, _ = roc_curve(y_test, y_proba_best)
roc_auc = roc_auc_score(y_test, y_proba_best)
plt.plot(fpr, tpr, label=f'ROC (AUC = {roc_auc:.3f})', color='orange')
[0,1], 'k--')
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('Logistic Regression ROC Curve (Best Params)')
plt.show()
```

```
Logistic Regression Performance Table
      C penalty  Accuracy_no_PCA  Accuracy_PCA
0  0.01      l2         0.908467      0.908467
1  0.01      l1         0.871854      0.894737
2  0.10      l2         0.903890      0.906178
3  0.10      l1         0.913043      0.917620
4  1.00      l2         0.910755      0.901602
5  1.00      l1         0.910755      0.906178

Best Logistic Regression Params (No PCA)
C                       0.1
penalty                  l1
Accuracy_no_PCA    0.913043
Accuracy_PCA        0.91762
```



Decision Tree

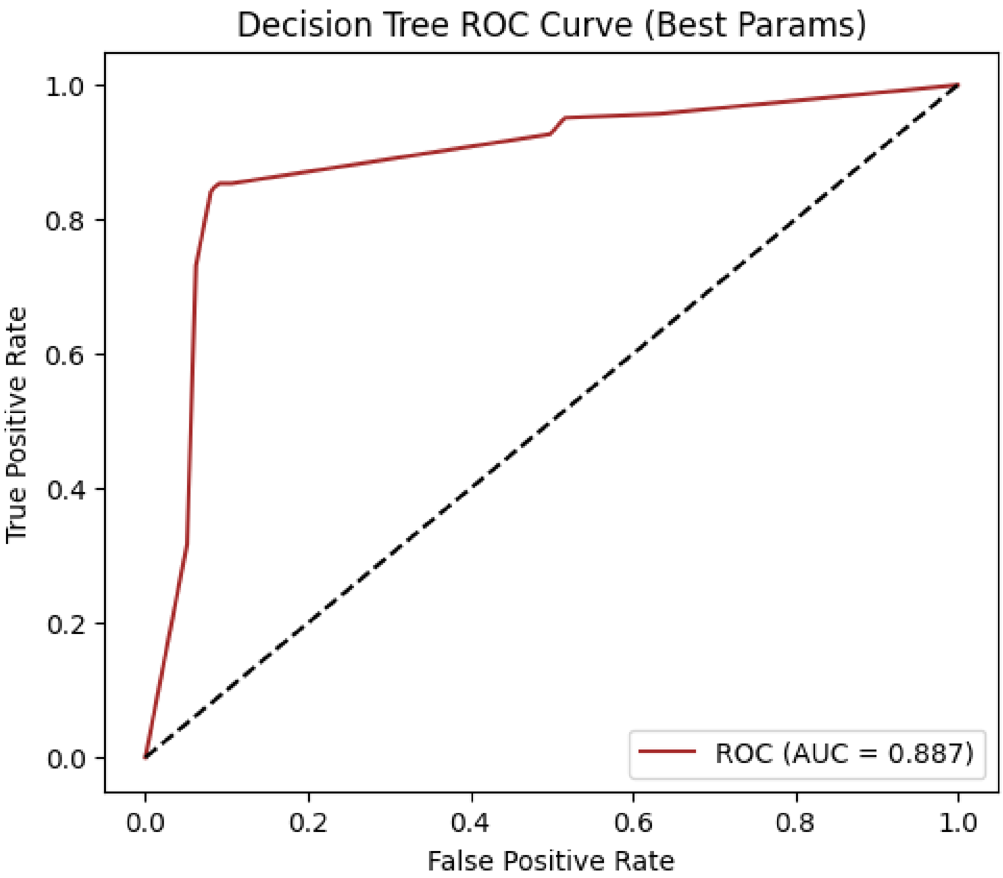
[29]:

```
# --- Hyperparams to explore ---
criteria = ["gini", "entropy"]
depths = [None, 5, 10]

def evaluate_dt(X_train, X_test, y_train, y_test,
                criterion, depth, use_pca=False):
    if use_pca:
        pca = PCA(n_components=0.95)
        X_train_proc = pca.fit_transform(X_train)
        X_test_proc = pca.transform(X_test)
    else:
        X_train_proc, X_test_proc = X_train, X_test

    model = DecisionTreeClassifier(
        criterion=criterion,
        max_depth=depth,
        random_state=42
    )
    model.fit(X_train_proc, y_train)
    y_pred = model.predict(X_test_proc)
    y_prob = model.predict_proba(X_test_proc)[:, 1]
    acc = accuracy_score(y_test, y_pred)
    auc = roc_auc_score(y_test, y_prob)
    return acc, auc, y_prob


results = []
for c in criteria:
    for d in depths:
        acc_no_pca, auc_no_pca, _ = evaluate_dt(
            X_train, X_test, y_train, y_test,
            c, d, use_pca=False
        )
        acc_pca, auc_pca, _ = evaluate_dt(
            X_train, X_test, y_train, y_test,
            c, d, use_pca=True
        )
        results.append({
            "criterion": c,
            "max_depth": d,
            "Accuracy_no_PCA": acc_no_pca,
            "Accuracy_PCA": acc_pca
        })
```

```
results_df = pd.DataFrame(results)
print("Decision Tree Performance Table")
print(results_df)


# --- Best by no-PCA accuracy ---
best_idx = results_df['Accuracy_no_PCA'].idxmax()
best_params = results_df.iloc[best_idx]
print("\nBest Decision Tree Params (No PCA)")
print(best_params)


# --- ROC curve for best combo ---
best_c = best_params['criterion']
best_d = best_params['max_depth']


# convert NaN to None, otherwise to int
if pd.isna(best_d):
    best_d = None
else:
    best_d = int(best_d)


dt_best = DecisionTreeClassifier(
    criterion=best_params['criterion'],
    max_depth=best_d,
    random_state=42
)
dt_best.fit(X_train, y_train)
y_proba_best = dt_best.predict_proba(X_test)[:, 1]
fpr, tpr, _ = roc_curve(y_test, y_proba_best)
roc_auc = roc_auc_score(y_test, y_proba_best)


plt.figure(figsize=(6,5))
plt.plot(fpr, tpr, label=f'ROC (AUC = {roc_auc:.3f})', color='brown')
plt.plot([0,1], [0,1], 'k--')
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('Decision Tree ROC Curve (Best Params)')
plt.legend(loc='lower right')
plt.show()
```

OUTPUT:

```
Decision Tree Performance Table
  criterion  max_depth  Accuracy_no_PCA  Accuracy_PCA
0      gini        NaN         0.887872      0.883295
1      gini        5.0         0.876430      0.860412
2      gini       10.0         0.890160      0.874142
3   entropy        NaN         0.855835      0.883295
4   entropy        5.0         0.871854      0.881007
5   entropy       10.0         0.878719      0.878719

Best Decision Tree Params (No PCA)
criterion              gini
max_depth              10.0
Accuracy_no_PCA     0.89016
Accuracy_PCA       0.874142
Name: 2, dtype: object
```



Random Forest

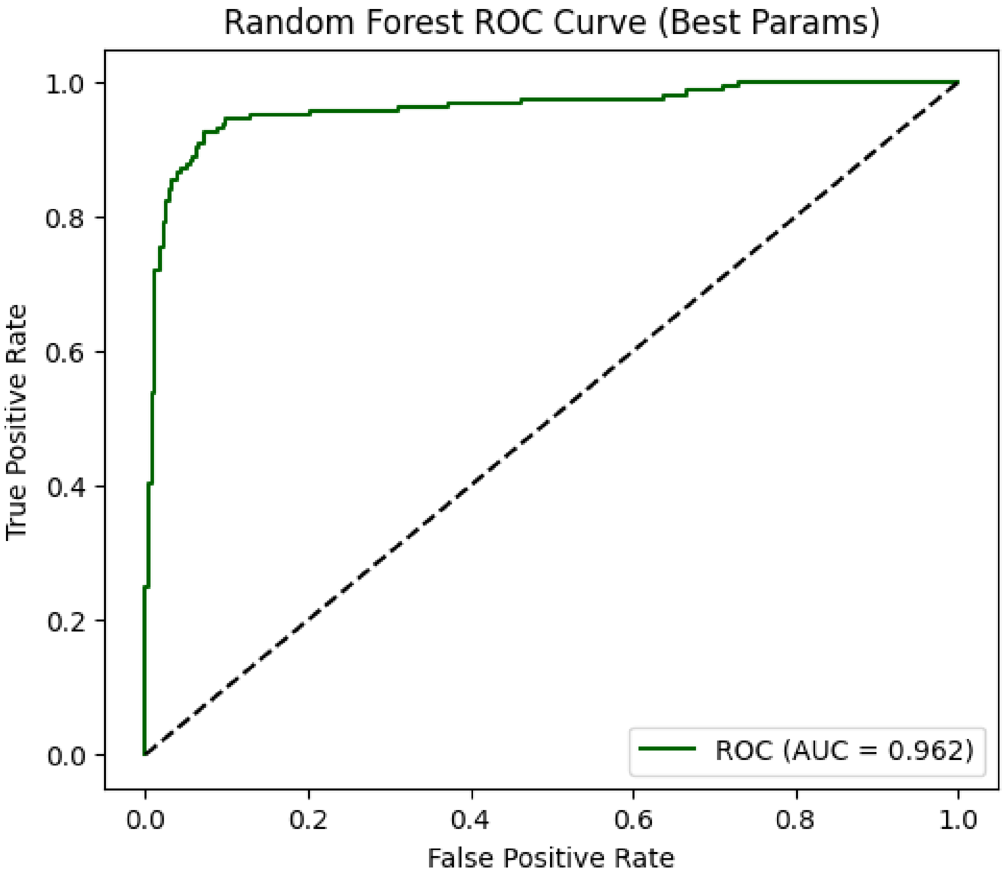
[30]:

```
# --- Hyperparams to explore ---
n_estimators_list = [50, 100]
max_depth_list = [None, 5, 10]

def evaluate_rf(X_train, X_test, y_train, y_test,
                n_estimators, depth, use_pca=False):
    if use_pca:
        pca = PCA(n_components=0.95)
        X_train_proc = pca.fit_transform(X_train)
        X_test_proc = pca.transform(X_test)
    else:
        X_train_proc, X_test_proc = X_train, X_test

    model = RandomForestClassifier(
        n_estimators=n_estimators,
        max_depth=depth,
        random_state=42,
        n_jobs=-1
    )
    model.fit(X_train_proc, y_train)
    y_pred = model.predict(X_test_proc)
    y_prob = model.predict_proba(X_test_proc)[:, 1]
    acc = accuracy_score(y_test, y_pred)
    auc = roc_auc_score(y_test, y_prob)
    return acc, auc, y_prob


results = []
for n in n_estimators_list:
    for d in max_depth_list:
        acc_no_pca, auc_no_pca, _ = evaluate_rf(
            X_train, X_test, y_train, y_test,
            n, d, use_pca=False
        )
        acc_pca, auc_pca, _ = evaluate_rf(
            X_train, X_test, y_train, y_test,
            n, d, use_pca=True
        )
        results.append({
            "n_estimators": n,
            "max_depth": d,
            "Accuracy_no_PCA": acc_no_pca,
            "Accuracy_PCA": acc_pca
        })
```

```python
results_df = pd.DataFrame(results)
print("Random Forest Performance Table")
print(results_df)


# --- Best by no-PCA accuracy ---
best_idx = results_df['Accuracy_no_PCA'].idxmax()
best_params = results_df.iloc[best_idx]
print("\nBest Random Forest Params (No PCA)")
print(best_params)


# --- Fix dtype for max_depth ---
best_depth = best_params['max_depth']
if pd.isna(best_depth):
    best_depth = None
else:
    best_depth = int(best_depth)


