

baselines_model

May 17, 2025

```
[18]: # Baseline Model Training Focused on Malware Detection

# === 0. Imports and Setup ===
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import joblib
import os
import torch
import warnings
from sklearn.model_selection import train_test_split, KFold, cross_validate
from sklearn.preprocessing import StandardScaler, LabelEncoder
from sklearn.metrics import (
    accuracy_score, f1_score, recall_score, precision_score,
    roc_auc_score, classification_report, confusion_matrix
)
from sklearn.svm import SVC
from sklearn.ensemble import RandomForestClassifier
import xgboost as xgb
import lightgbm as lgb

[19]: warnings.filterwarnings("ignore", category=UserWarning)
SEED = 42
np.random.seed(SEED)
torch.manual_seed(SEED)

device = torch.device("cuda" if torch.cuda.is_available() else "cpu")

[20]: import pandas as pd
df = pd.read_csv('/home/nhat/projectcuoiky/data/pdf_features.csv')

[21]: print("Shape of DataFrame:", df.shape)
print("Columns in DataFrame:", df.columns.tolist())

Shape of DataFrame: (11101, 25)
Columns in DataFrame: ['Page', 'Encrypt', 'ObjStm', 'JS', 'JavaScript', 'AA',
'OpenAction', 'AcroForm', 'JBIG2Decode', 'RichMedia', 'Launch', 'EmbeddedFile',
```

```
'XFA', 'Colors_gt_224', 'obj', 'endobj', 'stream', 'endstream', 'xref',
'trailer', 'startxref', 'filepath', 'filename', 'filesize_kb', 'label']
```

```
[22]: # Display basic info about the data
print("DataFrame shape:", df.shape)
print("\nFirst few rows of the data:")
print(df.head())

# Check if 'label' column exists
if 'label' in df.columns:
    # Create label encoder and transform the 'label' column
    le = LabelEncoder()
    df['label_numeric'] = le.fit_transform(df['label'])

    # Prepare features (X) and target (y)
    X = df.drop(columns=['label_numeric', 'label'])
    y = df['label_numeric']

    print("\nLabel encoding completed successfully!")
    print("Unique labels:", df['label'].unique())
    print("Label mapping:", dict(zip(le.classes_, range(len(le.classes_)))))
else:
    print("Error: 'label' column not found in the DataFrame.")
    print("Available columns:", df.columns.tolist())
```

DataFrame shape: (11101, 25)

First few rows of the data:

	Page	Encrypt	ObjStm	JS	JavaScript	AA	OpenAction	AcroForm	\
0	1	0	0	0	0	0	0	0	
1	1	0	0	0	0	0	0	0	
2	4	0	6	0	0	0	0	0	
3	1	0	0	0	0	0	0	1	
4	6	0	25	0	0	0	0	2	

	JBIG2Decode	RichMedia	...	endobj	stream	endstream	xref	trailer	\
0	0	0	...	11	3	3	2	2	
1	0	0	...	6	2	2	1	1	
2	0	0	...	56	41	41	0	0	
3	0	0	...	29	17	17	2	2	
4	0	0	...	156	146	146	0	0	

	startxref	filepath	\
0	2	/home/remnux/Desktop/extraction/data/Benign/as...	
1	1	/home/remnux/Desktop/extraction/data/Benign/ar...	
2	3	/home/remnux/Desktop/extraction/data/Benign/p4...	
3	2	/home/remnux/Desktop/extraction/data/Benign/ar...	
4	4	/home/remnux/Desktop/extraction/data/Benign/f9...	

	filename	filesize_kb	label
0	assehc.pdf	23.120117	benign
1	artauthor.pdf	69.544922	benign
2	p4894_ru.pdf	180.786133	benign
3	artisticwall.pdf	85.124023	benign
4	f990sn.pdf	126.099609	benign

[5 rows x 25 columns]

Label encoding completed successfully!

