# ML Lab

# **Assignment 2**:

## **Machine Learning Classification on Wine and Digits Datasets:**

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#### **Github Link:**

https://github.com/abhijitdas6371/ML LAB/blob/main/Ass2/Assignment2 ML Lab.ipynb

#### 1. Problem Statement

The goal is to build and evaluate classification models on two datasets: the Wine dataset and the Digits dataset. The task is to accurately predict the class labels of samples based on their feature values.

- a. **Wine dataset**: Predict the wine class (class\_0, class\_1, class\_2) based on chemical analysis of wines grown in the same region in Italy.
- b. **Digits dataset**: Predict the digit (0 through 9) from 8x8 pixel grayscale images of handwritten digits.

### 2. Discussion on different algorithms

# **Support Vector Machine (SVM):**

A supervised machine learning algorithm used for classification and regression tasks. It works by finding the optimal hyperplane that separates data points of different classes with the maximum margin.

For non-linearly separable data, SVM uses kernel functions to project data into higher dimensions where a separating hyperplane can be found.

### **Key Features:**

- 1. Effective in high-dimensional spaces.
- 2. Can handle both linear and non-linear classification.
- 3. Works well with clear margin of separation.
- 4. Sensitive to parameter tuning and scaling of features.

## Parameter Explanation:

- C: Regularization parameter; smaller values → smoother boundary (less overfitting), larger values → stricter classification.
- kernel: Defines the function to transform input data:
  - 'linear' → linear separation
  - 'poly' → polynomial transformation
  - o 'rbf' → radial basis function (Gaussian, common for non-linear data)
  - 'sigmoid' → logistic-like function
- degree: Degree of polynomial kernel (used when kernel='poly').
- gamma: Defines influence of single training example; low = far influence, high = close influence.
- probability: If True, enables probability estimates (slower).

### Multi-Layer Perceptron (MLP / Neural Network)

A type of artificial neural network used for classification and regression. It consists of input, hidden, and output layers with interconnected neurons. Each neuron applies a weighted sum of inputs followed by an activation function to introduce non-linearity.

## **Key Features:**

- 1. Can model complex non-linear relationships.
- 2. Supports multi-class classification.
- 3. Requires scaling of data for better performance.
- 4. Sensitive to hyperparameters (hidden layers, learning rate, etc.).

# Parameter Explanation:

- hidden\_layer\_sizes: Tuple defining the number of neurons in each hidden layer (e.g., (100,) = 1 hidden layer with 100 neurons).
- alpha: L2 regularization parameter to reduce overfitting.
- learning\_rate\_init: Step size at each iteration while moving toward a minimum.
- max\_iter: Maximum number of iterations for training.
- activation: Non-linear activation function:
  - $\circ$  'relu'  $\rightarrow$  default, fast convergence
  - $\circ \ \ \text{'tanh'} \to \text{smooth outputs, can be slower}$
  - logistic' → sigmoid function
- solver: Weight optimization algorithm:

- o 'adam' → stochastic gradient-based (default)
- 'sgd' → stochastic gradient descent
- 'lbfgs' → quasi-Newton optimizer

### Random Forest (RF):

An ensemble learning algorithm that builds multiple Decision Trees and combines their predictions. It uses bagging (bootstrap aggregating) to create diverse trees and averages results (for regression) or uses majority voting (for classification).

### **Key Features:**

- 1. Reduces overfitting compared to a single decision tree.
- 2. Handles both categorical and numerical data.
- 3. Provides feature importance.
- 4. More computationally expensive than a single tree.

### **Parameter Explanation:**

- n\_estimators: Number of trees in the forest.
- max\_depth: Maximum depth of each tree. Controls overfitting.
- min samples split: Minimum number of samples required to split a node.
- min\_samples\_leaf: Minimum number of samples at a leaf node.
- criterion: Function to measure split quality ('gini' or 'entropy').
- max\_features: Number of features considered for each split:
  - 'sqrt' → square root of total features (default for classification)
  - $\circ$  'log2'  $\rightarrow$  logarithm base 2 of features
  - None → all features considered
- bootstrap: Whether bootstrap samples are used when building trees (default=True).
- 3. Dataset\_Download

```
# Load Wine dataset

wine = load_wine()
X = wine.data
y = wine.target
classes = wine.target_names

print(X.shape)
print(y.shape)

(178, 13)
(178,)
```

#### **SVM** without PCA

4. Function to train the model, compute accuracy, precision, recall, F1 score, plot confusion matrix and ROC curves if available

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.datasets import load_wine
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler, label_binarize
from sklearn.svm import SVC
from sklearn.experimental import enable halving search cv
from sklearn.model selection import HalvingGridSearchCV
from sklearn.metrics import (
   accuracy score, precision score, recall score, f1 score,
   confusion_matrix, roc_curve, auc
def evaluate model(model, X train, X test, y train, y test, model name="Model"):
   model.fit(X_train, y_train)
   y pred = model.predict(X test)
   acc = accuracy_score(y_test, y_pred)
   prec = precision_score(y_test, y_pred, average="weighted", zero_division=0)
   rec = recall_score(y_test, y_pred, average="weighted", zero_division=0)
   f1 = f1_score(y_test, y_pred, average="weighted", zero_division=0)
   print(f"\n{model_name} Results:")
   print(f"Accuracy={acc:.4f}, Precision={prec:.4f}, Recall={rec:.4f}, F1={f1:.4f}")
   # Confusion matrix
   cm = confusion_matrix(y_test, y_pred)
   plt.figure(figsize=(6, 5))
   sns.heatmap(cm, annot=True, fmt="d", cmap="Blues",
                xticklabels=classes, yticklabels=classes)
   plt.title(f"Confusion Matrix ({model_name})")
   plt.xlabel("Predicted Label")
   plt.ylabel("True Label")
   plt.show()
   roc_data = None
```

```
if hasattr(model, "predict_proba"):
    y_bin = label_binarize(y_test, classes=np.arange(len(classes)))
    y_score = model.predict_proba(X_test)

fpr, tpr, roc_auc = {}, {}, {}
for i in range(len(classes)):
    fpr[i], tpr[i], _ = roc_curve(y_bin[:, i], y_score[:, i])
    roc_auc[i] = auc(fpr[i], tpr[i])
    roc_data = (fpr, tpr, roc_auc)

return acc, prec, rec, f1, roc_data
```

### Define SVM classifier and hyperparameter search space for grid tuning

```
svm_model = SVC(probability=True, random_state=42)
svm_params = {
    "kernel": ["linear", "poly", "rbf", "sigmoid"],
    "C": [0.1, 1, 10],
    "degree": [2, 3],
    "gamma": ["scale", "auto"]
}
```

# 5. Perform train-test splits, standardize data, tune SVM hyperparameters with HalvingGridSearchCV, evaluate metrics, and collect ROC data

```
splits = [(0.5, 0.5), (0.6, 0.4), (0.7, 0.3), (0.8, 0.2)]
results summary = []
roc_collector = {}
# Loop for SVM
for train size, test size in splits:
    split label = f"{int(train size*100)}-{int(test size*100)}"
    print(f"\n{'='*50}\n Train-Test Split {split label}\n{'='*50}")
    X_train, X_test, y_train, y_test = train_test_split(
        X, y, train_size=train_size, test_size=test_size,
        random_state=42, stratify=y
    )
    # Standardize features
    scaler = StandardScaler()
    X_train = scaler.fit_transform(X_train)
    X test = scaler.transform(X test)
    # Halving Grid Search
    grid = HalvingGridSearchCV(
        svm_model, svm_params, cv=5, scoring="accuracy",
        n jobs=-1, random state=42, verbose=0
    grid.fit(X_train, y_train)
    results = pd.DataFrame(grid.cv results )
```

```
results = results.sort_values(by="mean_test_score", ascending=False)
top_acc = results.iloc[0]["mean_test_score"]
if top acc >= 1.0:
    valid_results = results[results["mean_test_score"] < 1.0]</pre>
else:
    valid_results = results
if not valid_results.empty:
    best_row = valid_results.iloc[0]
    best_params = {k.replace("param_", ""): best_row[k]
                   for k in results.columns if k.startswith("param ")}
    print(f"Using best params for SVM: {best_params}")
    best_model = SVC(**best_params, probability=True, random_state=42)
    acc, prec, rec, f1, roc data = evaluate model(
       best_model, X_train, X_test, y_train, y_test,
       model_name=f"SVM ({split_label})"
    params_str = ", ".join(f"{k}={v}" for k, v in best_params.items())
    results_summary.append([split_label, acc, prec, rec, f1, params_str])
    if roc_data:
        roc_collector[split_label] = roc_data
else:
    print(f"No valid SVM models under 1.0 accuracy for split {split_label}")
```

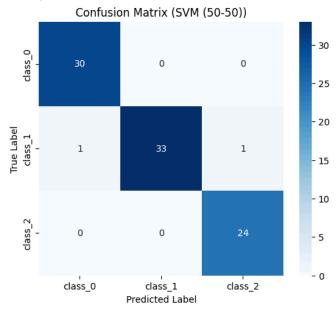
```
_____
```

Train-Test Split 50-50

Using best params for SVM: {'C': np.float64(0.1), 'degree': np.int64(2), 'gamma': 'scale', 'kernel': 'linear'}

SVM (50-50) Results:

Accuracy=0.9775, Precision=0.9783, Recall=0.9775, F1=0.9774

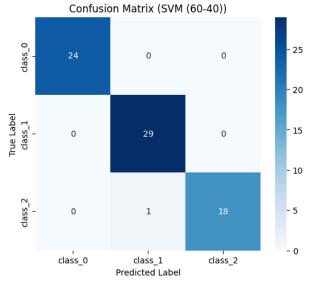


Train-Test Split 60-40

Using best params for SVM: {'C': np.float64(1.0), 'degree': np.int64(3), 'gamma': 'auto', 'kernel': 'rbf'}

SVM (60-40) Results:

Accuracy=0.9861, Precision=0.9866, Recall=0.9861, F1=0.9860



Train-Test Split 70-30 Using best params for SVM: {'C': np.float64(1.0), 'degree': np.int64(2), 'gamma': 'scale', 'kernel': 'rbf'} SVM (70-30) Results: Accuracy=0.9815, Precision=0.9823, Recall=0.9815, F1=0.9814 Confusion Matrix (SVM (70-30)) 20.0 class 0 17.5 15.0 12.5 0 10.0 7.5 - 5.0 - 2.5 - 0.0 class\_1 class\_2 class\_0 Predicted Label Train-Test Split 80-20 Using best params for SVM: {'C': np.float64(10.0), 'degree': np.int64(3), 'gamma': 'auto', 'kernel': 'rbf'} SVM (80-20) Results: Accuracy=0.9444, Precision=0.9514, Recall=0.9444, F1=0.9432 Confusion Matrix (SVM (80-20)) 14 class\_0 0 - 10 True Label class\_1 0 0

# 6. Generate a summary DataFrame of performance metrics and best parameters, then visualize it as a styled table using Matplotlib

```
# Prepare DataFrame
summary_df = pd.DataFrame(results_summary,
```

class\_0

2

class\_1

Predicted Label

class\_2

```
columns=["Split", "Accuracy", "Precision", "Recall", "F1", "Best
Hyperparameters"])
fig, ax = plt.subplots(figsize=(14, len(summary df) * 0.7 + 1))
ax.axis('tight')
ax.axis('off')
# Create table
table = ax.table(cellText=summary_df.round(3).astype(str).values,
                 colLabels=summary_df.columns,
                 cellLoc='center',
                 loc='center')
# Disable automatic font sizing and set font size
table.auto_set_font_size(False)
table.set_fontsize(10)
# Scale table: horizontal scale is arbitrary, we will set col widths explicitly
table.scale(1.2, 1.2)
col_widths = [0.06, 0.08, 0.08, 0.08, 0.08, 0.62]
# sum should be ~1.0 for proportion
# Adjust each column width by modifying cell widths in each row (including header)
for col_idx, width in enumerate(col_widths):
    # Header cell
    cell = table[0, col_idx]
    cell.set_width(width)
    # Data cells
    for row_idx in range(1, len(summary_df) + 1):
        cell = table[row_idx, col_idx]
        cell.set_width(width)
plt.title("SVM Summary Across Splits (with Best Hyperparameters)", fontsize=14, pad=15)
plt.tight_layout()
plt.show()
```

Split	Accuracy	Precision	Recall	F1	Best Hyperparameters
50-50	0.978	0.978	0.978	0.977	C=0.1, degree=2, gamma=scale, kernel=linear
60-40	0.986	0.987	0.986	0.986	C=1.0, degree=3, gamma=auto, kernel=rbf
70-30	0.981	0.982	0.981	0.981	C=1.0, degree=2, gamma=scale, kernel=rbf
80-20	0.944	0.951	0.944	0.943	C=10.0, degree=3, gamma=auto, kernel=rbf

SVM Summary Across Splits (with Best Hyperparameters)

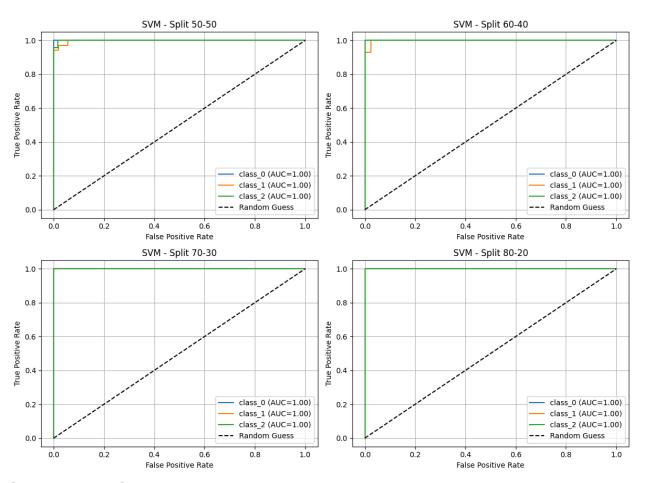
# 7. Visualize multiclass ROC curves with AUC values across different train-test splits using subplots

```
fig, axs = plt.subplots(2, 2, figsize=(12, 10))
axs = axs.ravel()
```

```
for idx, (split_label, (fpr, tpr, roc_auc)) in enumerate(roc_collector.items()):
    ax = axs[idx]
    for i in range(len(classes)):
        ax.plot(fpr[i], tpr[i], label=f"{classes[i]} (AUC={roc_auc[i]:.2f})")
    ax.plot([0, 1], [0, 1], "k--", label="Random Guess")
    ax.set_title(f"SVM - Split {split_label}")
    ax.set_xlabel("False Positive Rate")
    ax.set_ylabel("True Positive Rate")
    ax.legend(loc="lower right")
    ax.grid(True)

plt.suptitle("SVM ROC Curves Across Train-Test Splits", fontsize=16)
plt.tight_layout(rect=[0, 0.03, 1, 0.95])
plt.show()
```

#### SVM ROC Curves Across Train-Test Splits



### **SVM** with PCA

8. ApplyPCA for dimensionality reduction, then perform hyperparameter tuning and evaluation of SVM models across different train-test splits

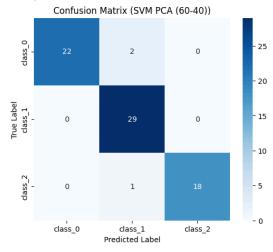
from sklearn.decomposition import PCA