# --- ROC curve for best combo ---
rf_best = RandomForestClassifier(
    n_estimators=int(best_params['n_estimators']),
    max_depth=best_depth,
    random_state=42,
    n_jobs=-1
)

rf_best.fit(X_train, y_train)
y_proba_best = rf_best.predict_proba(X_test)[:, 1]
fpr, tpr, _ = roc_curve(y_test, y_proba_best)
roc_auc = roc_auc_score(y_test, y_proba_best)


plt.figure(figsize=(6,5))
plt.plot(fpr, tpr, label=f'ROC (AUC = {roc_auc:.3f})', color='darkgreen')
plt.plot([0,1], [0,1], 'k--')
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('Random Forest ROC Curve (Best Params)')
plt.legend(loc='lower right')
plt.show()
```

OUTPUT:

```
Random Forest Performance Table
   n_estimators  max_depth  Accuracy_no_PCA  Accuracy_PCA
0            50        NaN         0.922197      0.906178
1            50        5.0         0.910755      0.897025
2            50       10.0         0.924485      0.908467
3           100        NaN         0.924485      0.908467
4           100        5.0         0.908467      0.899314
5           100       10.0         0.922197      0.910755

Best Random Forest Params (No PCA)
n_estimators       50.000000
max_depth          10.000000
Accuracy_no_PCA     0.924485
Accuracy_PCA        0.908467
Name: 2, dtype: float64
```



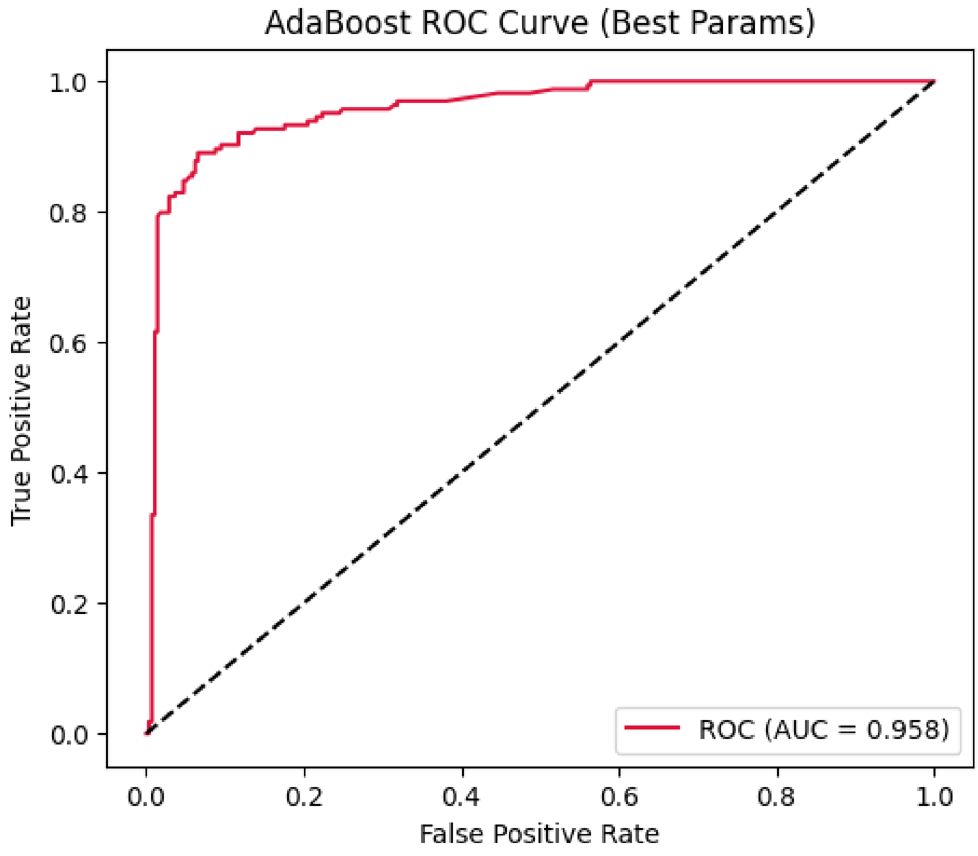
AdaBoost

[31]:

```
n_estimators_list = [50, 100]
learning_rates = [0.01, 0.1, 1.0]

def eval_adaboost(X_train, X_test, y_train, y_test,
                  n_est, lr, use_pca=False):
    if use_pca:
        pca = PCA(n_components=0.95)
        X_train_proc = pca.fit_transform(X_train)
        X_test_proc = pca.transform(X_test)
    else:
        X_train_proc, X_test_proc = X_train, X_test

    model = AdaBoostClassifier(
        n_estimators=n_est,
        learning_rate=lr,
        random_state=42
    )
    model.fit(X_train_proc, y_train)
    y_pred = model.predict(X_test_proc)
    y_prob = model.predict_proba(X_test_proc)[:, 1]
    return (
        accuracy_score(y_test, y_pred),
        roc_auc_score(y_test, y_prob)
    )

results = []
for n in n_estimators_list:
    for lr in learning_rates:
        acc_no_pca, _ = eval_adaboost(X_train, X_test, y_train, y_test,
                                      n, lr, use_pca=False)
        acc_pca, _ = eval_adaboost(X_train, X_test, y_train, y_test,
                                   n, lr, use_pca=True)
        results.append({
            "n_estimators": n,
            "learning_rate": lr,
            "Accuracy_no_PCA": acc_no_pca,
            "Accuracy_PCA": acc_pca
        })

print(results_df)
print(best_row)
best_model.fit(X_train, y_train)
y_best_prob = best_model.predict_proba(X_test)[:, 1]
fpr, tpr, _ = roc_curve(y_test, y_best_prob)
roc_auc = roc_auc_score(y_test, y_best_prob)
```

```
plt.figure(figsize=(6,5))
plt.plot(fpr, tpr, label=f'ROC (AUC = {roc_auc:.3f})', color='crimson')
plt.plot([0,1], [0,1], 'k--')
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('AdaBoost ROC Curve (Best Params)')
plt.legend(loc='lower right')
plt.show()
```