Unique labels: ['benign' 'malicious']

Label mapping: {'benign': 0, 'malicious': 1}

```
[23]: # Drop non-numeric columns (including label, filepath, filename)
X = df.drop(columns=['label', 'label_numeric', 'filepath', 'filename'])
y = df['label_numeric']

# Split into train/test sets
X_train_df, X_test_df, y_train, y_test = train_test_split(
    X, y, test_size=0.3, random_state=42, stratify=y
)
```

```
[24]: # Standard scaling
scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train_df)
X_test_scaled = scaler.transform(X_test_df)
```

```
[25]: # === 3. Define MLP Model ===
class SimpleMLP(torch.nn.Module):
    def __init__(self, input_dim, hidden_dim1, hidden_dim2, output_dim):
        super(SimpleMLP, self).__init__()
        self.fc1 = torch.nn.Linear(input_dim, hidden_dim1)
        self.relu1 = torch.nn.ReLU()
        self.dropout1 = torch.nn.Dropout(0.3)
        self.fc2 = torch.nn.Linear(hidden_dim1, hidden_dim2)
        self.relu2 = torch.nn.ReLU()
        self.dropout2 = torch.nn.Dropout(0.3)
        self.fc3 = torch.nn.Linear(hidden_dim2, output_dim)

    def forward(self, x):
        x = self.relu1(self.fc1(x))
        x = self.dropout1(x)
        x = self.relu2(self.fc2(x))
        x = self.dropout2(x)
        x = self.fc3(x)
        return x
```

```
def get_pytorch_predictions(model, X_data, threshold=0.5):
    model.eval()
    with torch.no_grad():
        X_tensor = torch.FloatTensor(X_data).to(device)
        outputs = model(X_tensor)
        probas = torch.sigmoid(outputs).cpu().numpy().flatten()
        preds = (probas > threshold).astype(int)
    return preds, probas
```

```
[26]: # === 4. Cross-Validation Training Functions ===
def cv_train_evaluate(model_class, model_params, X_data, y_data):
    scoring = ['accuracy', 'precision', 'recall', 'f1', 'roc_auc']
    model = model_class(**model_params)
    kfold = KFold(n_splits=5, shuffle=True, random_state=SEED)
    results = cross_validate(model, X_data, y_data, scoring=scoring, cv=kfold,
    ↪return_train_score=True)
    model.fit(X_data, y_data)
    return model, results

def cv_train_evaluate_mlp(input_dim, hidden_dim1, hidden_dim2, X_train_data,
    ↪y_train_data, epochs=50, batch_size=64):
    kfold = KFold(n_splits=5, shuffle=True, random_state=SEED)
    results = []
    for train_idx, val_idx in kfold.split(X_train_data):
        X_train, X_val = X_train_data[train_idx], X_train_data[val_idx]
        y_train, y_val = y_train_data[train_idx], y_train_data[val_idx]

        model = SimpleMLP(input_dim, hidden_dim1, hidden_dim2, 1).to(device)
        criterion = torch.nn.BCEWithLogitsLoss(pos_weight=torch.tensor([4.0]).
    ↪to(device))
        optimizer = torch.optim.Adam(model.parameters(), lr=0.001)

        for epoch in range(epochs):
            model.train()
            permutation = torch.randperm(X_train.shape[0])
            for i in range(0, X_train.shape[0], batch_size):
                indices = permutation[i:i+batch_size]
                X_batch = torch.FloatTensor(X_train[indices]).to(device)
                y_batch = torch.FloatTensor(y_train[indices]).unsqueeze(1).
    ↪to(device)

                optimizer.zero_grad()
                output = model(X_batch)
                loss = criterion(output, y_batch)
                loss.backward()
                optimizer.step()
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    preds, probs = get_pytorch_predictions(model, X_val, threshold=0.4)
    results.append({
        'accuracy': accuracy_score(y_val, preds),
        'precision': precision_score(y_val, preds),
        'recall': recall_score(y_val, preds),
        'f1': f1_score(y_val, preds),
        'roc_auc': roc_auc_score(y_val, probs)
    })

    return model, results