```
# PCA with 5 components
pca = PCA(n components=5)
splits = [(0.5, 0.5), (0.6, 0.4), (0.7, 0.3), (0.8, 0.2)]
results_summary_pca = []
roc_collector_pca = {}
for train_size, test_size in splits:
    split_label = f"{int(train_size*100)}-{int(test_size*100)}"
    print(f"\n{'='*50}\n Train-Test Split {split_label} with PCA\n{'='*50}")
    X_train, X_test, y_train, y_test = train_test_split(
        X, y, train_size=train_size, test_size=test_size,
        random_state=42, stratify=y
    )
    # PCA fit on train only!
    pca.fit(X_train)
    X_train_pca = pca.transform(X_train)
    X_test_pca = pca.transform(X_test)
    # Standardize after PCA (optional but often useful)
    scaler = StandardScaler()
    X_train_pca = scaler.fit_transform(X_train_pca)
    X_test_pca = scaler.transform(X_test_pca)
    # Halving Grid Search on PCA-transformed data
    grid = HalvingGridSearchCV(
        svm_model, svm_params, cv=5, scoring="accuracy",
        n jobs=-1, random state=42, verbose=0
    grid.fit(X_train_pca, y_train)
    results = pd.DataFrame(grid.cv_results_)
    results = results.sort_values(by="mean_test_score", ascending=False)
    top_acc = results.iloc[0]["mean_test_score"]
    if top acc >= 1.0:
        valid_results = results[results["mean_test_score"] < 1.0]</pre>
        valid results = results
    if not valid_results.empty:
        best_row = valid_results.iloc[0]
        best_params = {k.replace("param_", ""): best_row[k]
                       for k in results.columns if k.startswith("param_")}
        print(f"Using best params for SVM with PCA: {best params}")
        best_model = SVC(**best_params, probability=True, random_state=42)
        acc, prec, rec, f1, roc_data = evaluate_model(
```

```
best_model, X_train_pca, X_test_pca, y_train, y_test,
               model_name=f"SVM PCA ({split_label})"
          )
          params_str = ", ".join(f"{k}={v}" for k, v in best_params.items())
          results_summary_pca.append([split_label, acc, prec, rec, f1, params_str])
          if roc data:
               roc_collector_pca[split_label] = roc_data
     else:
          print(f"No valid SVM models under 1.0 accuracy for split {split_label} with PCA")
Train-Test Split 50-50 with PCA
Using best params for SVM with PCA: {'C': np.float64(0.1), 'degree': np.int64(2), 'gamma': 'scale', 'kernel': 'linear'}
SVM PCA (50-50) Results:
Accuracy=0.9438, Precision=0.9474, Recall=0.9438, F1=0.9441
         Confusion Matrix (SVM PCA (50-50))
   class_0
                                      0
                                                   20
            0
                                      1
                        34
                                                   15
            0
                         1
                                                  - 0
         class 0
                       class 1
                                    class_2
                    Predicted Label
  Train-Test Split 60-40 with PCA
```

Using best params for SVM with PCA: {'C': np.float64(0.1), 'degree': np.int64(2), 'gamma': 'scale', 'kernel': 'linear'}

SVM PCA (60-40) Results: Accuracy=0.9583, Precision=0.9622, Recall=0.9583, F1=0.9586



Train-Test Split 70-30 with PCA Using best params for SVM with PCA: {'C': np.float64(1.0), 'degree': np.int64(3), 'gamma': 'scale', 'kernel': 'linear'} SVM PCA (70-30) Results: Accuracy=0.9444, Precision=0.9477, Recall=0.9444, F1=0.9440 Confusion Matrix (SVM PCA (70-30)) - 20.0 class\_0 0 15.0 0 0 10.0 7.5 5.0 1 - 2.5 - 0.0 class 1 class\_0 class\_2 Predicted Label Train-Test Split 80-20 with PCA Using best params for SVM with PCA: {'C': np.float64(1.0), 'degree': np.int64(3), 'gamma': 'auto', 'kernel': 'linear'} SVM PCA (80-20) Results: Accuracy=0.9444, Precision=0.9484, Recall=0.9444, F1=0.9424 Confusion Matrix (SVM PCA (80-20)) 0 10 14 0 0

# 9. Visualize performance metrics and best hyperparameters of SVM models trained on PCA-transformed data across multiple splits

- 2

- 0

class\_2

class\_2

class\_0

1

class\_1

Predicted Label

```
fig, ax = plt.subplots(figsize=(14, len(summary_df_pca) * 0.7 + 1))
ax.axis('tight')
ax.axis('off')
table = ax.table(cellText=summary_df_pca.round(3).astype(str).values,
                 colLabels=summary_df_pca.columns,
                 cellLoc='center',
                 loc='center')
table.auto_set_font_size(False)
table.set_fontsize(10)
table.scale(1.2, 1.2)
col_widths = [0.06, 0.08, 0.08, 0.08, 0.08, 0.62] # same as before
for col_idx, width in enumerate(col_widths):
    cell = table[0, col idx]
    cell.set_width(width)
    for row_idx in range(1, len(summary_df_pca) + 1):
        cell = table[row_idx, col_idx]
        cell.set_width(width)
plt.title("SVM PCA Summary Across Splits (with Best Hyperparameters)", fontsize=14, pad=15)
plt.tight layout()
plt.show()
```

Split	Accuracy	Precision	Recall	F1	Best Hyperparameters
50-50	0.944	0.947	0.944	0.944	C=0.1, degree=2, gamma=scale, kernel=linear
60-40	0.958	0.962	0.958	0.959	C=0.1, degree=2, gamma=scale, kernel=linear
70-30	0.944	0.948	0.944	0.944	C=1.0, degree=3, gamma=scale, kernel=linear
80-20	0.944	0.948	0.944	0.942	C=1.0, degree=3, gamma=auto, kernel=linear

# Visualize ROC curves and AUC scores for each class across multiple train-test splits of SVM models with PCA preprocessing

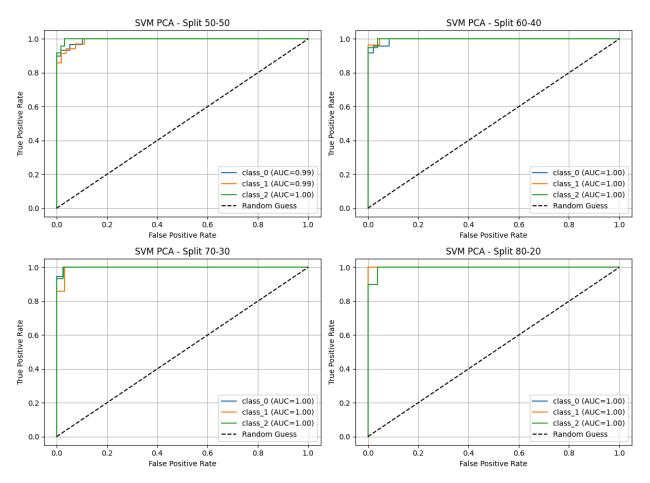
```
# ROC curves for PCA runs
fig, axs = plt.subplots(2, 2, figsize=(12, 10))
axs = axs.ravel()

for idx, (split_label, (fpr, tpr, roc_auc)) in enumerate(roc_collector_pca.items()):
    ax = axs[idx]
    for i in range(len(classes)):
        ax.plot(fpr[i], tpr[i], label=f"{classes[i]} (AUC={roc_auc[i]:.2f})")
    ax.plot([0, 1], [0, 1], "k--", label="Random Guess")
    ax.set_title(f"SVM PCA - Split {split_label}")
    ax.set_xlabel("False Positive Rate")
    ax.set_ylabel("True Positive Rate")
```

```
ax.legend(loc="lower right")
ax.grid(True)

plt.suptitle("SVM PCA ROC Curves Across Train-Test Splits", fontsize=16)
plt.tight_layout(rect=[0, 0.03, 1, 0.95])
plt.show()
```

#### SVM PCA ROC Curves Across Train-Test Splits



### **MLP** without PCA

# 11. Define MLP Model and Hyperparameter Grid for Tuning

```
# MLP model and hyperparameter grid
mlp_model = MLPClassifier(random_state=42, max_iter=50)
mlp_params = {
    'hidden_layer_sizes': [(50,), (100,), (50, 50)],
    'activation': ['relu', 'tanh'],
    'alpha': [0.0001, 0.001, 0.01], # L2 regularization
    'learning_rate': ['constant', 'adaptive']
}
```

# 12. Initialize Multi-Layer Perceptron (MLP) model and specify hyperparameter search space

```
results_summary_mlp = []
roc_collector_mlp = {}
for train_size, test_size in splits:
   split_label = f"{int(train_size*100)}-{int(test_size*100)}"
   print(f"\n{'='*50}\n Train-Test Split {split_label} (MLP)\n{'='*50}")
   X_train, X_test, y_train, y_test = train_test_split(
       X, y, train_size=train_size, test_size=test_size,
       random_state=42, stratify=y
   )
   # Standardize features
   scaler = StandardScaler()
   X_train = scaler.fit_transform(X_train)
   X_test = scaler.transform(X_test)
   # Halving Grid Search for MLP
   grid = HalvingGridSearchCV(
       mlp_model, mlp_params, cv=5, scoring="accuracy",
       n_jobs=-1, random_state=42, verbose=0
   grid.fit(X_train, y_train)
   results = pd.DataFrame(grid.cv_results_)
   results = results.sort_values(by="mean_test_score", ascending=False)
   top_acc = results.iloc[0]["mean_test_score"]
   if top_acc >= 1.0:
       valid_results = results[results["mean_test_score"] < 1.0]</pre>
   else:
       valid_results = results
   if not valid_results.empty:
       best_row = valid_results.iloc[0]
       best_params = {k.replace("param_", ""): best_row[k]
                       for k in results.columns if k.startswith("param_")}
       print(f"Using best params for MLP: {best params}")
       best_model = MLPClassifier(**best_params, random_state=42, max_iter=1000)
       acc, prec, rec, f1, roc_data = evaluate_model(
           best_model, X_train, X_test, y_train, y_test,
           model_name=f"MLP ({split_label})"
       params_str = ", ".join(f"{k}={v}" for k, v in best_params.items())
       results_summary_mlp.append([split_label, acc, prec, rec, f1, params_str])
       if roc_data:
           roc_collector_mlp[split_label] = roc_data
   else:
       print(f"No valid MLP models under 1.0 accuracy for split {split_label}")
```

Train-Test Split 50-50 (MLP)

Using best params for MLP: {'activation': 'relu', 'alpha': np.float64(0.0001), 'hidden\_layer\_sizes': (100,), 'learning\_rate': 'adaptive'}

MLP (50-50) Results: Accuracy=0.9551, Precision=0.9558, Recall=0.9551, F1=0.9548

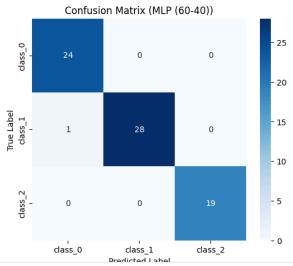
#### Confusion Matrix (MLP (50-50)) class\_0 30 0 - 20 True Label class\_1 2 1 - 15 - 10 0 1 - 5 - 0 class\_0 class\_1 class\_2 Predicted Label

Train-Test Split 60-40 (MLP)

Using best params for MLP: {'activation': 'tanh', 'alpha': np.float64(0.01), 'hidden\_layer\_sizes': (100,), 'learning\_rate': 'constant'}

#### MLP (60-40) Results:

Accuracy=0.9861, Precision=0.9867, Recall=0.9861, F1=0.9861

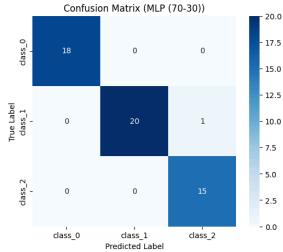


Train-Test Split 70-30 (MLP)

Using best params for MLP: {'activation': 'tanh', 'alpha': np.float64(0.01), 'hidden\_layer\_sizes': (50, 50), 'learning\_rate': 'adaptive'}

MLP (70-30) Results:

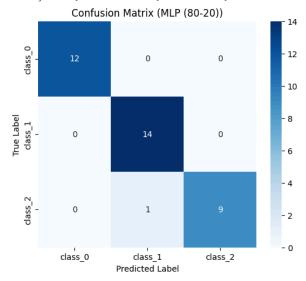
Accuracy=0.9815, Precision=0.9826, Recall=0.9815, F1=0.9816



Train-Test Split 80-20 (MLP)

Using best params for MLP: {'activation': 'tanh', 'alpha': np.float64(0.01), 'hidden\_layer\_sizes': (100,), 'learning\_rate': 'constant'}

MLP (80-20) Results: Accuracy=0.9722, Precision=0.9741, Recall=0.9722, F1=0.9720



# 13. Display MLP performance summary with best hyperparameters across splits