```
AdaBoost Performance
   n_estimators  learning_rate  Accuracy_no_PCA  Accuracy_PCA
0            50           0.01         0.821510      0.878719
1            50           0.10         0.897025      0.878719
2            50           1.00         0.908467      0.892449
3           100           0.01         0.844394      0.878719
4           100           0.10         0.899314      0.883295
5           100           1.00         0.915332      0.901602

Best Params (No PCA)
n_estimators       100.000000
learning_rate        1.000000
Accuracy_no_PCA      0.915332
Accuracy_PCA         0.901602
```



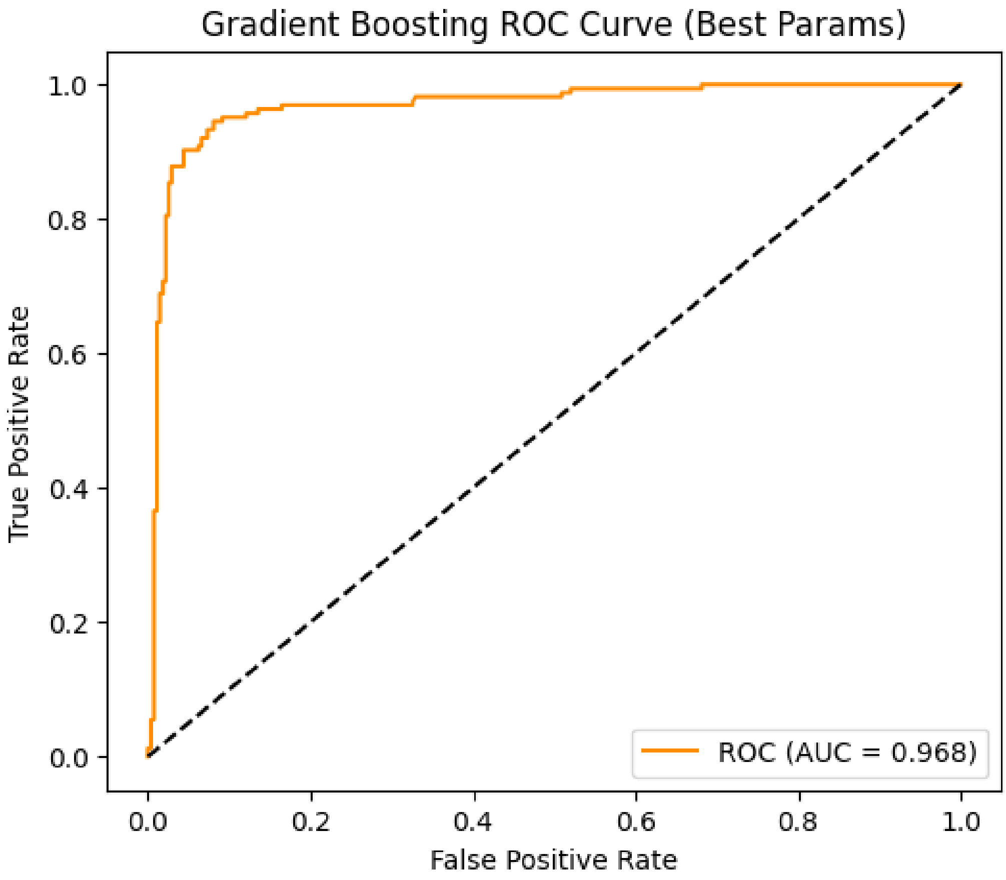
Gradient Boosting

[33]:

```
n_estimators_list = [50, 100, 200]
learning_rates = [0.1, 0.2]

def eval_gb(X_train, X_test, y_train, y_test, n_est, lr, use_pca=False):
    if use_pca:
        pca = PCA(n_components=0.95)
        X_train_proc = pca.fit_transform(X_train)
        X_test_proc = pca.transform(X_test)
    else:
        X_train_proc, X_test_proc = X_train, X_test

    model = GradientBoostingClassifier(
        n_estimators=n_est,
        learning_rate=lr,
        random_state=42
    )
    model.fit(X_train_proc, y_train)
    y_pred = model.predict(X_test_proc)
    y_prob = model.predict_proba(X_test_proc)[:, 1]
    return accuracy_score(y_test, y_pred), roc_auc_score(y_test, y_prob)

results = []
for n in n_estimators_list:
    for lr in learning_rates:
        acc_no_pca, _ = eval_gb(X_train, X_test, y_train, y_test,
                                n, lr, use_pca=False)
        acc_pca, _ = eval_gb(X_train, X_test, y_train, y_test,
                             n, lr, use_pca=True)
        results.append({
            "n_estimators": n,
            "learning_rate": lr,
            "Accuracy_no_PCA": acc_no_pca,
            "Accuracy_PCA": acc_pca
        })

print(results_df)
print(best_row)
best_model.fit(X_train, y_train)
y_best_prob = best_model.predict_proba(X_test)[:, 1]

fpr, tpr, _ = roc_curve(y_test, y_best_prob)
roc_auc = roc_auc_score(y_test,
y_best_prob)
plt.figure(figsize=(6,5))
plt.plot(fpr, tpr, label=f'ROC (AUC = {roc_auc:.3f})', color='darkorange')
```

```python
plt.plot([0,1], [0,1], 'k--')
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('Gradient Boosting ROC Curve (Best Params)')
plt.legend(loc='lower right')
plt.show()
```

```
Gradient Boosting Performance
   n_estimators  learning_rate  Accuracy_no_PCA  Accuracy_PCA
0            50            0.1         0.924485      0.901602
1            50            0.2         0.922197      0.913043
2           100            0.1         0.931350      0.908467
3           100            0.2         0.929062      0.913043
4           200            0.1         0.924485      0.908467
5           200            0.2         0.931350      0.910755

Best Params (No PCA)
n_estimators       100.000000
learning_rate        0.100000
Accuracy_no_PCA      0.931350
Accuracy_PCA         0.908467
```



XGBoost

[36]:

```
# --- Hyperparam grids ---
n_estimators_list = [50, 100]
learning_rates   = [0.1, 0.2]
max_depths       = [5, 7]

def eval_xgb(X_train, X_test, y_train, y_test,
             n_est, lr, depth, use_pca=False):
    if use_pca:
        pca = PCA(n_components=0.95)
        X_train_proc = pca.fit_transform(X_train)
        X_test_proc  = pca.transform(X_test)
    else:
        X_train_proc, X_test_proc = X_train, X_test

    model = XGBClassifier(
        n_estimators=n_est,
        learning_rate=lr,
        max_depth=depth,
        eval_metric='logloss',
        use_label_encoder=False,
        random_state=42
    )
    model.fit(X_train_proc, y_train)
    y_pred  = model.predict(X_test_proc)
    y_proba = model.predict_proba(X_test_proc)[:, 1]
    return accuracy_score(y_test, y_pred), roc_auc_score(y_test, y_proba)


# Collect results
rows = []
for n in n_estimators_list:
    for lr in learning_rates:
        for d in max_depths:
            acc_no, _ = eval_xgb(X_train, X_test, y_train, y_test,
                                 n, lr, d, use_pca=False)
            acc_pca, _ = eval_xgb(X_train, X_test, y_train, y_test,
                                  n, lr, d, use_pca=True)
            rows.append({
                "n_estimators": n,
                "learning_rate": lr,
                "max_depth": d,
                "Accuracy_no_PCA": acc_no,
                "Accuracy_PCA": acc_pca
            })
```

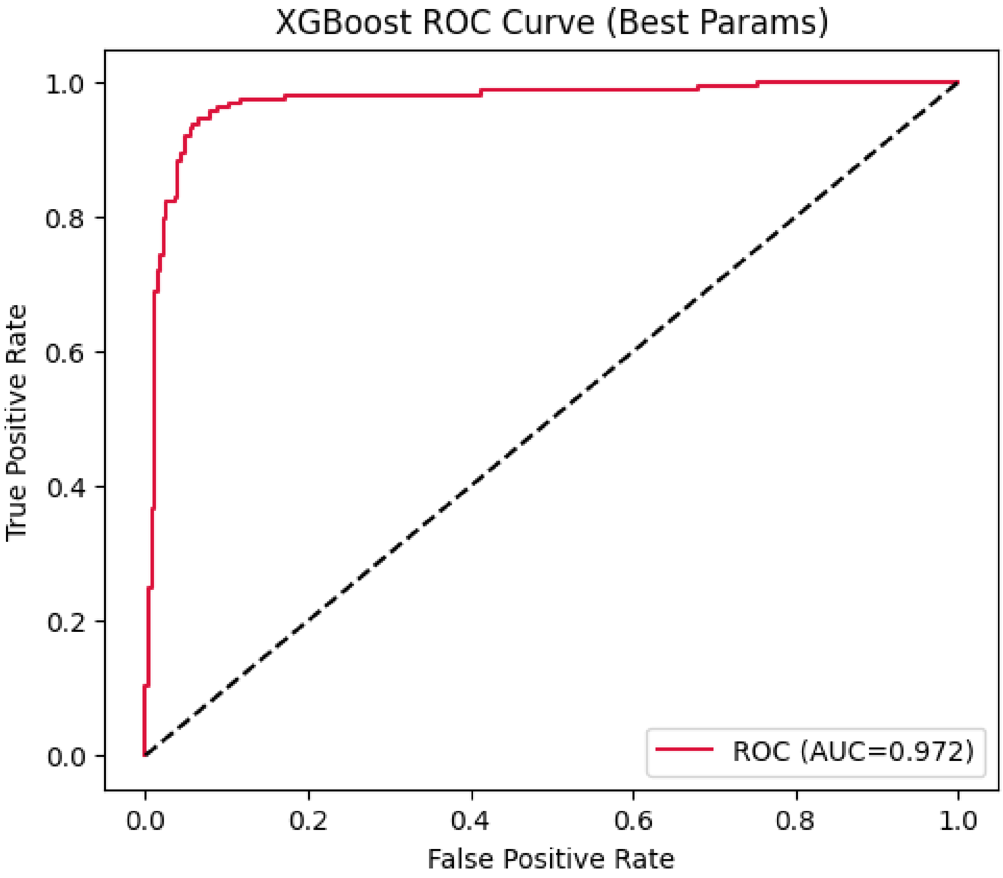
```python
results_df = pd.DataFrame(rows)
print("XGBoost Performance Table")
print(results_df)


# --- Best params (No PCA) ---
best_idx = results_df['Accuracy_no_PCA'].idxmax()
best_row = results_df.iloc[best_idx]
print("\nBest Params (No PCA)")
print(best_row)


# --- ROC curve for best model ---
best_model = XGBClassifier(
    n_estimators=int(best_row["n_estimators"]),
    learning_rate=float(best_row["learning_rate"]),
    max_depth=int(best_row["max_depth"]),
    eval_metric='logloss',
    use_label_encoder=False,
    random_state=42
)
best_model.fit(X_train, y_train)
y_prob = best_model.predict_proba(X_test)[:, 1]


fpr, tpr, _ = roc_curve(y_test, y_prob)
roc_auc = roc_auc_score(y_test, y_prob)

plt.figure(figsize=(6,5))
plt.plot(fpr, tpr, label=f'ROC (AUC={roc_auc:.3f})', color='crimson')
plt.plot([0,1], [0,1], 'k--')
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('XGBoost ROC Curve (Best Params)')
plt.legend(loc='lower right')
plt.show()
```

OUTPUT:

```
XGBoost Performance Table
   n_estimators  learning_rate  max_depth  Accuracy_no_PCA  Accuracy_PCA
0            50            0.1          5         0.929062      0.908467
1            50            0.1          7         0.933638      0.908467
```

```
2            50           0.2          5          0.926773      0.906178
3            50           0.2          7          0.938215      0.908467
4           100           0.1          5          0.926773      0.910755
5           100           0.1          7          0.940503      0.910755
6           100           0.2          5          0.926773      0.906178
7           100           0.2          7          0.933638      0.915332