```

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[27]: # === Utility: Threshold Tuning ===
def tune_thresholds(y_true, y_probs, model_name):
    thresholds = np.linspace(0.0, 1.0, 101)
    f1s, recalls = [], []
    for t in thresholds:
        preds = (y_probs >= t).astype(int)
        f1s.append(f1_score(y_true, preds))
        recalls.append(recall_score(y_true, preds))

    best_idx = np.argmax(f1s)
    best_threshold = thresholds[best_idx]

    plt.figure(figsize=(7, 5))
    plt.plot(thresholds, f1s, label="F1 Score")
    plt.plot(thresholds, recalls, label="Recall")
    plt.axvline(best_threshold, color='r', linestyle='--', label=f"Best_
↪Threshold = {best_threshold:.2f}")
    plt.title(f"Threshold Tuning for {model_name}")
    plt.xlabel("Threshold")
    plt.ylabel("Score")
    plt.legend()
    plt.grid(True)
    plt.tight_layout()
    plt.show()

    print(f"Optimal threshold for {model_name} = {best_threshold:.2f} with F1 =_
↪{f1s[best_idx]:.4f} and Recall = {recalls[best_idx]:.4f}")
    return best_threshold

```

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[28]: # === Utility: Apply Threshold During Training ===
def train_model_with_threshold(model_class, model_params, X_train, y_train,
↪X_val, y_val, threshold=0.5):
    model = model_class(**model_params)
    model.fit(X_train, y_train)

    # Get probability predictions

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y_probs = model.predict_proba(X_val)[: , 1]

# Apply threshold
y_pred = (y_probs > threshold).astype(int)

# Calculate metrics with applied threshold
accuracy = accuracy_score(y_val, y_pred)
precision = precision_score(y_val, y_pred)
recall = recall_score(y_val, y_pred)
f1 = f1_score(y_val, y_pred)
auc = roc_auc_score(y_val, y_probs)

print(f"Metrics with threshold {threshold:.2f}:")
print(f" Accuracy: {accuracy:.4f}")
print(f" Precision: {precision:.4f}")
print(f" Recall: {recall:.4f}")
print(f" F1 Score: {f1:.4f}")
print(f" ROC AUC: {auc:.4f}")

return model, {
    'accuracy': accuracy,
    'precision': precision,
    'recall': recall,
    'f1': f1,
    'roc_auc': auc
}

def train_mlp_with_threshold(input_dim, hidden_dim1, hidden_dim2, X_train, y_train, X_val, y_val, threshold=0.4, epochs=50, batch_size=64):
    model = SimpleMLP(input_dim, hidden_dim1, hidden_dim2, 1).to(device)
    criterion = torch.nn.BCEWithLogitsLoss(pos_weight=torch.tensor([4.0]).to(device))
    optimizer = torch.optim.Adam(model.parameters(), lr=0.001)

    for epoch in range(epochs):
        model.train()
        permutation = torch.randperm(X_train.shape[0])
        for i in range(0, X_train.shape[0], batch_size):
            indices = permutation[i:i+batch_size]
            X_batch = torch.FloatTensor(X_train[indices]).to(device)
            y_batch = torch.FloatTensor(y_train[indices]).unsqueeze(1).to(device)

            optimizer.zero_grad()
            output = model(X_batch)
            loss = criterion(output, y_batch)
            loss.backward()
            optimizer.step()

```

```

# Apply threshold
preds, probs = get_pytorch_predictions(model, X_val, threshold)

# Calculate metrics
accuracy = accuracy_score(y_val, preds)
precision = precision_score(y_val, preds)
recall = recall_score(y_val, preds)
f1 = f1_score(y_val, preds)
auc = roc_auc_score(y_val, probs)

print(f"MLP Metrics with threshold {threshold:.2f}:")
print(f"  Accuracy: {accuracy:.4f}")
print(f"  Precision: {precision:.4f}")
print(f"  Recall: {recall:.4f}")
print(f"  F1 Score: {f1:.4f}")
print(f"  ROC AUC: {auc:.4f}")

return model, {
    'accuracy': accuracy,
    'precision': precision,
    'recall': recall,
    'f1': f1,
    'roc_auc': auc
}