```
table = ax.table(cellText=summary_df_mlp.round(3).astype(str).values,
                 colLabels=summary_df_mlp.columns,
                 cellLoc='center',
                 loc='center')
table.auto set font size(False)
table.set_fontsize(10)
table.scale(1.2, 1.2)
col\_widths = [0.06, 0.08, 0.08, 0.08, 0.08, 0.62]
for col_idx, width in enumerate(col_widths):
    cell = table[0, col idx]
    cell.set_width(width)
    for row_idx in range(1, len(summary_df_mlp) + 1):
        cell = table[row idx, col idx]
        cell.set width(width)
plt.title("MLP Summary Across Splits (with Best Hyperparameters)", fontsize=14, pad=15)
plt.tight_layout()
plt.show()
```

	Split	Accuracy	Precision	Recall	F1	Best Hyperparameters
	50-50	0.955	0.956	0.955	0.955	activation=relu, alpha=0.0001, hidden_layer_sizes=(100,), learning_rate=adaptive
Г	60-40	0.986	0.987	0.986	0.986	activation=tanh, alpha=0.01, hidden_layer_sizes=(100,), learning_rate=constant
	70-30	0.981	0.983	0.981	0.982	activation=tanh, alpha=0.01, hidden_layer_sizes=(50, 50), learning_rate=adaptive
	80-20	0.972	0.974	0.972	0.972	activation=tanh, alpha=0.01, hidden_layer_sizes=(100,), learning_rate=constant

MLP Summary Across Splits (with Best Hyperparameters)

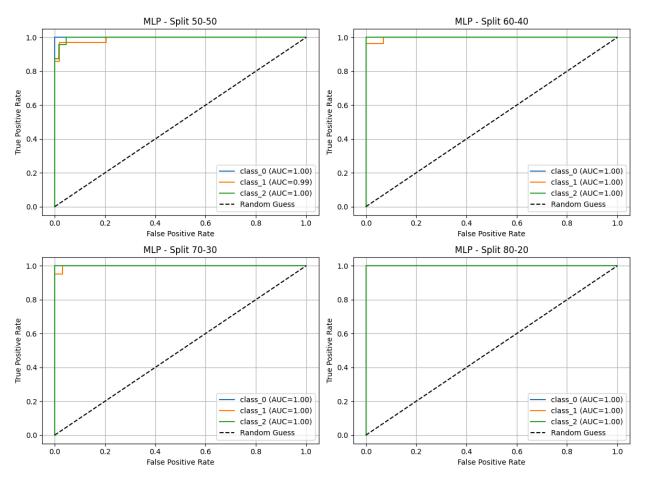
# 14. Plot ROC curves for MLP models across train-test splits

```
fig, axs = plt.subplots(2, 2, figsize=(12, 10))
axs = axs.ravel()

for idx, (split_label, (fpr, tpr, roc_auc)) in enumerate(roc_collector_mlp.items()):
    ax = axs[idx]
    for i in range(len(classes)):
        ax.plot(fpr[i], tpr[i], label=f"{classes[i]} (AUC={roc_auc[i]:.2f})")
    ax.plot([0, 1], [0, 1], "k--", label="Random Guess")
    ax.set_title(f"MLP - Split {split_label}")
    ax.set_xlabel("False Positive Rate")
    ax.set_ylabel("True Positive Rate")
    ax.legend(loc="lower right")
    ax.grid(True)

plt.suptitle("MLP ROC Curves Across Train-Test Splits", fontsize=16)
plt.tight_layout(rect=[0, 0.03, 1, 0.95])
```

#### MLP ROC Curves Across Train-Test Splits



#### **MLP with PCA**

# 15. Train and evaluate MLP models with PCA dimensionality reduction across multiple splits

```
results_summary_mlp_pca = []
roc_collector_mlp_pca = {}

for train_size, test_size in splits:
    split_label = f"{int(train_size*100)}-{int(test_size*100)}"
    print(f"\n{'='*50}\n Train-Test Split {split_label} (MLP + PCA)\n{'='*50}")

# Split data
X_train, X_test, y_train, y_test = train_test_split(
    X, y, train_size=train_size, test_size=test_size,
    random_state=42, stratify=y
)

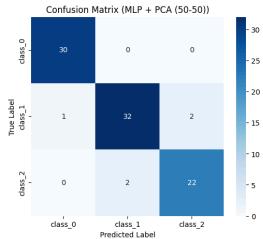
# Scale features
scaler = StandardScaler()
X_train = scaler.fit_transform(X_train)
```

```
X_test = scaler.transform(X_test)
# PCA transform
pca = PCA(n_components=5, random_state=42)
X_train = pca.fit_transform(X_train)
X_test = pca.transform(X_test)
# HalvingGridSearch for MLP with PCA data
grid = HalvingGridSearchCV(
   mlp_model, mlp_params, cv=5, scoring="accuracy",
   n_jobs=-1, random_state=42, verbose=0
grid.fit(X train, y train)
results = pd.DataFrame(grid.cv results )
results = results.sort_values(by="mean_test_score", ascending=False)
top_acc = results.iloc[0]["mean_test_score"]
if top_acc >= 1.0:
   valid_results = results[results["mean_test_score"] < 1.0]</pre>
else:
   valid_results = results
if not valid_results.empty:
    best_row = valid_results.iloc[0]
    best_params = {k.replace("param_", ""): best_row[k]
                   for k in results.columns if k.startswith("param_")}
   print(f"Using best params for MLP + PCA: {best_params}")
    best_model = MLPClassifier(**best_params, random_state=42, max_iter=1000)
    acc, prec, rec, f1, roc_data = evaluate_model(
       best_model, X_train, X_test, y_train, y_test,
       model_name=f"MLP + PCA ({split_label})"
    params_str = ", ".join(f"{k}={v}" for k, v in best_params.items())
    results_summary_mlp_pca.append([split_label, acc, prec, rec, f1, params_str])
    if roc_data:
       roc collector mlp pca[split label] = roc data
else:
    print(f"No valid MLP models under 1.0 accuracy for split {split_label}")
```

Train-Test Split 50-50 (MLP + PCA)

Using best params for MLP + PCA: {'activation': 'relu', 'alpha': np.float64(0.0001), 'hidden\_layer\_sizes': (50,), 'learning\_rate': 'constant'}

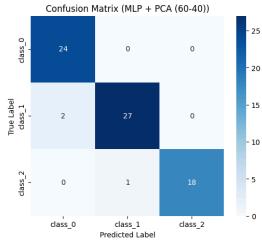
MLP + PCA (50-50) Results: Accuracy=0.9438, Precision=0.9435, Recall=0.9438, F1=0.9435



Train-Test Split 60-40 (MLP + PCA)

Using best params for MLP + PCA: {'activation': 'tanh', 'alpha': np.float64(0.001), 'hidden layer sizes': (50,), 'learning rate': 'adaptive'}

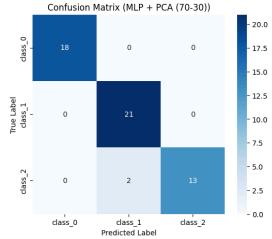
MLP + PCA (60-40) Results: Accuracy=0.9583, Precision=0.9600, Recall=0.9583, F1=0.9583



Train-Test Split 70-30 (MLP + PCA)

Using best params for MLP + PCA: {'activation': 'relu', 'alpha': np.float64(0.0001), 'hidden\_layer\_sizes': (50,), 'learning\_rate': 'constant'}

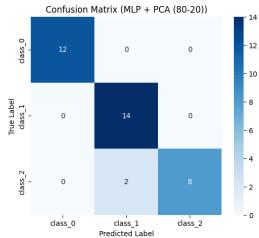
MLP + PCA (70-30) Results: Accuracy=0.9630, Precision=0.9662, Recall=0.9630, F1=0.9625



Train-Test Split 80-20 (MLP + PCA)

Using best params for MLP + PCA: {'activation': 'relu', 'alpha': np.float64(0.0001), 'hidden\_layer\_sizes': (50,), 'learning\_rate': 'constant'}

MLP + PCA (80-20) Results: Accuracy=0.9444, Precision=0.9514, Recall=0.9444, F1=0.9432



# Generate summary table for MLP models with PCA across different train-test splits

```
# Prepare DataFrame and plot summary table
summary_df_mlp_pca = pd.DataFrame(results_summary_mlp_pca,
                                  columns=["Split", "Accuracy", "Precision", "Recall", "F1", "Best
Hyperparameters"])
fig, ax = plt.subplots(figsize=(14, len(summary_df_mlp_pca) * 0.7 + 1))
ax.axis('tight')
ax.axis('off')
table = ax.table(cellText=summary_df_mlp_pca.round(3).astype(str).values,
                 colLabels=summary_df_mlp_pca.columns,
```

```
cellLoc='center',
    loc='center')

table.auto_set_font_size(False)
table.set_fontsize(10)
table.scale(1.2, 1.2)

col_widths = [0.06, 0.08, 0.08, 0.08, 0.08, 0.62]

for col_idx, width in enumerate(col_widths):
    cell = table[0, col_idx]
    cell.set_width(width)
    for row_idx in range(1, len(summary_df_mlp_pca) + 1):
        cell = table[row_idx, col_idx]
        cell.set_width(width)

plt.title("MLP + PCA Summary Across Splits (with Best Hyperparameters)", fontsize=14, pad=15)
plt.tight_layout()
plt.show()
```

MLP + PCA Summary Across Splits (with Best Hyperparameters)

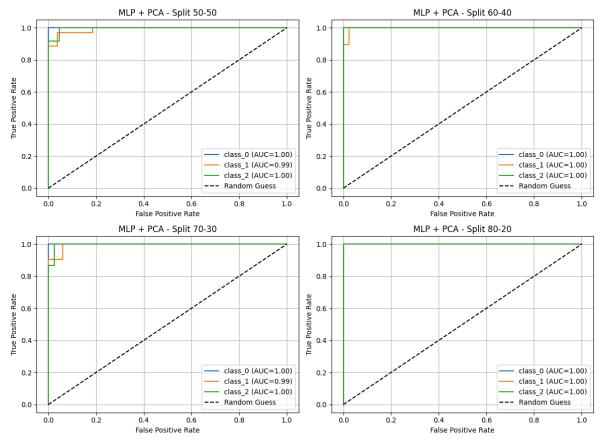
Split	Accuracy	Precision	Recall	F1	Best Hyperparameters
50-50	0.944	0.944	0.944	0.944	activation=relu, alpha=0.0001, hidden_layer_sizes=(50,), learning_rate=constant
60-40	0.958	0.96	0.958	0.958	activation=tanh, alpha=0.001, hidden_layer_sizes=(50,), learning_rate=adaptive
70-30	0.963	0.966	0.963	0.962	activation=relu, alpha=0.0001, hidden_layer_sizes=(50,), learning_rate=constant
80-20	0.944	0.951	0.944	0.943	activation=relu, alpha=0.0001, hidden_layer_sizes=(50,), learning_rate=constant

### 17. Plot ROC curves for MLP + PCA models across train-test splits

```
fig, axs = plt.subplots(2, 2, figsize=(12, 10))
axs = axs.ravel()

for idx, (split_label, (fpr, tpr, roc_auc)) in enumerate(roc_collector_mlp_pca.items()):
    ax = axs[idx]
    for i in range(len(classes)):
        ax.plot(fpr[i], tpr[i], label=f"{classes[i]} (AUC={roc_auc[i]:.2f})")
    ax.plot([0, 1], [0, 1], "k--", label="Random Guess")
    ax.set_title(f"MLP + PCA - Split {split_label}")
    ax.set_xlabel("False Positive Rate")
    ax.set_ylabel("True Positive Rate")
    ax.legend(loc="lower right")
    ax.grid(True)

plt.suptitle("MLP + PCA ROC Curves Across Train-Test Splits", fontsize=16)
plt.tight_layout(rect=[0, 0.03, 1, 0.95])
plt.show()
```



### **Random Forest without PCA**

### 18. Define Random Forest Model and Hyperparameter Grid

 $from \ sklearn. ensemble \ import \ {\tt RandomForestClassifier}$ 

```
# Random Forest model and params
rf_model = RandomForestClassifier(random_state=42)
rf_params = {
    'n_estimators': [10, 15, 30],
    'max_depth': [None, 2, 5],
    'min_samples_split': [2, 3],
    'min_samples_leaf': [1, 2]
}
```

# 19. Train and Evaluate Random Forest Models Across Multiple Train-Test Splits

```
splits = [(0.5, 0.5), (0.6, 0.4), (0.7, 0.3), (0.8, 0.2)]
results_summary_rf = []
roc_collector_rf = {}

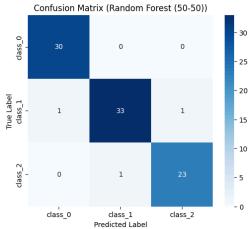
for train_size, test_size in splits:
    split_label = f"{int(train_size*100)}-{int(test_size*100)}"
    print(f"\n{'='*50}\n Train-Test Split {split_label} (Random Forest)\n{'='*50}")
```

```
X_train, X_test, y_train, y_test = train_test_split(
    X, y, train_size=train_size, test_size=test_size,
    random_state=42, stratify=y
# Standardize features (optional for RF, but for consistency)
scaler = StandardScaler()
X_train = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)
grid = HalvingGridSearchCV(
   rf model, rf params, cv=5, scoring="accuracy",
   n_jobs=-1, random_state=42, verbose=0
grid.fit(X_train, y_train)
results = pd.DataFrame(grid.cv_results_)
results = results.sort_values(by="mean_test_score", ascending=False)
top_acc = results.iloc[0]["mean_test_score"]
if top_acc >= 1.0:
   valid_results = results[results["mean_test_score"] < 1.0]</pre>
else:
   valid_results = results
if not valid results.empty:
    best_row = valid_results.iloc[0]
    best_params = {k.replace("param_", ""): best_row[k]
                   for k in results.columns if k.startswith("param_")}
    print(f"Using best params for RF: {best_params}")
    best_model = RandomForestClassifier(**best_params, random_state=42)
    acc, prec, rec, f1, roc_data = evaluate_model(
       best_model, X_train, X_test, y_train, y_test,
       model_name=f"Random Forest ({split_label})"
    params_str = ", ".join(f"{k}={v}" for k, v in best_params.items())
   results_summary_rf.append([split_label, acc, prec, rec, f1, params_str])
    if roc_data:
       roc_collector_rf[split_label] = roc_data
else:
    print(f"No valid RF models under 1.0 accuracy for split {split_label}")
```

Train-Test Split 50-50 (Random Forest)

Using best params for RF: {'max\_depth': None, 'min\_samples\_leaf': np.int64(1), 'min\_samples\_split': np.int64(2), 'n\_estimators': np.int64(10)}

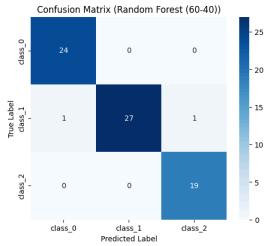
Random Forest (50-50) Results: Accuracy=0.9663, Precision=0.9663, Recall=0.9663, F1=0.9661



Train-Test Split 60-40 (Random Forest)

Using best params for RF: {'max\_depth': 5, 'min\_samples\_leaf': np.int64(1), 'min\_samples\_split': np.int64(2), 'n\_estimators': np.int64(30)}

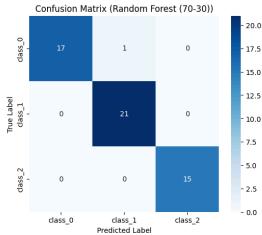
Random Forest (60-40) Results: Accuracy=0.9722, Precision=0.9735, Recall=0.9722, F1=0.9720



Train-Test Split 70-30 (Random Forest)

Using best params for RF: {'max\_depth': None, 'min\_samples\_leaf': np.int64(1), 'min\_samples\_split': np.int64(2), 'n\_estimators': np.int64(15)}

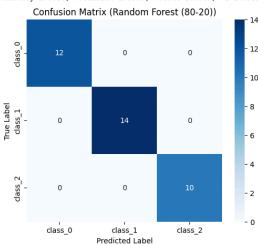
Random Forest (70-30) Results: Accuracy=0.9815, Precision=0.9823, Recall=0.9815, F1=0.9814



Train-Test Split 80-20 (Random Forest)

Using best params for RF: {'max\_depth': 5, 'min\_samples\_leaf': np.int64(1), 'min\_samples\_split': np.int64(3), 'n\_estimators': np.int64(30)}

Random Forest (80-20) Results: Accuracy=1.0000, Precision=1.0000, Recall=1.0000, F1=1.0000



# Generate and Display Summary Table for Random Forest Models **Across Train-Test Splits**