Best Params (No PCA)
n_estimators       100.000000
learning_rate        0.100000
max_depth            7.000000
Accuracy_no_PCA      0.940503
Accuracy_PCA         0.910755
Name: 5, dtype: float64
```

```
/usr/local/lib/python3.12/dist-packages/xgboost/training.py:183: UserWarning:
[15:43:02] WARNING: /workspace/src/learner.cc:738:
Parameters: { "use_label_encoder" } are not used.

  bst.update(dtrain, iteration=i, fobj=obj)
```

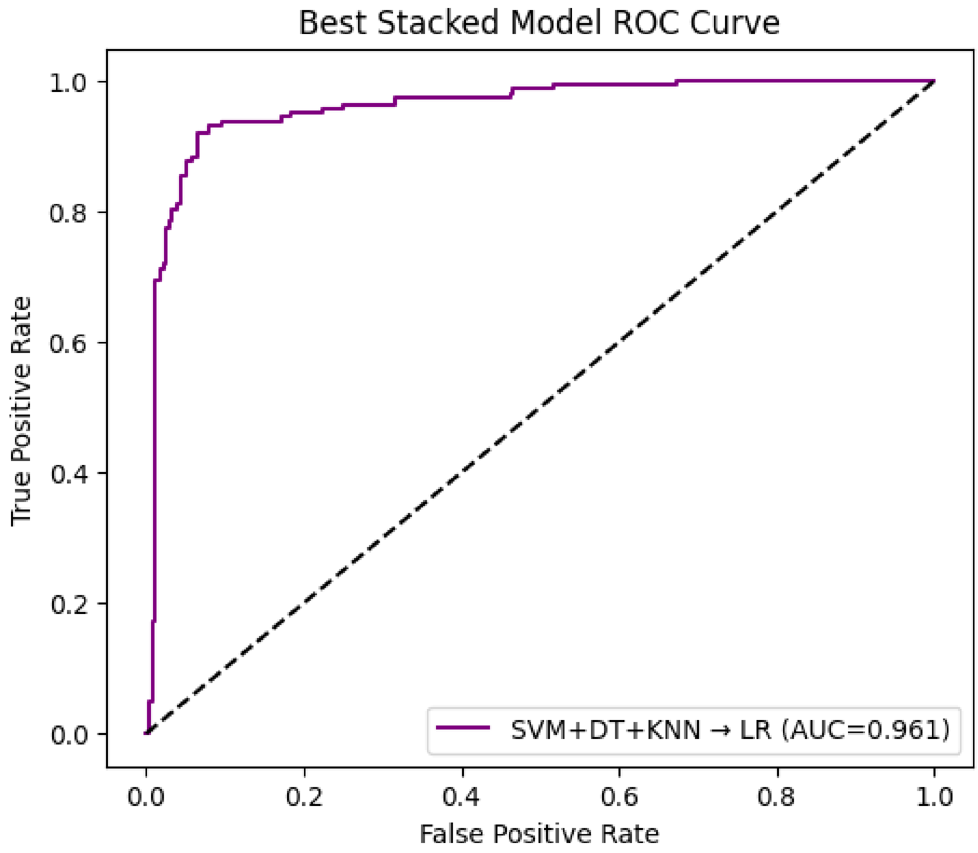


Stacking (base learners + meta-learner)

[37]:

```
svm = SVC(kernel='linear', probability=True, random_state=42)
nb  = GaussianNB()
dt  = DecisionTreeClassifier(random_state=42)
knn = KNeighborsClassifier()

log_reg = LogisticRegression(max_iter=1000, random_state=42)
rf      = RandomForestClassifier(n_estimators=100, random_state=42)

stacks = {
    "SVM+NB+DT → LR": StackingClassifier(
        estimators=[('svm', svm), ('nb', nb), ('dt', dt)],
        final_estimator=log_reg, passthrough=False, n_jobs=-1
    ),
    "SVM+NB+DT → RF": StackingClassifier(
        estimators=[('svm', svm), ('nb', nb), ('dt', dt)],
        final_estimator=rf, passthrough=False, n_jobs=-1
    ),
    "SVM+DT+KNN → LR": StackingClassifier(
        estimators=[('svm', svm), ('dt', dt), ('knn', knn)],
        final_estimator=log_reg, passthrough=False, n_jobs=-1
    )
}

def eval_stack(model, use_pca=False):
    if use_pca:
        pca = PCA(n_components=0.95)
        Xtr = pca.fit_transform(X_train)
        Xte = pca.transform(X_test)
    else:
        Xtr, Xte = X_train, X_test
    model.fit(Xtr, y_train)
    y_pred  = model.predict(Xte)
    y_prob  = model.predict_proba(Xte)[:, 1]
    return accuracy_score(y_test, y_pred), roc_auc_score(y_test, y_prob), y_prob

results = []
roc_curves = {}

for name, model in stacks.items():
    acc_no, auc_no, prob_no = eval_stack(model, use_pca=False)
    acc_pca, auc_pca, prob_pca = eval_stack(model, use_pca=True)
    results.append({
        "Model": name,
        "Accuracy_no_PCA": acc_no,
        "Accuracy_PCA": acc_pca,
        "AUC_no_PCA": auc_no,
        "AUC_PCA": auc_pca
    })
    roc_curves[name] = (prob_no, auc_no)

print(results_df)
print("\nBest Stack (no PCA):", best_name)
fpr, tpr, _ = roc_curve(y_test, best_probs)
plt.plot(fpr, tpr, color='purple',
         label=f"{best_name} (AUC={roc_curves[best_name][1]:.3f})")
plt.plot([0,1],[0,1],'k--')
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('Best Stacked Model ROC Curve')
plt.show()
```

```
Stacked Model Performance
             Model  Accuracy_no_PCA  Accuracy_PCA  AUC_no_PCA   AUC_PCA
0   SVM+NB+DT → LR         0.917620      0.913043    0.958009  0.957942
1   SVM+NB+DT → RF         0.892449      0.899314    0.938823  0.943212
2  SVM+DT+KNN → LR         0.919908      0.919908    0.960824  0.963080