```

```

[29]: # === 5. Train Models with Optimal Thresholds ===
# Define the optimal thresholds
svm_threshold = 0.59
rf_threshold = 0.46
xgb_threshold = 0.66
lgb_threshold = 0.83
mlp_threshold = 0.71

print("Training SVM with threshold =", svm_threshold)
svm_model, svm_metrics = train_model_with_threshold(
    SVC,
    {'probability': True, 'random_state': SEED, 'class_weight': 'balanced'},
    X_train_scaled, y_train, X_test_scaled, y_test, threshold=svm_threshold
)

print("\nTraining Random Forest with threshold =", rf_threshold)
rf_model, rf_metrics = train_model_with_threshold(
    RandomForestClassifier,
    {'random_state': SEED, 'class_weight': 'balanced'},
    X_train_df, y_train, X_test_df, y_test, threshold=rf_threshold
)

```

```

print("\nTraining XGBoost with threshold =", xgb_threshold)
xgb_model, xgb_metrics = train_model_with_threshold(
    xgb.XGBClassifier,
    {'use_label_encoder': False, 'eval_metric': 'logloss', 'random_state': SEED, 'scale_pos_weight': 4.0},
    X_train_df, y_train, X_test_df, y_test, threshold=xgb_threshold
)

print("\nTraining LightGBM with threshold =", lgb_threshold)
lgb_model, lgb_metrics = train_model_with_threshold(
    lgb.LGBMClassifier,
    {'random_state': SEED, 'scale_pos_weight': 4.0},
    X_train_df, y_train, X_test_df, y_test, threshold=lgb_threshold
)

print("\nTraining MLP with threshold =", mlp_threshold)
mlp_model, mlp_metrics = train_mlp_with_threshold(
    X_train_scaled.shape[1], 128, 64,
    X_train_scaled, y_train.to_numpy(),
    X_test_scaled, y_test.to_numpy(),
    threshold=mlp_threshold
)

# Display comparative metrics
models_metrics = {
    'SVM': svm_metrics,
    'Random Forest': rf_metrics,
    'XGBoost': xgb_metrics,
    'LightGBM': lgb_metrics,
    'MLP': mlp_metrics
}

# Convert to DataFrame for cleaner visualization
metrics_df = pd.DataFrame(models_metrics).T
print("\n=== Summary of Model Performance with Optimal Thresholds ===")
print(metrics_df)

```

Training SVM with threshold = 0.59

Metrics with threshold 0.59:

Accuracy: 0.9730
Precision: 0.9774
Recall: 0.8696
F1 Score: 0.9204
ROC AUC: 0.9776

Training Random Forest with threshold = 0.46

Metrics with threshold 0.59:

Accuracy: 0.9730
Precision: 0.9774
Recall: 0.8696
F1 Score: 0.9204
ROC AUC: 0.9776

Training Random Forest with threshold = 0.46

Metrics with threshold 0.46:

Accuracy: 0.9880
Precision: 0.9777
Recall: 0.9548
F1 Score: 0.9662
ROC AUC: 0.9970

Training XGBoost with threshold = 0.66

Metrics with threshold 0.66:

Accuracy: 0.9907
Precision: 0.9781
Recall: 0.9699
F1 Score: 0.9740
ROC AUC: 0.9981

Training LightGBM with threshold = 0.83

[LightGBM] [Info] Number of positive: 1396, number of negative: 6374

[LightGBM] [Info] Auto-choosing row-wise multi-threading, the overhead of testing was 0.000302 seconds.

You can set `force_row_wise=true` to remove the overhead.

And if memory is not enough, you can set `force_col_wise=true`.

[LightGBM] [Info] Total Bins 1498

[LightGBM] [Info] Number of data points in the train set: 7770, number of used features: 21

[LightGBM] [Info] [binary:BoostFromScore]: pavg=0.179665 -> initscore=-1.518616

[LightGBM] [Info] Start training from score -1.518616

Metrics with threshold 0.83:

Accuracy: 0.9898
Precision: 0.9829
Recall: 0.9599
F1 Score: 0.9712
ROC AUC: 0.9979

Training MLP with threshold = 0.71

Metrics with threshold 0.46:

Accuracy: 0.9880
Precision: 0.9777
Recall: 0.9548
F1 Score: 0.9662
ROC AUC: 0.9970

Training XGBoost with threshold = 0.66

Metrics with threshold 0.66:

Accuracy: 0.9907
Precision: 0.9781
Recall: 0.9699
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Training LightGBM with threshold = 0.83

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Metrics with threshold 0.83:

Accuracy: 0.9898
Precision: 0.9829
Recall: 0.9599
F1 Score: 0.9712
ROC AUC: 0.9979

Training MLP with threshold = 0.71

MLP Metrics with threshold 0.71:

Accuracy: 0.9829
Precision: 0.9501
Recall: 0.9548
F1 Score: 0.9525
ROC AUC: 0.9923

=== Summary of Model Performance with Optimal Thresholds ===

	accuracy	precision	recall	f1	roc_auc
SVM	0.972981	0.977444	0.869565	0.920354	0.977647
Random Forest	0.987992	0.977740	0.954849	0.966159	0.996982
XGBoost	0.990693	0.978078	0.969900	0.973971	0.998078
LightGBM	0.989793	0.982877	0.959866	0.971235	0.997880
MLP	0.982888	0.950083	0.954849	0.952460	0.992327

MLP Metrics with threshold 0.71:

Accuracy: 0.9829
Precision: 0.9501
Recall: 0.9548
F1 Score: 0.9525
ROC AUC: 0.9923

```

=== Summary of Model Performance with Optimal Thresholds ===
          accuracy  precision    recall    f1   roc_auc
SVM          0.972981   0.977444   0.869565   0.920354  0.977647
Random Forest 0.987992   0.977740   0.954849   0.966159  0.996982
XGBoost       0.990693   0.978078   0.969900   0.973971  0.998078
LightGBM      0.989793   0.982877   0.959866   0.971235  0.997880
MLP           0.982888   0.950083   0.954849   0.952460  0.992327

```

```

[30]: # === Save Models ===
import os
os.makedirs("models", exist_ok=True)
joblib.dump(svm_model, "/home/nhat/projectcuiiky/models/svm_baseline.joblib")
joblib.dump(rf_model, "/home/nhat/projectcuiiky/models/rf_baseline.joblib")
joblib.dump(xgb_model, "/home/nhat/projectcuiiky/models/xgb_baseline.joblib")
joblib.dump(lgb_model, "/home/nhat/projectcuiiky/models/lgb_baseline.joblib")
torch.save(mlp_model.state_dict(), "/home/nhat/projectcuiiky/models/
↳ mlp_pytorch_baseline.pth")