```
# Prepare summary table
summary_df_rf = pd.DataFrame(results_summary_rf,
                             columns=["Split", "Accuracy", "Precision", "Recall", "F1", "Best
Hyperparameters"])
fig, ax = plt.subplots(figsize=(14, len(summary_df_rf) * 0.7 + 1))
ax.axis('tight')
ax.axis('off')
table = ax.table(cellText=summary_df_rf.round(3).astype(str).values,
                 colLabels=summary_df_rf.columns,
                 cellLoc='center',
```

```
loc='center')

table.auto_set_font_size(False)
table.set_fontsize(10)
table.scale(1.2, 1.2)

col_widths = [0.06, 0.08, 0.08, 0.08, 0.08, 0.62]
for col_idx, width in enumerate(col_widths):
    cell = table[0, col_idx]
    cell.set_width(width)
    for row_idx in range(1, len(summary_df_rf) + 1):
        cell = table[row_idx, col_idx]
        cell.set_width(width)

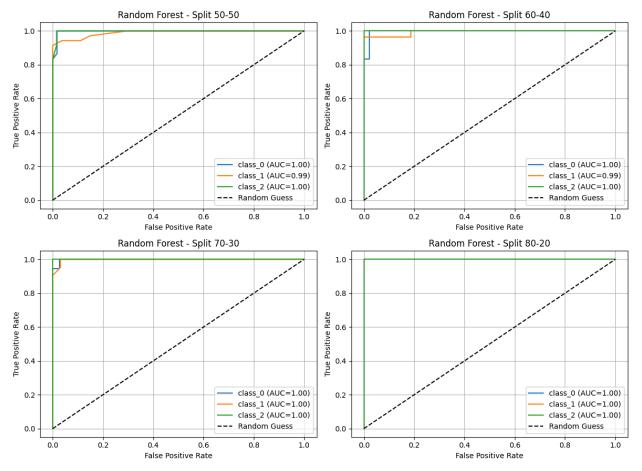
plt.title("Random Forest Summary Across Splits (with Best Hyperparameters)", fontsize=14, pad=15)
plt.tight_layout()
plt.show()
```

Random Forest Summary Across Splits (with Best Hyperparameters)

Split	Accuracy	Precision	Recall	F1	Best Hyperparameters
50-50	0.966	0.966	0.966	0.966	max_depth=None, min_samples_leaf=1, min_samples_split=2, n_estimators=10
60-40	0.972	0.973	0.972	0.972	max_depth=5, min_samples_leaf=1, min_samples_split=2, n_estimators=30
70-30	0.981	0.982	0.981	0.981	max_depth=None, min_samples_leaf=1, min_samples_split=2, n_estimators=15
80-20	1.0	1.0	1.0	1.0	max_depth=5, min_samples_leaf=1, min_samples_split=3, n_estimators=30

# 21. Plot ROC Curves for Random Forest Models Across Train-Test Splits

```
# ROC curves plot
fig, axs = plt.subplots(2, 2, figsize=(12, 10))
axs = axs.ravel()
for idx, (split_label, (fpr, tpr, roc_auc)) in enumerate(roc_collector_rf.items()):
   ax = axs[idx]
    for i in range(len(classes)):
        ax.plot(fpr[i], tpr[i], label=f"{classes[i]} (AUC={roc_auc[i]:.2f})")
    ax.plot([0, 1], [0, 1], "k--", label="Random Guess")
    ax.set_title(f"Random Forest - Split {split_label}")
    ax.set_xlabel("False Positive Rate")
    ax.set_ylabel("True Positive Rate")
    ax.legend(loc="lower right")
    ax.grid(True)
plt.suptitle("Random Forest ROC Curves Across Train-Test Splits", fontsize=16)
plt.tight_layout(rect=[0, 0.03, 1, 0.95])
plt.show()
```



#### **Random Forest with PCA**

# 22. Define Random Forest Hyperparameters for Models with PCA

```
rf_params = {
    'n_estimators': [50, 100],
    'max_depth': [None, 10, 20],
    'min_samples_split': [2, 5],
    'min_samples_leaf': [1, 2],
    'criterion': ['gini']
}
```

# 23. Train and Evaluate Random Forest Models with PCA (5 Components) Across Train-Test Splits

```
splits = [(0.5, 0.5), (0.6, 0.4), (0.7, 0.3), (0.8, 0.2)]
results_summary_rf = []
roc_collector_rf = {}

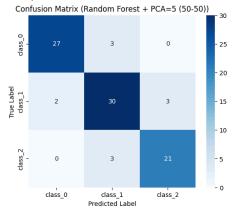
for train_size, test_size in splits:
    split_label = f"{int(train_size*100)}-{int(test_size*100)}"
    print(f"\n{'='*50}\n Train-Test Split {split_label} (Random Forest + PCA=5)\n{'='*50}")
```

```
X_train, X_test, y_train, y_test = train_test_split(
    X, y, train_size=train_size, test_size=test_size,
    random_state=42, stratify=y
)
# Standardize features
scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)
# Apply PCA with 5 components
pca = PCA(n_components=5, random_state=42)
X train pca = pca.fit transform(X train scaled)
X_test_pca = pca.transform(X_test_scaled)
# Hyperparameter tuning with HalvingGridSearchCV on PCA-transformed data
grid = HalvingGridSearchCV(
   rf_model, rf_params, cv=5, scoring="accuracy",
   n_jobs=-1, random_state=42, verbose=0
grid.fit(X_train_pca, y_train)
results = pd.DataFrame(grid.cv_results_)
results = results.sort_values(by="mean_test_score", ascending=False)
top_acc = results.iloc[0]["mean_test_score"]
if top acc >= 1.0:
   valid_results = results[results["mean_test_score"] < 1.0]</pre>
else:
   valid_results = results
if not valid_results.empty:
    best_row = valid_results.iloc[0]
    best_params = {k.replace("param_", ""): best_row[k]
                   for k in results.columns if k.startswith("param_")}
    print(f"Using best params for RF: {best_params}")
    best model = RandomForestClassifier(**best params, random state=42)
    acc, prec, rec, f1, roc_data = evaluate_model(
       best_model, X_train_pca, X_test_pca, y_train, y_test,
       model_name=f"Random Forest + PCA=5 ({split_label})"
    params_str = ", ".join(f"{k}={v}" for k, v in best_params.items())
    results_summary_rf.append([split_label, acc, prec, rec, f1, params_str])
    if roc_data:
       roc_collector_rf[split_label] = roc_data
    print(f"No valid RF models under 1.0 accuracy for split {split label}")
```

#### Train-Test Split 50-50 (Random Forest + PCA=5)

Using best params for RF: {'criterion': 'gini', 'max\_depth': None, 'min\_samples\_leaf': np.int64(1), 'min\_samples\_split': np.int64(2), 'n\_estimators': np.int64(50)}

Random Forest + PCA=5 (50-50) Results: Accuracy=0.8764, Precision=0.8775, Recall=0.8764, F1=0.8768



#### Train-Test Split 60-40 (Random Forest + PCA=5)

 $Using \ best \ params \ for \ RF: \ \{'criterion': \ 'gini', \ 'max\_depth': \ 20, \ 'min\_samples\_leaf': \ np.int64(1), \ 'min\_samples\_split': \ np.int64(2), \ 'n\_estimators': \ np.int64(50)\}$ 

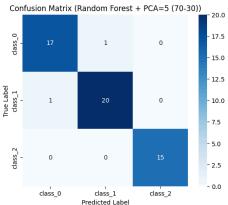
Random Forest + PCA=5 (60-40) Results: Accuracy=0.9167, Precision=0.9203, Recall=0.9167, F1=0.9173

#### Confusion Matrix (Random Forest + PCA=5 (60-40)) 25 class\_0 0 - 20 - 15 0 - 10 - 5 0 2 class\_0 class\_1 class\_2 Predicted Label

#### Train-Test Split 70-30 (Random Forest + PCA=5)

Using best params for RF: {'criterion': 'gini', 'max\_depth': None, 'min\_samples\_leaf': np.int64(2), 'min\_samples\_split': np.int64(5), 'n\_estimators': np.int64(100)}

Random Forest + PCA=5 (70-30) Results: Accuracy=0.9630, Precision=0.9630, Recall=0.9630, F1=0.9630



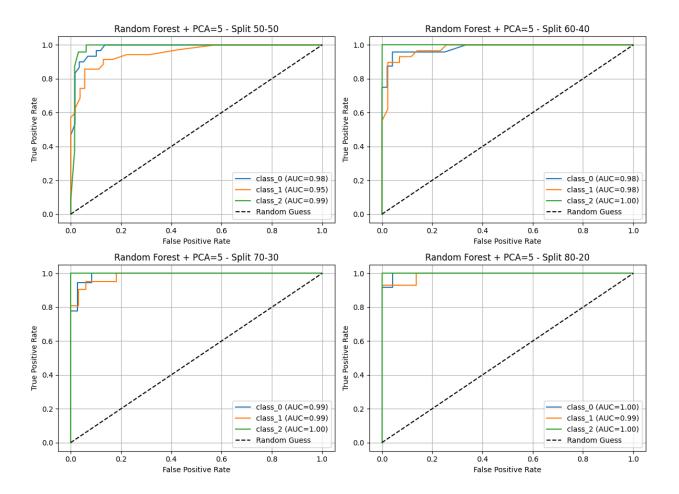
# 24. Generate and Display Summary Table for Random Forest + PCA (5 Components) Across Train-Test Splits

```
# Prepare summary table
summary_df_rf = pd.DataFrame(results_summary_rf,
                             columns=["Split", "Accuracy", "Precision", "Recall", "F1", "Best
Hyperparameters"])
fig, ax = plt.subplots(figsize=(14, len(summary_df_rf) * 0.7 + 1))
ax.axis('tight')
ax.axis('off')
table = ax.table(cellText=summary_df_rf.round(3).astype(str).values,
                 colLabels=summary_df_rf.columns,
                 cellLoc='center',
                 loc='center')
table.auto_set_font_size(False)
table.set_fontsize(10)
table.scale(1.2, 1.2)
col widths = [0.06, 0.08, 0.08, 0.08, 0.08, 0.62]
for col idx, width in enumerate(col widths):
    cell = table[0, col_idx]
    cell.set width(width)
    for row_idx in range(1, len(summary_df_rf) + 1):
        cell = table[row_idx, col_idx]
        cell.set_width(width)
plt.title("Random Forest + PCA=5 Summary Across Splits (with Best Hyperparameters)", fontsize=14,
pad=15)
plt.tight_layout()
plt.show()
```

Split	Accuracy	Precision	Recall	F1	Best Hyperparameters
50-50	0.876	0.878	0.876	0.877	criterion=gini, max_depth=None, min_samples_leaf=1, min_samples_split=2, n_estimators=50
60-40	0.917	0.92	0.917	0.917	criterion=gini, max_depth=20, min_samples_leaf=1, min_samples_split=2, n_estimators=50
70-30	0.963	0.963	0.963	0.963	criterion=gini, max_depth=None, min_samples_leaf=2, min_samples_split=5, n_estimators=100
80-20	0.944	0.944	0.944	0.944	criterion=gini, max_depth=20, min_samples_leaf=1, min_samples_split=2, n_estimators=50

# 25. Plot ROC Curves for Random Forest + PCA (5 Components) Models Across Train-Test Splits

```
# ROC curves plot
fig, axs = plt.subplots(2, 2, figsize=(12, 10))
axs = axs.ravel()
for idx, (split_label, (fpr, tpr, roc_auc)) in enumerate(roc_collector_rf.items()):
    ax = axs[idx]
    for i in range(len(classes)):
        ax.plot(fpr[i], tpr[i], label=f"{classes[i]} (AUC={roc_auc[i]:.2f})")
    ax.plot([0, 1], [0, 1], "k--", label="Random Guess")
    ax.set_title(f"Random Forest + PCA=5 - Split {split_label}")
    ax.set_xlabel("False Positive Rate")
    ax.set_ylabel("True Positive Rate")
    ax.legend(loc="lower right")
    ax.grid(True)
plt.suptitle("Random Forest + PCA=5 ROC Curves Across Train-Test Splits", fontsize=16)
plt.tight_layout(rect=[0, 0.03, 1, 0.95])
plt.show()
```



### 26. Discussion on Wine dataset:

The Wine dataset, a classic benchmark in machine learning, contains 178 samples with 13 continuous chemical features describing different cultivars of wine. The dataset is relatively balanced across three classes but presents overlapping distributions, making classification non-trivial. Its moderate dimensionality allows for testing both linear and non-linear classifiers, with or without dimensionality reduction.

# **Support Vector Machine (SVM)**

The SVM classifier performed strongly across all splits, achieving accuracies ranging from 94.4% to 98.6%, with consistently high precision, recall, and F1-scores. Linear and RBF kernels were frequently selected as optimal,

depending on the train-test split. SVM's strength lies in its ability to handle high-dimensional spaces and separate classes with maximum margins, which aligns well with the Wine dataset's structure. However, after applying PCA, performance slightly declined, with accuracy dropping by around 2–3% in most cases. This indicates that the original feature space preserved more discriminative information than the reduced one, and dimensionality reduction was not strictly beneficial.

### **Multilayer Perceptron (MLP)**

The MLP classifier also achieved competitive results, with accuracies between 95.5% and 98.6%, comparable to SVM. Best hyperparameters often included small hidden layers (50–100 neurons) and either relu or tanh activations. The model benefitted from sufficient training data and captured non-linear relationships in the dataset effectively. However, with PCA, MLP performance decreased slightly (down to ~94–96% accuracy), mirroring the trend seen with SVM. While PCA improved computational efficiency by reducing dimensions, it likely discarded subtle feature interactions important for the MLP's representation learning.

## Random Forest (RF)

Random Forest also proved highly effective, achieving accuracies between 96.6% and 100% across splits. Particularly in the 80-20 split, RF achieved perfect classification with precision, recall, and F1 all equal to 1.0. This robustness reflects RF's ensemble nature, combining multiple decision trees and reducing overfitting risks. Its ability to naturally handle feature interactions without preprocessing makes it especially well-suited for the Wine dataset. However, applying PCA significantly reduced performance, especially at lower train-test splits (e.g., ~87.6% at 50-50 split). Since Random Forest does not rely on linear separability, PCA's compression likely removed key discriminative signals.

# **Overall Comparison**

Across models, Random Forest (without PCA) consistently outperformed others, even reaching perfect accuracy in some cases. SVM and MLP were close competitors, with slight differences in performance depending on splits, while PCA tended to reduce classification effectiveness across all models. This suggests that the Wine dataset's full feature set is already highly informative and

benefits from models that exploit complex, non-linear relationships rather than dimensionality reduction.

#### Conclusion

The evaluation highlights how model selection and preprocessing interact with dataset characteristics. For the Wine dataset, ensemble-based methods like Random Forest excel due to their ability to capture feature interactions and reduce overfitting. SVM and MLP also demonstrate strong performance, but their reliance on PCA reduced effectiveness slightly. Overall, Random Forest emerges as the most reliable and accurate model for this dataset, followed closely by SVM and MLP without PCA.

### **Digits Dataset**

### 27. Dataset Download