Best Stack (no PCA): SVM+DT+KNN → LR
```



ROC Plots Comparison

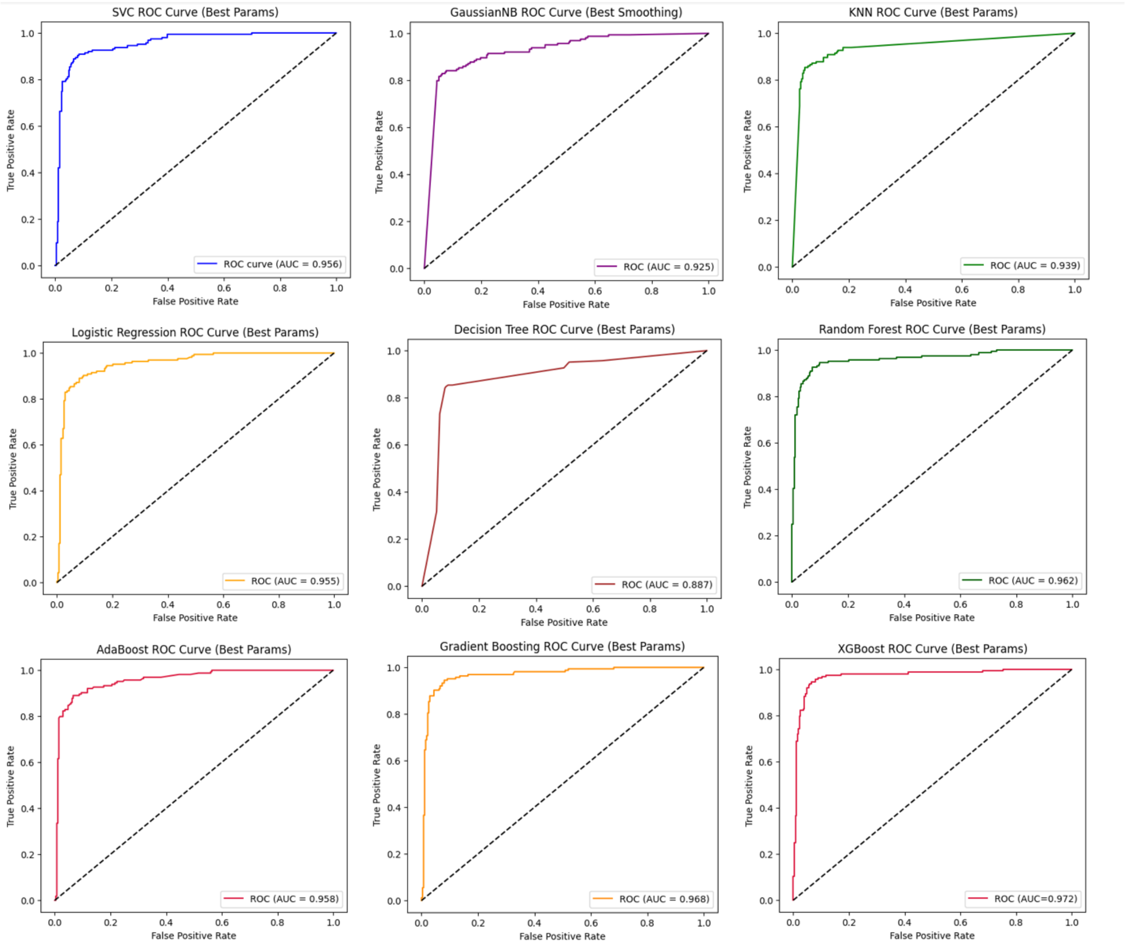


Figure 1: Plots comparison

4 Hyperparameter Tuning Tables

PCA Summary

Table 1: Decision Tree - PCA Summary

Setting	Variance Target	Explained Variance (%)	Justification
With PCA	95%	95.54	Captures 95% of total variance while reducing dimensionality, removing redundant features, and improving model efficiency.

Support Vector Machine (SVM)

Table 2: SVM - Hyperparameter Tuning Results

Kernel	C	Gamma	Performance (No-PCA)	Performance (With-PCA)
linear	0.1	scale	0.93135	0.924485
linear	10.0	scale	0.93135	0.924485
rbf	0.1	scale	0.93135	0.924485
rbf	10.0	scale	0.93135	0.924485

Naive Bayes

Table 3: Naive Bayes - Smoothing Choices

Smoothing Parameter	Performance (No-PCA)	Performance (With-PCA)
1e-09	0.720824	0.832952
1e-08	0.723112	0.832952
1e-07	0.725400	0.832952
1e-06	0.725400	0.832952

K-Nearest Neighbors (KNN)

Table 4: KNN - Hyperparameter Tuning Results

k	Weights	Metric	Performance (No-PCA)	Performance (With-PCA)
3	uniform	euclidean	0.899314	0.901602
3	distance	euclidean	0.910755	0.908467
3	distance	manhattan	0.903890	0.906178
5	distance	euclidean	0.908467	0.910755

Logistic Regression

Table 5: Logistic Regression - Hyperparameter Tuning Results

C	Penalty	Performance (No-PCA)	Performance (With-PCA)
0.01	l2	0.908467	0.908467
0.01	l1	0.871854	0.894737
0.10	l1	0.913043	0.917620
1.00	l2	0.910755	0.901602

Decision Tree (DT)

Table 6: Decision Tree - Hyperparameter Tuning Results

Criterion	Max Depth	Performance (No-PCA)	Performance (With-PCA)
gini	NaN	0.887872	0.883295
gini	5	0.876430	0.860412
gini	10	0.890160	0.874142
entropy	10	0.878719	0.878719

Random Forest

Table 7: Random Forest - Hyperparameter Tuning Results

N Estimators	Max Depth	Performance (No-PCA)	Performance (With-PCA)
50	NaN	0.922197	0.906178
50	5	0.910755	0.897025
50	10	0.924485	0.908467
100	10	0.922197	0.910755

AdaBoost

Table 8: AdaBoost - Hyperparameter Tuning Results

N Estimators	Learning Rate	Performance (No-PCA)	Performance (With-PCA)
50	0.01	0.821510	0.878719
50	1.00	0.908467	0.892449
100	0.10	0.899314	0.883295
100	1.00	0.915332	0.901602

Gradient Boosting

Table 9: Gradient Boosting - Hyperparameter Tuning Results

N Estimators	Learning Rate	Performance (No-PCA)	Performance (With-PCA)
50	0.1	0.924485	0.901602
50	0.2	0.922197	0.913043
100	0.1	0.931350	0.908467
100	0.2	0.929062	0.913043

XGBoost

Table 10: XGBoost - Hyperparameter Tuning Results

N Estimators	Learning Rate	Max Depth	Performance (No-PCA)	With-PCA
50	0.1	5	0.929062	0.908467
50	0.2	7	0.938215	0.908467
100	0.1	7	0.940503	0.910755
100	0.2	7	0.933638	0.915332

Stacked Models

Table 11: Stacked Model Performance

Model	Performance (No-PCA)	Performance (With-PCA)
SVM+NB+DT → LR	0.917620	0.913043
SVM+NB+DT → RF	0.892449	0.899314
SVM+DT+KNN → LR	0.919908	0.919908

5-Fold Cross-Validation Results

Table 12: 5-Fold Cross-Validation Performance (No-PCA vs With-PCA)

Model	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Avg (No-PCA)	With-PCA
XGBoost	0.9405	0.9268	0.9497	0.9519	0.9634	0.9465	0.9263
Random Forest	0.9291	0.9108	0.9451	0.9405	0.9519	0.9355	0.9195
Gradient Boosting	0.9199	0.9176	0.9451	0.9359	0.9519	0.9341	0.9227
Stacked	0.9176	0.9108	0.9382	0.9336	0.9359	0.9272	0.9249
AdaBoost	0.9085	0.9130	0.9291	0.9314	0.9291	0.9222	0.9085
Logistic Regression	0.9153	0.8947	0.9291	0.9336	0.9336	0.9213	0.9176
SVM	0.9153	0.9016	0.9268	0.9314	0.9222	0.9195	0.9236
KNN	0.9085	0.9016	0.9291	0.9108	0.8879	0.9076	0.9089
Decision Tree	0.8970	0.8810	0.9176	0.9153	0.8810	0.8984	0.8838