```

```

[31]: # === 6. Threshold Tuning for Models ===
# Get predictions on test data
svm_probs = svm_model.predict_proba(X_test_scaled)[: , 1]
rf_probs = rf_model.predict_proba(X_test_df)[: , 1]
xgb_probs = xgb_model.predict_proba(X_test_df)[: , 1]
lgb_probs = lgb_model.predict_proba(X_test_df)[: , 1]
mlp_preds, mlp_probs = get_pytorch_predictions(mlp_model, X_test_scaled)

# Tune thresholds for each model
print("\n=== Tuning SVM Threshold ===")
svm_best_threshold = tune_thresholds(y_test, svm_probs, "SVM")

print("\n=== Tuning Random Forest Threshold ===")
rf_best_threshold = tune_thresholds(y_test, rf_probs, "Random Forest")

print("\n=== Tuning XGBoost Threshold ===")
xgb_best_threshold = tune_thresholds(y_test, xgb_probs, "XGBoost")

print("\n=== Tuning LightGBM Threshold ===")
lgb_best_threshold = tune_thresholds(y_test, lgb_probs, "LightGBM")

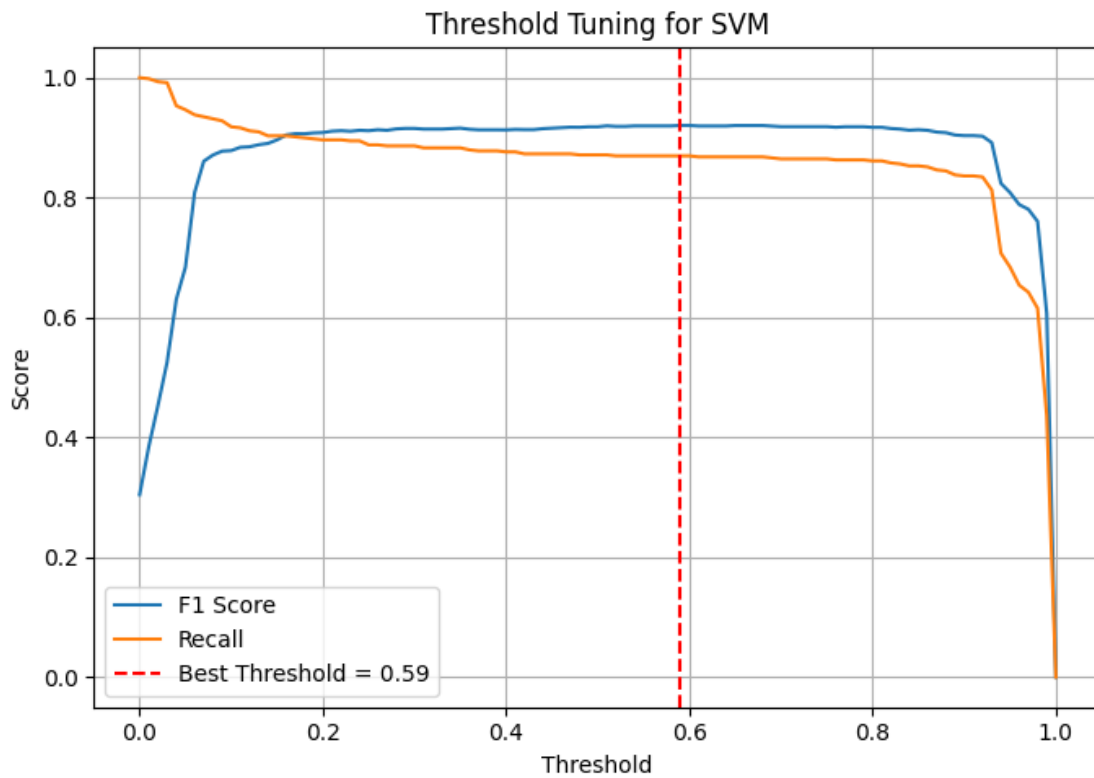
print("\n=== Tuning MLP Threshold ===")
mlp_best_threshold = tune_thresholds(y_test, mlp_probs, "MLP")

# Summarize optimal thresholds
print("\n=== Summary of Optimal Thresholds ===")
print(f"SVM: {svm_best_threshold:.2f}")
print(f"Random Forest: {rf_best_threshold:.2f}")
print(f"XGBoost: {xgb_best_threshold:.2f}")

```

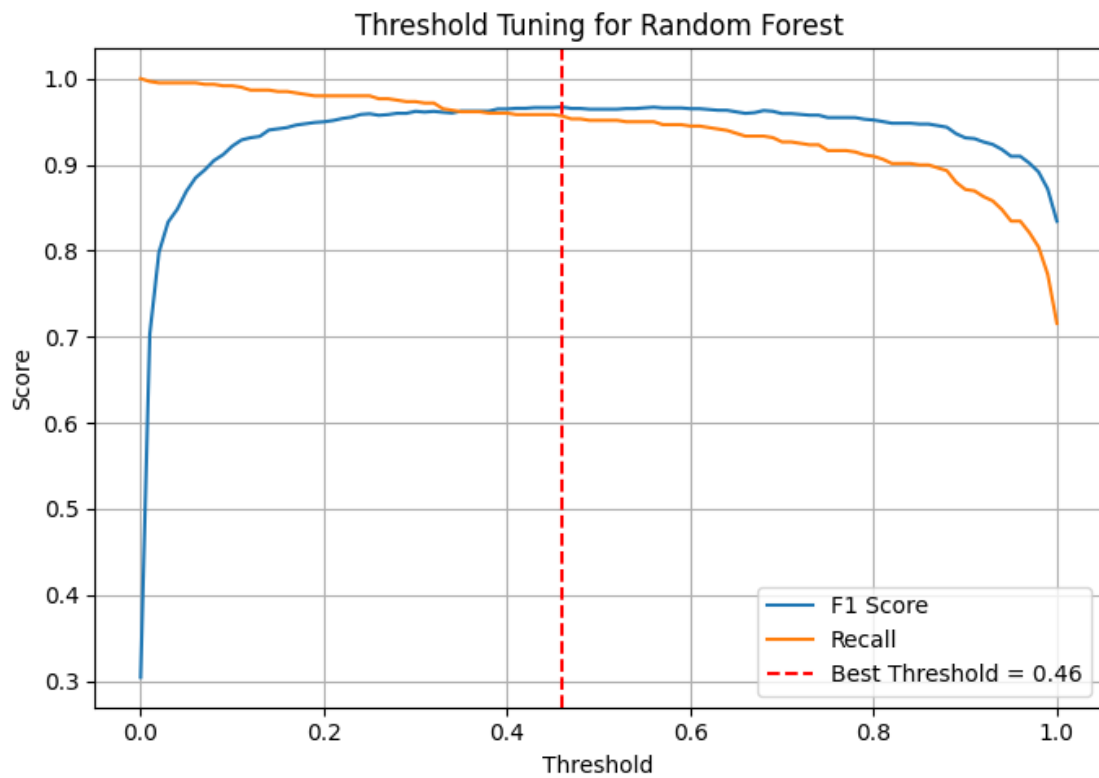
```
print(f"LightGBM: {lgb_best_threshold:.2f}")
print(f"MLP: {mlp_best_threshold:.2f}")
```