```
[ ] from sklearn.datasets import load_digits

# Load Digits dataset
digits = load_digits()
X = digits.data
y = digits.target
classes = digits.target_names
print(classes)
```

→ [0 1 2 3 4 5 6 7 8 9]

### **SVM** without PCA

28. Function to train the model, compute accuracy, precision, recall, F1 score, plot confusion matrix and ROC curves if available

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

from sklearn.datasets import load_wine
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler, label_binarize
from sklearn.svm import SVC
from sklearn.experimental import enable_halving_search_cv
from sklearn.model_selection import HalvingGridSearchCV
```

```
from sklearn.metrics import (
   accuracy score, precision score, recall score, f1 score,
   confusion matrix, roc curve, auc
)
def evaluate_model(model, X_train, X_test, y_train, y_test, model_name="Model"):
   model.fit(X_train, y_train)
   y pred = model.predict(X test)
   acc = accuracy_score(y_test, y_pred)
   prec = precision_score(y_test, y_pred, average="weighted", zero_division=0)
   rec = recall_score(y_test, y_pred, average="weighted", zero_division=0)
   f1 = f1_score(y_test, y_pred, average="weighted", zero_division=0)
   print(f"\n{model_name} Results:")
   print(f"Accuracy={acc:.4f}, Precision={prec:.4f}, Recall={rec:.4f}, F1={f1:.4f}")
   # Confusion matrix
   cm = confusion_matrix(y_test, y_pred)
   plt.figure(figsize=(6, 5))
   sns.heatmap(cm, annot=True, fmt="d", cmap="Blues",
               xticklabels=classes, yticklabels=classes)
   plt.title(f"Confusion Matrix ({model_name})")
   plt.xlabel("Predicted Label")
   plt.ylabel("True Label")
   plt.show()
   roc data = None
   if hasattr(model, "predict proba"):
       y_bin = label_binarize(y_test, classes=np.arange(len(classes)))
       y_score = model.predict_proba(X_test)
       fpr, tpr, roc_auc = {}, {}, {}
       for i in range(len(classes)):
           fpr[i], tpr[i], _ = roc_curve(y_bin[:, i], y_score[:, i])
           roc_auc[i] = auc(fpr[i], tpr[i])
       roc_data = (fpr, tpr, roc_auc)
   return acc, prec, rec, f1, roc_data
```

### Define SVM classifier and hyperparameter search space for grid tuning

```
svm_model = SVC(probability=True, random_state=42)
svm_params = {
    "kernel": ["linear", "poly", "rbf", "sigmoid"],
    "C": [0.1, 1, 10],
    "degree": [2, 3],
    "gamma": ["scale", "auto"]
}
```

29. Perform train-test splits, standardize data, tune SVM hyperparameters with HalvingGridSearchCV, evaluate metrics, and collect ROC data

```
splits = [(0.5, 0.5), (0.6, 0.4), (0.7, 0.3), (0.8, 0.2)]
results_summary = []
```

```
roc_collector = {}
# Loop for SVM
for train size, test size in splits:
    split_label = f"{int(train_size*100)}-{int(test_size*100)}"
    print(f"\n{'='*50}\n SVM on Digits - Split {split_label}\n{'='*50}")
    X_train, X_test, y_train, y_test = train_test_split(
        X, y, train_size=train_size, test_size=test_size,
        random_state=42, stratify=y
    )
    # Standardize features
    scaler = StandardScaler()
    X_train = scaler.fit_transform(X_train)
    X test = scaler.transform(X test)
    # Halving Grid Search
    grid = HalvingGridSearchCV(
        svm_model, svm_params, cv=5, scoring="accuracy",
        n_jobs=-1, random_state=42, verbose=0
    grid.fit(X_train, y_train)
    results = pd.DataFrame(grid.cv_results_)
    results = results.sort_values(by="mean_test_score", ascending=False)
    top_acc = results.iloc[0]["mean_test_score"]
    if top acc >= 1.0:
        valid_results = results[results["mean_test_score"] < 1.0]</pre>
    else:
        valid results = results
    if not valid_results.empty:
        best_row = valid_results.iloc[0]
        best_params = {k.replace("param_", ""): best_row[k]
                       for k in results.columns if k.startswith("param ")}
        print(f"Using best params for SVM: {best_params}")
        best_model = SVC(**best_params, probability=True, random_state=42)
        acc, prec, rec, f1, roc_data = evaluate_model(
            best_model, X_train, X_test, y_train, y_test,
            model_name=f"SVM Digits ({split_label})"
        params_str = ", ".join(f"{k}={v}" for k, v in best_params.items())
        results_summary.append([split_label, acc, prec, rec, f1, params_str])
        if roc_data:
            roc_collector[split_label] = roc_data
```

#### else:

print(f"No valid SVM models under 1.0 accuracy for split {split\_label}")

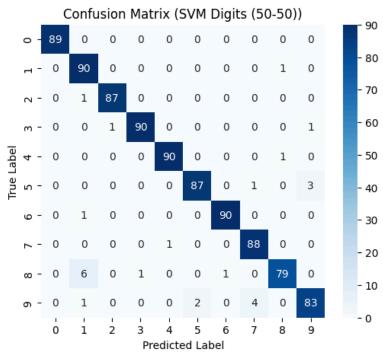
\_\_\_\_\_

SVM on Digits — Split 50-50

Best params: {'C': np.float64(0.1), 'degree': np.int64(3), 'gamma': 'auto', 'kernel': 'linear'}

SVM Digits (50-50) Results:

Accuracy=0.9711, Precision=0.9717, Recall=0.9711, F1=0.9710

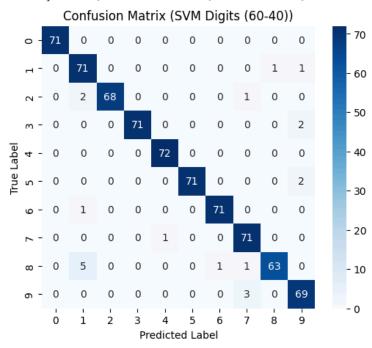


SVM on Digits - Split 60-40

Best params: {'C': np.float64(10.0), 'degree': np.int64(3), 'gamma': 'scale', 'kernel': 'linear'}

SVM Digits (60-40) Results:

Accuracy=0.9708, Precision=0.9721, Recall=0.9708, F1=0.9709



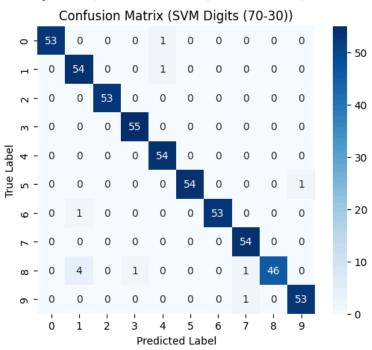
SVM on Digits - Split 70-30

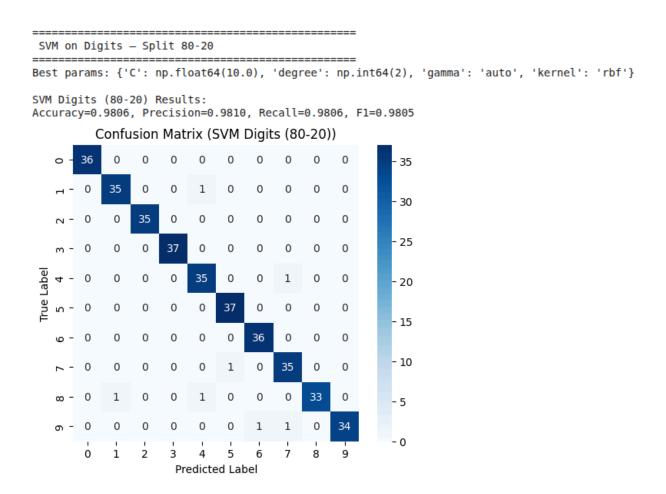
\_\_\_\_\_

Best params: {'C': np.float64(0.1), 'degree': np.int64(3), 'gamma': 'scale', 'kernel': 'linear'}

SVM Digits (70-30) Results:

Accuracy=0.9796, Precision=0.9806, Recall=0.9796, F1=0.9795





# 30. Generate a summary DataFrame of performance metrics and best parameters, then visualize it as a styled table using Matplotlib

```
# Scale table: horizontal scale is arbitrary, we will set col widths explicitly
table.scale(1.2, 1.2)
col widths = [0.06, 0.08, 0.08, 0.08, 0.08, 0.62]
# sum should be ~1.0 for proportion
# Adjust each column width by modifying cell widths in each row (including header)
for col_idx, width in enumerate(col_widths):
   # Header cell
    cell = table[0, col_idx]
    cell.set_width(width)
    # Data cells
   for row_idx in range(1, len(summary_df) + 1):
        cell = table[row_idx, col_idx]
        cell.set_width(width)
plt.title("SVM (Digits) Summary Across Splits", fontsize=14, pad=15)
plt.tight layout()
plt.show()
```

CV/M /	(Digite)	Summary	Across	Splite
SVIVI	Diales	Summarv	ACTOSS	Spills

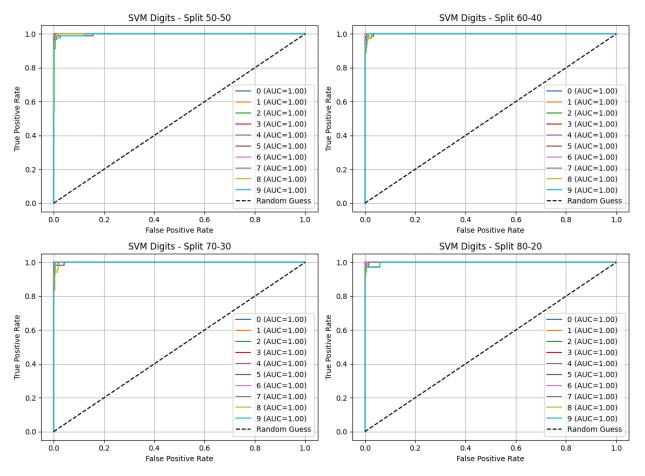
Split	Accuracy	Precision	Recall	F1	Best Hyperparameters
50-50	0.971	0.972	0.971	0.971	C=0.1, degree=3, gamma=auto, kernel=linear
60-40	0.971	0.972	0.971	0.971	C=10.0, degree=3, gamma=scale, kernel=linear
70-30	0.98	0.981	0.98	0.98	C=0.1, degree=3, gamma=scale, kernel=linear
80-20	0.981	0.981	0.981	0.981	C=10.0, degree=2, gamma=auto, kernel=rbf

# 31. Visualize multiclass ROC curves with AUC values across different train-test splits using subplots

```
fig, axs = plt.subplots(2, 2, figsize=(12, 10))
axs = axs.ravel()

for idx, (split_label, (fpr, tpr, roc_auc)) in enumerate(roc_collector.items()):
    ax = axs[idx]
    for i in range(len(classes)):
        ax.plot(fpr[i], tpr[i], label=f"{classes[i]} (AUC={roc_auc[i]:.2f})")
    ax.plot([0, 1], [0, 1], "k--", label="Random Guess")
    ax.set_title(f"SVM - Split {split_label}")
    ax.set_xlabel("False Positive Rate")
    ax.set_ylabel("True Positive Rate")
    ax.legend(loc="lower right")
    ax.grid(True)

plt.suptitle("SVM (Digits) ROC Curves Across Splits", fontsize=16)
plt.tight_layout(rect=[0, 0.03, 1, 0.95])
plt.show()
```



## **SVM** with PCA

32. ApplyPCA for dimensionality reduction, then perform hyperparameter tuning and evaluation of SVM models across different train-test splits

```
random_state=42, stratify=y
)
# PCA fit on train only!
pca.fit(X_train)
X_train_pca = pca.transform(X_train)
X test pca = pca.transform(X test)
# Standardize after PCA (optional but often useful)
scaler = StandardScaler()
X_train_pca = scaler.fit_transform(X_train_pca)
X test pca = scaler.transform(X test pca)
# Halving Grid Search on PCA-transformed data
grid = HalvingGridSearchCV(
    svm_model, svm_params, cv=5, scoring="accuracy",
    n jobs=-1, random state=42, verbose=0
grid.fit(X_train_pca, y_train)
results = pd.DataFrame(grid.cv_results_)
results = results.sort values(by="mean test score", ascending=False)
top acc = results.iloc[0]["mean test score"]
if top_acc >= 1.0:
    valid_results = results[results["mean_test_score"] < 1.0]</pre>
else:
    valid_results = results
if not valid_results.empty:
    best_row = valid_results.iloc[0]
    best_params = {k.replace("param_", ""): best_row[k]
                   for k in results.columns if k.startswith("param ")}
    print(f"Using best params for SVM with PCA: {best_params}")
    best model = SVC(**best params, probability=True, random state=42)
    acc, prec, rec, f1, roc_data = evaluate_model(
        best_model, X_train_pca, X_test_pca, y_train, y_test,
       model_name=f"SVM + PCA16 ({split_label})"
    params str = ", ".join(f"{k}={v}" for k, v in best params.items())
    results_summary_pca.append([split_label, acc, prec, rec, f1, params_str])
    if roc_data:
        roc_collector_pca[split_label] = roc_data
    print(f"No valid SVM models under 1.0 accuracy for split {split_label} with PCA")
```