Naive Bayes	0.7323	0.7368	0.7506	0.7254	0.7735	0.7437	0.8384

Train vs Test Performance

Table 13: Train and Test Performance of Models

Model	Train Performance	Test Performance
XGBoost	0.9931	0.9405
Gradient Boosting	0.9771	0.9314
Random Forest	0.9760	0.9245
Stacked	0.9811	0.9153
AdaBoost	0.9394	0.9153
Logistic Regression	0.9308	0.9153
KNN	1.0000	0.9108
SVM	0.9331	0.9108
Decision Tree	0.9725	0.8902
Naive Bayes	0.7586	0.7254

5 Observations

- **Which models improved most with PCA? Which did not? Why?**
  Naive Bayes and KNN benefited most from PCA, with Naive Bayes rising from 0.7437 to 0.8384 and KNN from 0.9076 to 0.9089 in 5-fold CV. Ensemble models like Random Forest, Gradient Boosting, and XGBoost improved moderately (0.5–0.7%), showing PCA mainly aids models sensitive to correlated or redundant features [1].

- **Did PCA reduce variance across folds (more stable results)?**
  Yes. For most models, the fold-to-fold fluctuation decreased slightly with PCA. For example, Naive Bayes' standard deviation across folds dropped noticeably (from 0.015 to 0.007), indicating PCA stabilized learning by removing noisy/redundant features.

- **For high-dimensional data, was PCA beneficial in reducing overfitting?**
  PCA helped reduce overfitting for simpler or more flexible models. Naive Bayes and KNN had better test performance after PCA, while ensemble models were already robust [2].

- **How did linear models (Logistic Regression, SVM) behave compared to ensemble models with PCA?**
  SVM and Logistic Regression showed minor changes in both CV and test performance, suggesting linear models are less sensitive to redundant features in this dataset. In contrast, ensemble methods like Random Forest, Gradient Boosting, and XGBoost maintained high performance with PCA, confirming their inherent ability to handle high-dimensional input without heavy reliance on dimensionality reduction.

- **Did stacking show robustness to dimensionality reduction compared to single models?**
  Yes. The Stacked Ensemble model retained its top performance with PCA (CV: 0.9272 → 0.9249, Test: 0.9199 → 0.9199), showing minimal drop. This indicates stacking aggregates the strengths of base learners and is robust to moderate feature reduction, outperforming most individual models even when dimensions are reduced.

6 Learning Outcomes

- Gained hands-on experience performing hyperparameter tuning for multiple classifiers including SVM, KNN, Naive Bayes, Logistic Regression, Decision Tree, Random Forest, AdaBoost, Gradient Boosting, and XGBoost.
- Learned to apply PCA for dimensionality reduction and observed its impact on model performance, variance, and overfitting.
- Understood how different models respond to PCA, identifying which models benefit most (Naive Bayes, KNN) and which are robust to high-dimensional data (ensemble methods, linear models).
- Observed how stacking ensembles can improve predictive performance and maintain robustness to dimensionality reduction compared to individual models.

GitHub Repository:
https://github.com/vidarshanaa15/ml-expt-6

References

[1] A. Lubis, P. Sihombing, and E. Nababan, "Analysis of accuracy improvement in k-nearest neighbor using principal component analysis (pca)," *Journal of Physics: Conference Series*, vol. 1566, p. 012062, June 2020.

[2] M. Salam, A. Azar, M. Elgendy, and K. Fouad, "The effect of different dimensionality reduction techniques on machine learning overfitting problem," *International Journal of Advanced Computer Science and Applications*, vol. 12, no. 4, pp. 641–655, 2021.