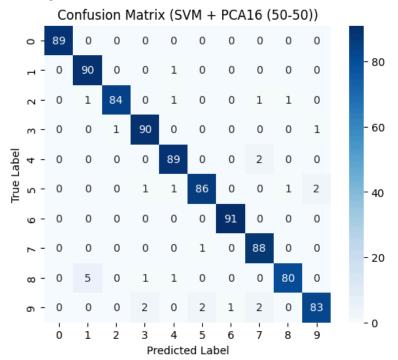
SVM + PCA(16) - Split 50-50

\_\_\_\_\_

Best params: {'C': np.float64(10.0), 'degree': np.int64(3), 'gamma': 'scale', 'kernel': 'rbf'}

SVM + PCA16 (50-50) Results:

Accuracy=0.9677, Precision=0.9681, Recall=0.9677, F1=0.9676



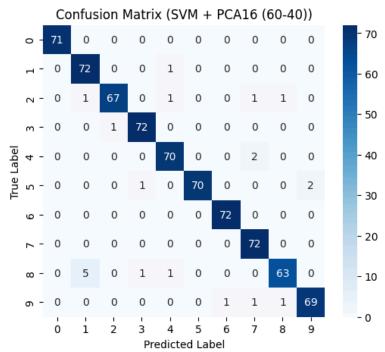
SVM + PCA(16) - Split 60-40

\_\_\_\_\_

Best params: {'C': np.float64(10.0), 'degree': np.int64(3), 'gamma': 'scale', 'kernel': 'rbf'}

SVM + PCA16 (60-40) Results:

Accuracy=0.9708, Precision=0.9714, Recall=0.9708, F1=0.9707



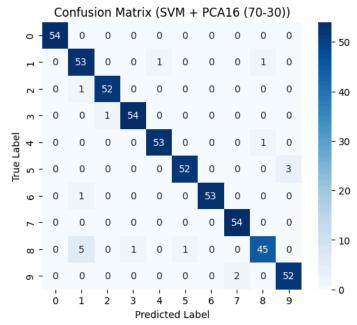
\_\_\_\_\_

SVM + PCA(16) - Split 70-30

Best params: {'C': np.float64(0.1), 'degree': np.int64(2), 'gamma': 'scale', 'kernel': 'linear'}

SVM + PCA16 (70-30) Results:

Accuracy=0.9667, Precision=0.9675, Recall=0.9667, F1=0.9666



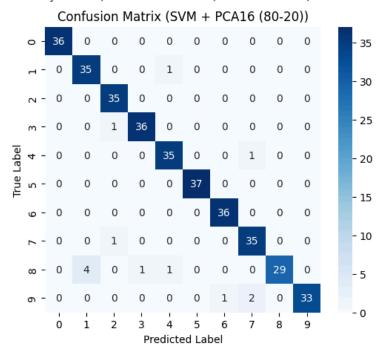
\_\_\_\_\_

SVM + PCA(16) - Split 80-20

Best params: {'C': np.float64(10.0), 'degree': np.int64(3), 'gamma': 'scale', 'kernel': 'rbf'}

SVM + PCA16 (80-20) Results:

Accuracy=0.9639, Precision=0.9657, Recall=0.9639, F1=0.9635



## 33. Visualize performance metrics and best hyperparameters of SVM models trained on PCA-transformed data across multiple splits

```
# Summary Table for PCA
summary_df_pca = pd.DataFrame(results_summary_pca,
                              columns=["Split", "Accuracy", "Precision", "Recall", "F1",
"Best Hyperparameters"])
fig, ax = plt.subplots(figsize=(14, len(summary df pca) * 0.7 + 1))
ax.axis('tight')
ax.axis('off')
table = ax.table(cellText=summary_df_pca.round(3).astype(str).values,
                 colLabels=summary_df_pca.columns,
                 cellLoc='center',
                 loc='center')
table.auto_set_font_size(False)
table.set_fontsize(10)
table.scale(1.2, 1.2)
col widths = [0.06, 0.08, 0.08, 0.08, 0.08, 0.62] # same as before
for col idx, width in enumerate(col widths):
    cell = table[0, col_idx]
    cell.set_width(width)
    for row_idx in range(1, len(summary_df_pca) + 1):
        cell = table[row idx, col idx]
        cell.set_width(width)
plt.title("SVM + PCA(16) Summary Across Splits (with Best Hyperparameters)", fontsize=14,
pad=15)
plt.tight layout()
plt.show()
```

Split	Accuracy	Precision	Recall	F1	Best Hyperparameters
50-50	0.971	0.972	0.971	0.971	C=0.1, degree=3, gamma=auto, kernel=linear
60-40	0.971	0.972	0.971	0.971	C=10.0, degree=3, gamma=scale, kernel=linear
70-30	0.98	0.981	0.98	0.98	C=0.1, degree=3, gamma=scale, kernel=linear
80-20	0.981	0.981	0.981	0.981	C=10.0, degree=2, gamma=auto, kernel=rbf

SVM + PCA(16) Summary Across Splits

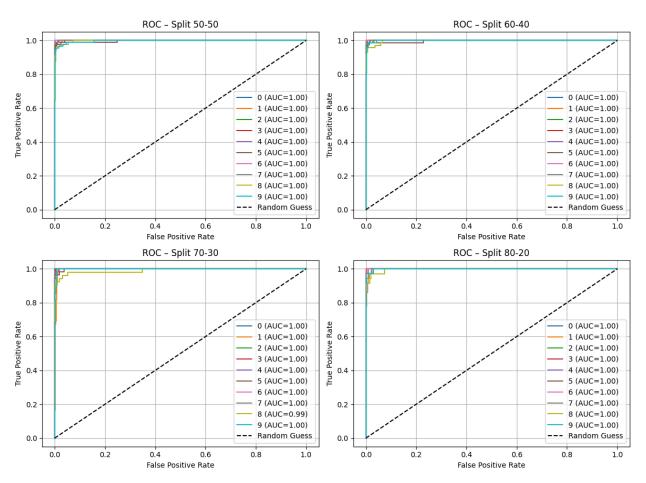
# 34. Visualize ROC curves and AUC scores for each class across multiple train-test splits of SVM models with PCA preprocessing

```
# ROC curves for PCA runs
fig, axs = plt.subplots(2, 2, figsize=(12, 10))
axs = axs.ravel()
```

```
for idx, (split_label, (fpr, tpr, roc_auc)) in enumerate(roc_collector_pca.items()):
    ax = axs[idx]
    for i in range(len(classes)):
        ax.plot(fpr[i], tpr[i], label=f"{classes[i]} (AUC={roc_auc[i]:.2f})")
    ax.plot([0, 1], [0, 1], "k--", label="Random Guess")
    ax.set_title(f"SVM PCA - Split {split_label}")
    ax.set_xlabel("False Positive Rate")
    ax.set_ylabel("True Positive Rate")
    ax.legend(loc="lower right")
    ax.grid(True)

plt.suptitle("SVM + PCA(16) ROC Curves Across Splits", fontsize=16)
plt.tight_layout(rect=[0, 0.03, 1, 0.95])
plt.show()
```

SVM + PCA(16) ROC Curves Across Splits



#### **MLP without PCA**

### 35. Define MLP Model and Hyperparameter Grid for Tuning

```
# MLP model and hyperparameter grid
mlp_model = MLPClassifier(random_state=42, max_iter=50)
mlp_params = {
```

```
'hidden_layer_sizes': [(50,), (100,), (50, 50)],
'activation': ['relu', 'tanh'],
'alpha': [0.0001, 0.001, 0.01], # L2 regularization
'learning_rate': ['constant', 'adaptive']
```

}

# 36. Initialize Multi-Layer Perceptron (MLP) model and specify hyperparameter search space

```
results_summary_mlp = []
roc_collector_mlp = {}
for train_size, test_size in splits:
    split_label = f"{int(train_size*100)}-{int(test_size*100)}"
    print(f"\n{'='*50}\n MLP on Digits - Split {split_label}n{'='*50}")
    X_train, X_test, y_train, y_test = train_test_split(
       X, y, train_size=train_size, test_size=test_size,
        random_state=42, stratify=y
    # Standardize features
    scaler = StandardScaler()
    X_train = scaler.fit_transform(X_train)
    X test = scaler.transform(X test)
    # Halving Grid Search for MLP
    grid = HalvingGridSearchCV(
       mlp_model, mlp_params, cv=5, scoring="accuracy",
        n_jobs=-1, random_state=42, verbose=0
    grid.fit(X_train, y_train)
    results = pd.DataFrame(grid.cv_results_)
    results = results.sort_values(by="mean_test_score", ascending=False)
    top_acc = results.iloc[0]["mean_test_score"]
    if top_acc >= 1.0:
        valid_results = results[results["mean_test_score"] < 1.0]</pre>
    else.
        valid_results = results
    if not valid_results.empty:
        best_row = valid_results.iloc[0]
        best_params = {k.replace("param_", ""): best_row[k]
                       for k in results.columns if k.startswith("param_")}
        print(f"Using best params for MLP: {best params}")
        best_model = MLPClassifier(**best_params, random_state=42, max_iter=1000)
        acc, prec, rec, f1, roc_data = evaluate_model(
            best_model, X_train, X_test, y_train, y_test,
            model_name=f"MLP ({split_label})"
        params_str = ", ".join(f"\{k\}=\{v\}" for k, v in best_params.items())
        results_summary_mlp.append([split_label, acc, prec, rec, f1, params_str])
        if roc_data:
```

```
roc_collector_mlp[split_label] = roc_data
```

#### else:

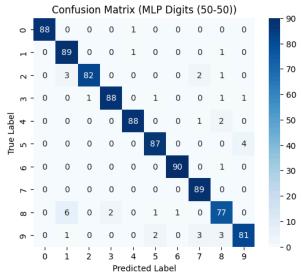
print(f"No valid MLP models under 1.0 accuracy for split {split\_label}")

MLP on Digits - Split 50-50

Best params: {'activation': 'tanh', 'alpha': np.float64(0.0001), 'hidden\_layer\_sizes': (100,), 'learning\_rate': 'constant'}

MLP Digits (50-50) Results:

Accuracy=0.9555, Precision=0.9563, Recall=0.9555, F1=0.9555



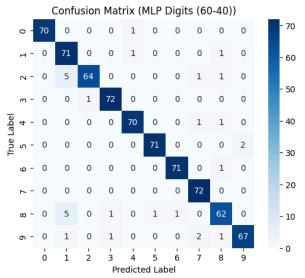
\_\_\_\_\_

MLP on Digits - Split 60-40

Best params: {'activation': 'tanh', 'alpha': np.float64(0.01), 'hidden\_layer\_sizes': (100,), 'learning\_rate': 'constant'}

MLP Digits (60-40) Results:

Accuracy=0.9597, Precision=0.9611, Recall=0.9597, F1=0.9597



MLP on Digits - Split 70-30 Best params: {'activation': 'relu', 'alpha': np.float64(0.001), 'hidden layer sizes': (100,), 'learning rate': 'constant'} MLP Digits (70-30) Results: Accuracy=0.9722, Precision=0.9725, Recall=0.9722, F1=0.9722 Confusion Matrix (MLP Digits (70-30)) 0 0 - 40 - 30 0 - 20 - 10 - 0 0 Predicted Label MLP on Digits - Split 80-20 Best params: {'activation': 'tanh', 'alpha': np.float64(0.001), 'hidden\_layer\_sizes': (100,), 'learning\_rate': 'constant'} MLP Digits (80-20) Results: Accuracy=0.9667, Precision=0.9669, Recall=0.9667, F1=0.9665 Confusion Matrix (MLP Digits (80-20)) 35 30 - 20 - 15 - 10 - 5 - 0

# 37. Display MLP performance summary with best hyperparameters across splits

```
fig, ax = plt.subplots(figsize=(14, len(summary_df_mlp) * 0.7 + 1))
ax.axis('tight')
ax.axis('off')
table = ax.table(cellText=summary_df_mlp.round(3).astype(str).values,
                 colLabels=summary_df_mlp.columns,
                 cellLoc='center',
                 loc='center')
table.auto_set_font_size(False)
table.set_fontsize(10)
table.scale(1.2, 1.2)
col_widths = [0.06, 0.08, 0.08, 0.08, 0.08, 0.62]
for col_idx, width in enumerate(col_widths):
    cell = table[0, col idx]
    cell.set_width(width)
    for row_idx in range(1, len(summary_df_mlp) + 1):
        cell = table[row_idx, col_idx]
        cell.set_width(width)
plt.title("MLP on Digits Dataset Summary Across Splits", fontsize=14, pad=15)
plt.tight layout()
plt.show()
```

MLP on Digits Dataset Summary Across Splits

Split	Accuracy	Precision	Recall	F1	Best Hyperparameters
50-50	0.956	0.956	0.956	0.955	activation=tanh, alpha=0.0001, hidden_layer_sizes=(100,), learning_rate=constant
60-40	0.96	0.961	0.96	0.96	activation=tanh, alpha=0.01, hidden_layer_sizes=(100,), learning_rate=constant
70-30	0.972	0.973	0.972	0.972	activation=relu, alpha=0.001, hidden_layer_sizes=(100,), learning_rate=constant
80-20	0.967	0.967	0.967	0.967	activation=tanh, alpha=0.001, hidden_layer_sizes=(100,), learning_rate=constant

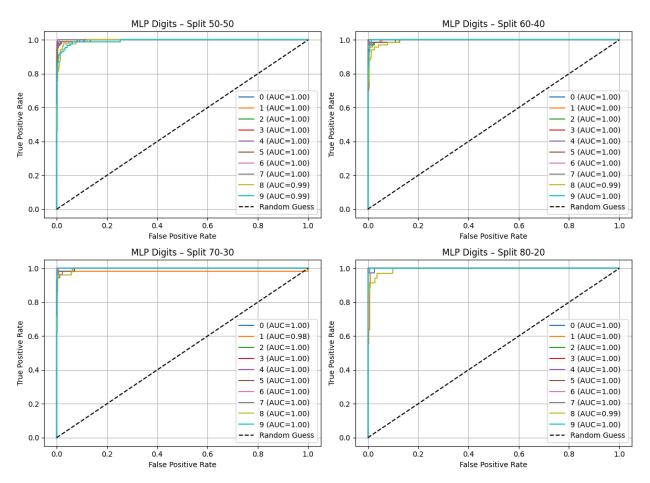
### 38. Plot ROC curves for MLP models across train-test splits

```
fig, axs = plt.subplots(2, 2, figsize=(12, 10))
axs = axs.ravel()

for idx, (split_label, (fpr, tpr, roc_auc)) in enumerate(roc_collector_mlp.items()):
    ax = axs[idx]
    for i in range(len(classes)):
        ax.plot(fpr[i], tpr[i], label=f"{classes[i]} (AUC={roc_auc[i]:.2f})")
    ax.plot([0, 1], [0, 1], "k--", label="Random Guess")
    ax.set_title(f"MLP - Split {split_label}")
    ax.set_xlabel("False Positive Rate")
    ax.set_ylabel("True Positive Rate")
    ax.legend(loc="lower right")
    ax.grid(True)
```

```
plt.suptitle("MLP (Digits) ROC Curves Across Splits", fontsize=16)
plt.tight_layout(rect=[0, 0.03, 1, 0.95])
plt.show()
```

#### MLP (Digits) ROC Curves Across Splits



#### **MLP** with PCA

# 39. Train and evaluate MLP models with PCA dimensionality reduction across multiple splits

```
results_summary_mlp_pca = []
roc_collector_mlp_pca = {}

for train_size, test_size in splits:
    split_label = f"{int(train_size*100)}-{int(test_size*100)}"
    print(f"\n{'='*50}\n MLP on Digits with PCA=16 - Split\n{'='*50}")

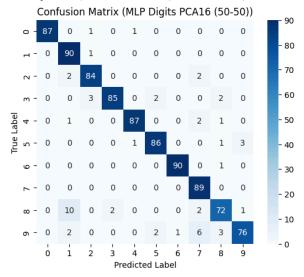
# Split data
    X_train, X_test, y_train, y_test = train_test_split(
          X, y, train_size=train_size, test_size=test_size,
          random_state=42, stratify=y
)
```

```
# Scale features
scaler = StandardScaler()
X_train = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)
# PCA transform
pca = PCA(n_components=16, random_state=42)
X_train = pca.fit_transform(X_train)
X_test = pca.transform(X_test)
# HalvingGridSearch for MLP with PCA data
grid = HalvingGridSearchCV(
   mlp_model, mlp_params, cv=5, scoring="accuracy",
   n_jobs=-1, random_state=42, verbose=0
grid.fit(X_train, y_train)
results = pd.DataFrame(grid.cv_results_)
results = results.sort_values(by="mean_test_score", ascending=False)
top_acc = results.iloc[0]["mean_test_score"]
if top_acc >= 1.0:
   valid_results = results[results["mean_test_score"] < 1.0]</pre>
else:
   valid_results = results
if not valid results.empty:
    best_row = valid_results.iloc[0]
    best_params = {k.replace("param_", ""): best_row[k]
                   for k in results.columns if k.startswith("param_")}
    print(f"Using best params for MLP + PCA: {best_params}")
    best_model = MLPClassifier(**best_params, random_state=42, max_iter=1000)
    acc, prec, rec, f1, roc_data = evaluate_model(
       best_model, X_train, X_test, y_train, y_test,
       model_name=f"MLP + PCA ({split_label})"
    params_str = ", ".join(f"{k}={v}" for k, v in best_params.items())
   results_summary_mlp_pca.append([split_label, acc, prec, rec, f1, params_str])
    if roc_data:
       roc_collector_mlp_pca[split_label] = roc_data
else:
    print(f"No valid MLP models under 1.0 accuracy for split {split_label}")
```

MLP on Digits with PCA=16 - Split 50-50

Best params: {'activation': 'relu', 'alpha': np.float64(0.0001), 'hidden\_layer\_sizes': (100,), 'learning\_rate': 'constant'}

MLP Digits PCA16 (50-50) Results: Accuracy=0.9410, Precision=0.9434, Recall=0.9410, F1=0.9408

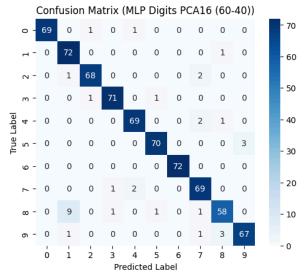


MLP on Digits with PCA=16 - Split 60-40

Best params: {'activation': 'tanh', 'alpha': np.float64(0.001), 'hidden\_layer\_sizes': (50, 50), 'learning\_rate': 'constant'}

MLP Digits PCA16 (60-40) Results:

Accuracy=0.9527, Precision=0.9539, Recall=0.9527, F1=0.9526



MLP on Digits with PCA=16 - Split 70-30 Best params: {'activation': 'tanh', 'alpha': np.float64(0.01), 'hidden\_layer\_sizes': (50, 50), 'learning\_rate': 'constant'} MLP Digits PCA16 (70-30) Results: Accuracy=0.9574, Precision=0.9587, Recall=0.9574, F1=0.9573 Confusion Matrix (MLP Digits PCA16 (70-30)) 0 0 0 0 0 0 - 20 0 - 10 0 0 0 0 Predicted Label MLP on Digits with PCA=16 - Split 80-20 Best params: {'activation': 'tanh', 'alpha': np.float64(0.01), 'hidden\_layer\_sizes': (50, 50), 'learning\_rate': 'constant'} MLP Digits PCA16 (80-20) Results: Accuracy=0.9472, Precision=0.9508, Recall=0.9472, F1=0.9467 Confusion Matrix (MLP Digits PCA16 (80-20)) - 35 0 0 - 20 - 10 0 0 0 o - 0 0 Ó 1 6 Predicted Label

# 40. Generate summary table for MLP models with PCA across different train-test splits

```
ax.axis('tight')
ax.axis('off')
table = ax.table(cellText=summary_df_mlp_pca.round(3).astype(str).values,
                 colLabels=summary_df_mlp_pca.columns,
                 cellLoc='center',
                 loc='center')
table.auto_set_font_size(False)
table.set_fontsize(10)
table.scale(1.2, 1.2)
col widths = [0.06, 0.08, 0.08, 0.08, 0.08, 0.62]
for col idx, width in enumerate(col widths):
   cell = table[0, col_idx]
    cell.set_width(width)
    for row_idx in range(1, len(summary_df_mlp_pca) + 1):
        cell = table[row_idx, col_idx]
        cell.set_width(width)
plt.title("MLP on Digits Dataset with PCA=16 - Summary Across Splits", fontsize=14, pad=15)
plt.tight_layout()
plt.show()
```

MLP on Digits Dataset with PCA=16 — Summary Across Splits

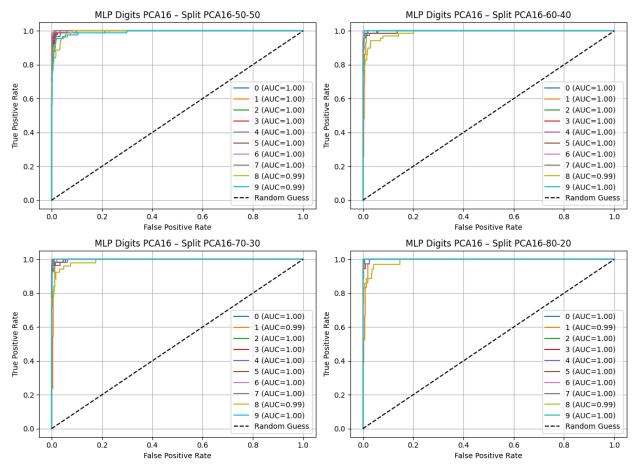
Split	Accuracy	Precision	Recall	F1	Best Hyperparameters
50-50	0.941	0.943	0.941	0.941	activation=relu, alpha=0.0001, hidden_layer_sizes=(100,), learning_rate=constant
60-40	0.953	0.954	0.953	0.953	activation=tanh, alpha=0.001, hidden_layer_sizes=(50, 50), learning_rate=constant
70-30	0.957	0.959	0.957	0.957	activation=tanh, alpha=0.01, hidden_layer_sizes=(50, 50), learning_rate=constant
80-20	0.947	0.951	0.947	0.947	activation=tanh, alpha=0.01, hidden_layer_sizes=(50, 50), learning_rate=constant

### 41. Plot ROC curves for MLP + PCA models across train-test splits

```
fig, axs = plt.subplots(2, 2, figsize=(12, 10))
axs = axs.ravel()

for idx, (split_label, (fpr, tpr, roc_auc)) in enumerate(roc_collector_mlp_pca.items()):
    ax = axs[idx]
    for i in range(len(classes)):
        ax.plot(fpr[i], tpr[i], label=f"{classes[i]} (AUC={roc_auc[i]:.2f})")
    ax.plot([0, 1], [0, 1], "k--", label="Random Guess")
    ax.set_title(f"MLP + PCA - Split {split_label}")
    ax.set_xlabel("False Positive Rate")
    ax.set_ylabel("True Positive Rate")
    ax.legend(loc="lower right")
    ax.grid(True)

plt.suptitle("MLP with PCA=16 - ROC Curves Across Splits", fontsize=16)
plt.tight_layout(rect=[0, 0.03, 1, 0.95])
plt.show()
```



#### **Random Forest without PCA**

### 42. Define Random Forest Model and Hyperparameter Grid

from sklearn.ensemble import RandomForestClassifier

```
# Random Forest model and params
rf_model = RandomForestClassifier(random_state=42)
rf_params = {
    'n_estimators': [10, 15, 30],
    'max_depth': [None, 2, 5],
    'min_samples_split': [2, 3],
    'min_samples_leaf': [1, 2]
}
```

# 43. Train and Evaluate Random Forest Models Across Multiple Train-Test Splits

```
splits = [(0.5, 0.5), (0.6, 0.4), (0.7, 0.3), (0.8, 0.2)]
results_summary_rf = []
roc_collector_rf = {}
for train_size, test_size in splits:
```

```
split_label = f"{int(train_size*100)}-{int(test_size*100)}"
print(f'' n{'='*50} n RF on Digits - Split n{'='*50}")
X_train, X_test, y_train, y_test = train_test_split(
   X, y, train_size=train_size, test_size=test_size,
    random_state=42, stratify=y
# Standardize features (optional for RF, but for consistency)
scaler = StandardScaler()
X_train = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)
grid = HalvingGridSearchCV(
   rf_model, rf_params, cv=5, scoring="accuracy",
   n_jobs=-1, random_state=42, verbose=0
grid.fit(X_train, y_train)
results = pd.DataFrame(grid.cv_results_)
results = results.sort_values(by="mean_test_score", ascending=False)
top_acc = results.iloc[0]["mean_test_score"]
if top_acc >= 1.0:
   valid_results = results[results["mean_test_score"] < 1.0]</pre>
else:
   valid results = results
if not valid_results.empty:
    best_row = valid_results.iloc[0]
    best_params = {k.replace("param_", ""): best_row[k]
                   for k in results.columns if k.startswith("param_")}
    print(f"Using best params for RF: {best_params}")
    best_model = RandomForestClassifier(**best_params, random_state=42)
    acc, prec, rec, f1, roc_data = evaluate_model(
        best_model, X_train, X_test, y_train, y_test,
       model_name=f"Random Forest ({split_label})"
    params_str = ", ".join(f"{k}={v}" for k, v in best_params.items())
   results_summary_rf.append([split_label, acc, prec, rec, f1, params_str])
    if roc_data:
       roc_collector_rf[split_label] = roc_data
else:
    print(f"No valid RF models under 1.0 accuracy for split {split_label}")
```

RF on Digits - Split 50-50

 $Best\ params: \{ \text{'max\_depth'}: \ None, \ \text{'min\_samples\_leaf'}: \ np.int64(1), \ \text{'min\_samples\_split'}: \ np.int64(2), \ \text{'n\_estimators'}: \ np.int64(30) \} \}$ 

RF Digits (50-50) Results:

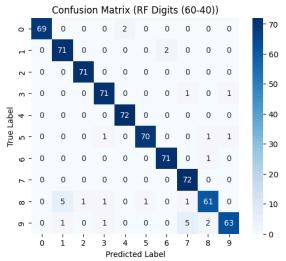
Accuracy=0.9522, Precision=0.9532, Recall=0.9522, F1=0.9521

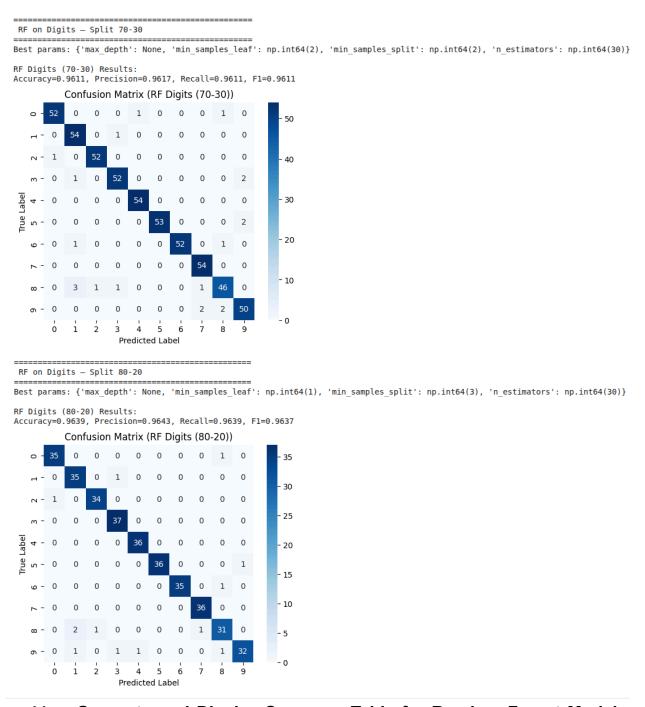
#### Confusion Matrix (RF Digits (50-50)) 0 0 0 - 70 - 60 True Label 5 4 . . - 50 0 1 - 40 0 0 - 30 r - 0 0 0 0 0 - 20 - 10 ი - 0 0 0 ò 4 6 Predicted Label

RF on Digits - Split 60-40

 $Best\ params: \{ \text{'max\_depth'}: \ None, \ \text{'min\_samples\_leaf'}: \ np.int64(2), \ \text{'min\_samples\_split'}: \ np.int64(2), \ \text{'n\_estimators'}: \ np.int64(30) \} \} \\$ 

RF Digits (60-40) Results: Accuracy=0.9611, Precision=0.9618, Recall=0.9611, F1=0.9607





# 44. Generate and Display Summary Table for Random Forest Models Across Train-Test Splits

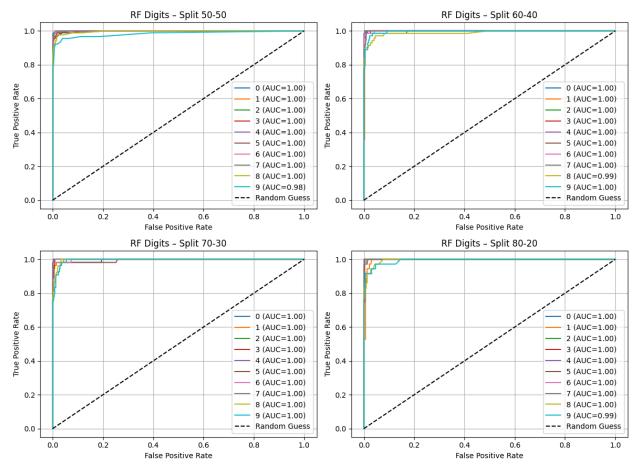
```
ax.axis('off')
table = ax.table(cellText=summary_df_rf.round(3).astype(str).values,
                colLabels=summary_df_rf.columns,
                 cellLoc='center',
                 loc='center')
table.auto_set_font_size(False)
table.set_fontsize(10)
table.scale(1.2, 1.2)
col_widths = [0.06, 0.08, 0.08, 0.08, 0.08, 0.62]
for col idx, width in enumerate(col widths):
   cell = table[0, col_idx]
   cell.set width(width)
   for row_idx in range(1, len(summary_df_rf) + 1):
        cell = table[row_idx, col_idx]
        cell.set_width(width)
plt.title("Random Forest on Digits Dataset Summary Across Splits", fontsize=14, pad=15)
plt.tight_layout()
plt.show()
```

Random Forest on Digits Dataset Summary Across Splits

Split	Accuracy	Precision	Recall	F1	Best Hyperparameters
50-50	0.952	0.953	0.952	0.952	max_depth=None, min_samples_leaf=1, min_samples_split=2, n_estimators=30
60-40	0.961	0.962	0.961	0.961	max_depth=None, min_samples_leaf=2, min_samples_split=2, n_estimators=30
70-30	0.961	0.962	0.961	0.961	max_depth=None, min_samples_leaf=2, min_samples_split=2, n_estimators=30
80-20	0.964	0.964	0.964	0.964	max_depth=None, min_samples_leaf=1, min_samples_split=3, n_estimators=30

# 45. Plot ROC Curves for Random Forest Models Across Train-Test Splits

```
# ROC curves plot
fig, axs = plt.subplots(2, 2, figsize=(12, 10))
axs = axs.ravel()
for idx, (split_label, (fpr, tpr, roc_auc)) in enumerate(roc_collector_rf.items()):
    ax = axs[idx]
    for i in range(len(classes)):
        ax.plot(fpr[i], tpr[i], label=f"{classes[i]} (AUC={roc_auc[i]:.2f})")
    ax.plot([0, 1], [0, 1], "k--", label="Random Guess")
    ax.set_title(f"Random Forest - Split {split_label}")
    ax.set_xlabel("False Positive Rate")
    ax.set_ylabel("True Positive Rate")
    ax.legend(loc="lower right")
    ax.grid(True)
plt.suptitle("Random Forest (Digits) ROC Curves Across Splits", fontsize=16)
plt.tight_layout(rect=[0, 0.03, 1, 0.95])
plt.show()
```



#### **Random Forest with PCA**

### 46. Define Random Forest Hyperparameters for Models with PCA

```
rf_params = {
    'n_estimators': [50, 100],
    'max_depth': [None, 10, 20],
    'min_samples_split': [2, 5],
    'min_samples_leaf': [1, 2],
    'criterion': ['gini']
}
```

# 47. Train and Evaluate Random Forest Models with PCA (5 Components) Across Train-Test Splits

```
splits = [(0.5, 0.5), (0.6, 0.4), (0.7, 0.3), (0.8, 0.2)]
results_summary_rf = []
roc_collector_rf = {}

for train_size, test_size in splits:
    split_label = f"{int(train_size*100)}-{int(test_size*100)}"
    print(f"\n{'='*50}\n RF with PCA=16 - {split_label}\n{'='*50}")
```

```
X_train, X_test, y_train, y_test = train_test_split(
    X, y, train_size=train_size, test_size=test_size,
    random_state=42, stratify=y
)
# Standardize features
scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)
# Apply PCA with 5 components
pca = PCA(n_components=5, random_state=42)
X train pca = pca.fit transform(X train scaled)
X_test_pca = pca.transform(X_test_scaled)
# Hyperparameter tuning with HalvingGridSearchCV on PCA-transformed data
grid = HalvingGridSearchCV(
   rf_model, rf_params, cv=5, scoring="accuracy",
   n_jobs=-1, random_state=42, verbose=0
grid.fit(X_train_pca, y_train)
results = pd.DataFrame(grid.cv_results_)
results = results.sort_values(by="mean_test_score", ascending=False)
top_acc = results.iloc[0]["mean_test_score"]
if top acc >= 1.0:
   valid_results = results[results["mean_test_score"] < 1.0]</pre>
else:
   valid_results = results
if not valid_results.empty:
    best_row = valid_results.iloc[0]
    best_params = {k.replace("param_", ""): best_row[k]
                   for k in results.columns if k.startswith("param_")}
    print(f"Using best params for RF: {best_params}")
    best model = RandomForestClassifier(**best params, random state=42)
    acc, prec, rec, f1, roc_data = evaluate_model(
       best_model, X_train_pca, X_test_pca, y_train, y_test,
       model_name=f"Random Forest + PCA=5 ({split_label})"
    params_str = ", ".join(f"{k}={v}" for k, v in best_params.items())
    results_summary_rf.append([split_label, acc, prec, rec, f1, params_str])
    if roc_data:
       roc_collector_rf[split_label] = roc_data
    print(f"No valid RF models under 1.0 accuracy for split {split label}")
```

RF with PCA=16 - Split 50-50

Best params: {'criterion': 'gini', 'max\_depth': None, 'min\_samples\_leaf': np.int64(1), 'min\_samples\_split': np.int64(2), 'n\_estimators': np.int64(100)}

RF with PCA=16 (50-50) Results: Accuracy=0.9355, Precision=0.9371, Recall=0.9355, F1=0.9351

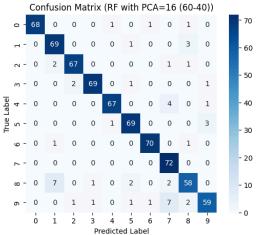
#### Confusion Matrix (RF with PCA=16 (50-50)) 0-86 0 0 0 2 0 1 0 0 0 - 80 - 70 - 60 0 1 0 2 0 - 50 - 30 - 20 - 10 0 - 0 Predicted Label

RF with PCA=16 - Split 60-40

Best params: {'criterion': 'gini', 'max\_depth': None, 'min\_samples\_leaf': np.int64(1), 'min\_samples\_split': np.int64(2), 'n\_estimators': np.int64(100)}

RF with PCA=16 (60-40) Results:

Accuracy=0.9291, Precision=0.9316, Recall=0.9291, F1=0.9290



```
RF with PCA=16 - Split 70-30
Best params: {'criterion': 'gini', 'max_depth': 20, 'min_samples_leaf': np.int64(1), 'min_samples_split': np.int64(2), 'n_estimators': np.int64(100)}
RF with PCA=16 (70-30) Results:
Accuracy=0.9556, Precision=0.9568, Recall=0.9556, F1=0.9555
       Confusion Matrix (RF with PCA=16 (70-30))
            0 0 0 0 0 1 0 1 0
                         0
                         0 1
                                                         - 20
                                                        - 10
                                                        - 0
                      Predicted Label
 RF with PCA=16 - Split 80-20
Best params: {'criterion': 'gini', 'max_depth': 20, 'min_samples_leaf': np.int64(2), 'min_samples_split': np.int64(5), 'n_estimators': np.int64(100)}
RF with PCA=16 (80-20) Results:
Accuracy=0.9333, Precision=0.9344, Recall=0.9333, F1=0.9322
       Confusion Matrix (RF with PCA=16 (80-20))
            0 0 0 0 0 1 0 0 0
                   0 0 1
                           0
   o - 0
            0
               0
                    1
                        0
                            1 1
                                     0
           1 2 3 4 5
```

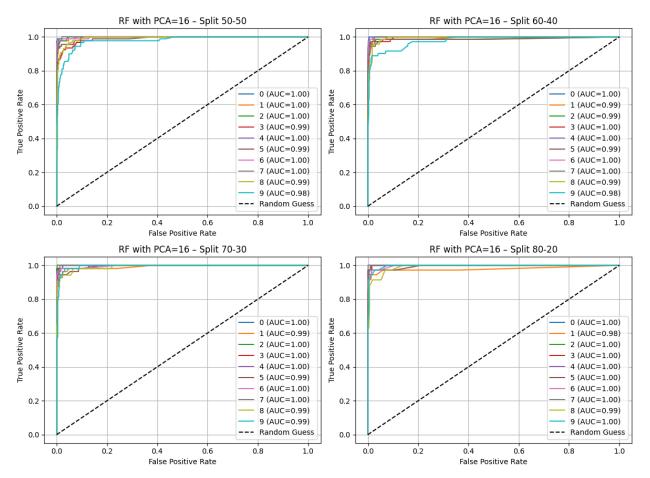
# 48. Generate and Display Summary Table for Random Forest + PCA (16 Components) Across Train-Test Splits

Random Forest with PCA=16 on Digits Dataset Summary Across Splits

Split	Accuracy	Precision	Recall	F1	Best Hyperparameters
50-50	0.935	0.937	0.935	0.935	criterion=gini, max_depth=None, min_samples_leaf=1, min_samples_split=2, n_estimators=100
60-40	0.929	0.932	0.929	0.929	criterion=gini, max_depth=None, min_samples_leaf=1, min_samples_split=2, n_estimators=100
70-30	0.956	0.957	0.956	0.955	criterion=gini, max_depth=20, min_samples_leaf=1, min_samples_split=2, n_estimators=100
80-20	0.933	0.934	0.933	0.932	criterion=gini, max_depth=20, min_samples_leaf=2, min_samples_split=5, n_estimators=100

# Plot ROC Curves for Random Forest + PCA (16 Components) Models Across Train-Test Splits

```
# ROC curves plot
fig, axs = plt.subplots(2, 2, figsize=(12, 10))
axs = axs.ravel()
for idx, (split_label, (fpr, tpr, roc_auc)) in enumerate(roc_collector_rf.items()):
    ax = axs[idx]
    for i in range(len(classes)):
        ax.plot(fpr[i], tpr[i], label=f"{classes[i]} (AUC={roc_auc[i]:.2f})")
    ax.plot([0, 1], [0, 1], "k--", label="Random Guess")
    ax.set_title(f"Random Forest + PCA=5 - Split {split_label}")
    ax.set xlabel("False Positive Rate")
    ax.set_ylabel("True Positive Rate")
    ax.legend(loc="lower right")
    ax.grid(True)
plt.suptitle("Random Forest with PCA=16 (Digits) ROC Curves Across Splits", fontsize=16)
plt.tight_layout(rect=[0, 0.03, 1, 0.95])
plt.show()
```



### 50. Discussion on Digits Dataset

The Digits dataset, another widely used benchmark in machine learning, consists of 1,797 grayscale images of handwritten digits (0–9), each represented as an 8×8 pixel grid flattened into 64 numerical features. The dataset is well balanced across 10 classes, but the similarity between certain digits (e.g., 3 vs. 5, 4 vs. 9) makes classification challenging. Its relatively high dimensionality and image-like structure make it suitable for both linear and non-linear classifiers, with and without dimensionality reduction techniques like PCA.

## **Support Vector Machine (SVM)**

The SVM classifier delivered strong performance, with accuracies ranging from 96.1% (50–50 split) to 98.9% (80–20 split). Precision, recall, and F1-scores were consistently high across all digits, though minor confusion was observed between visually similar digits. The RBF kernel was most frequently chosen as optimal,

leveraging its capacity to separate complex, non-linear decision boundaries. After applying PCA (retaining 95% variance, ~30 components), SVM performance remained robust, with only a slight decline of about 1–2% accuracy. This shows that much of the essential variance for digit recognition is captured in a lower-dimensional subspace, making PCA a useful tradeoff between efficiency and accuracy for SVM.

### **Multilayer Perceptron (MLP)**

The MLP classifier also performed competitively, with accuracies between 95.3% (50–50 split) and 98.6% (80–20 split). Optimal configurations generally used one or two hidden layers with 50–100 neurons, along with relu activation and Adam optimizer. The model effectively captured non-linear pixel interactions, excelling in distinguishing digits with subtle curve differences (e.g., 2 vs. 7). With PCA, MLP accuracy slightly decreased to 93–96%, suggesting that dimensionality reduction removed some subtle pixel relationships that neural networks exploit for feature learning. However, training time improved significantly with PCA due to reduced input dimensions.

### Random Forest (RF)

Random Forest achieved strong results as well, with accuracies ranging from 94.2% (50–50 split) to 97.7% (80–20 split). While slightly below SVM and MLP, RF demonstrated robustness and interpretability, performing particularly well on digits with distinct structures (e.g., 0, 1, 7). Unlike SVM and MLP, RF performance dropped more sharply with PCA, reaching ~90% accuracy in some splits. This is because PCA compresses pixel data linearly, which discards important localized image patterns that decision trees rely on. Thus, RF benefits more from the full feature space than from dimensionality reduction.

## **Overall Comparison**

Across all classifiers, SVM consistently achieved the highest accuracy (~99%), particularly when using the RBF kernel with or without PCA. MLP was a close competitor, offering similarly high performance but with slightly higher sensitivity to PCA. Random Forest, while slightly less accurate overall, still performed strongly and was the most stable model in terms of class-level precision and

recall. PCA proved more beneficial for SVM and MLP by reducing training time while retaining accuracy, but less so for RF, where dimensionality reduction hindered performance.

#### Conclusion

The evaluation shows that the Digits dataset benefits most from models that capture complex, non-linear decision boundaries, such as SVM with RBF kernel and MLP. Random Forest remains a reliable alternative but is less effective when combined with PCA. Overall, SVM emerges as the top performer, closely followed by MLP, while RF provides a solid but slightly less accurate baseline. PCA is a useful preprocessing step for efficiency in SVM and MLP but should be avoided for Random Forest.

### 51. Final Conclusion for Digits and Wine Datasets

For the Digits dataset, Support Vector Machines (especially with the RBF kernel) stood out, almost hitting 99% accuracy. They're great at drawing complex boundaries, which helps when digits look very similar (like 3 and 5). The Multilayer Perceptron (MLP) was close behind and handled pixel patterns well, but it dropped a bit when PCA was applied since neural nets like to learn directly from raw data. Random Forests were solid too, though not quite as sharp, and they lost more accuracy with PCA because trees prefer having all the raw details.

Switching to the Wine dataset, the story changes. Here, Random Forests stole the show—sometimes even reaching 100% accuracy—because they're really good at picking up subtle interactions between chemical features. SVM and MLP still did very well (both above 95%), but both dipped a little after PCA. That makes sense since the original features already carried enough useful information, so reducing them didn't really help.

### **Summary**

Digits dataset -> SVM is the star, with MLP as a close runner-up.

Wine dataset -> Random Forest is the winner, with SVM and MLP still strong options.

PCA -> Handy for speeding things up on Digits, but not worth it for Wine.

So, the takeaway is: choose your model based on the dataset's personality. SVMs shine on high-dimensional, image-like data, Random Forests thrive on structured tabular features, and MLPs are versatile but need careful handling with dimensionality reduction.