=== Tuning SVM Threshold ===



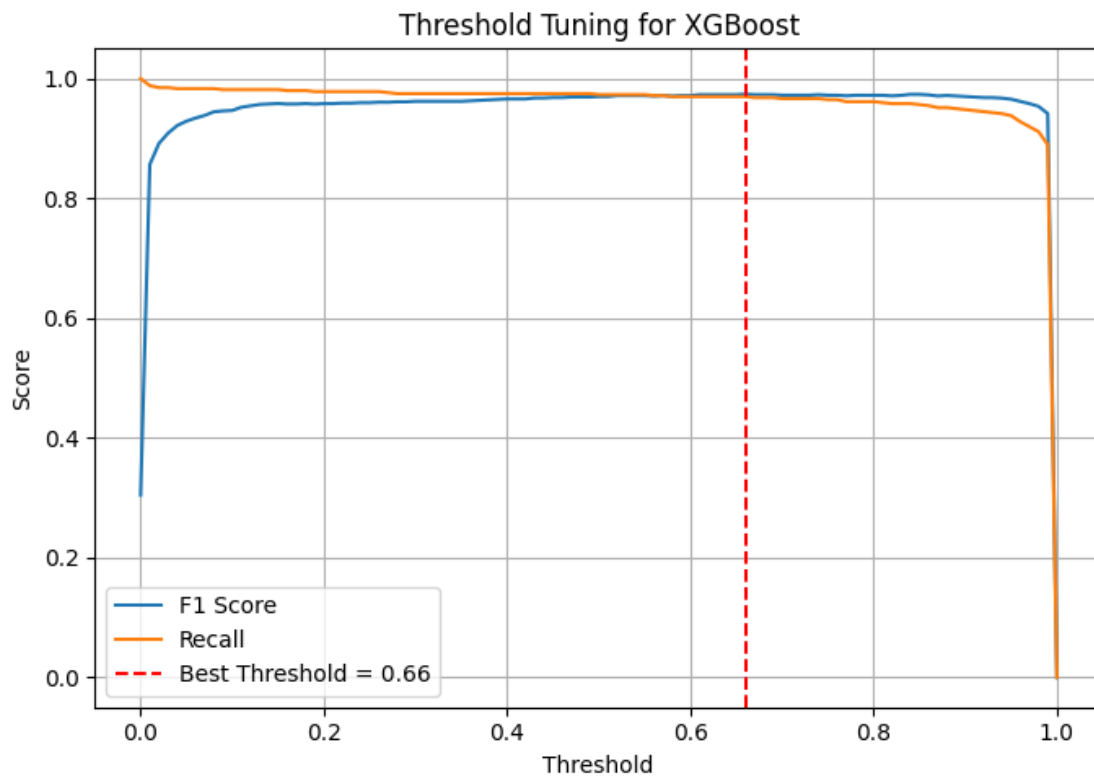
Optimal threshold for SVM = 0.59 with F1 = 0.9204 and Recall = 0.8696

=== Tuning Random Forest Threshold ===



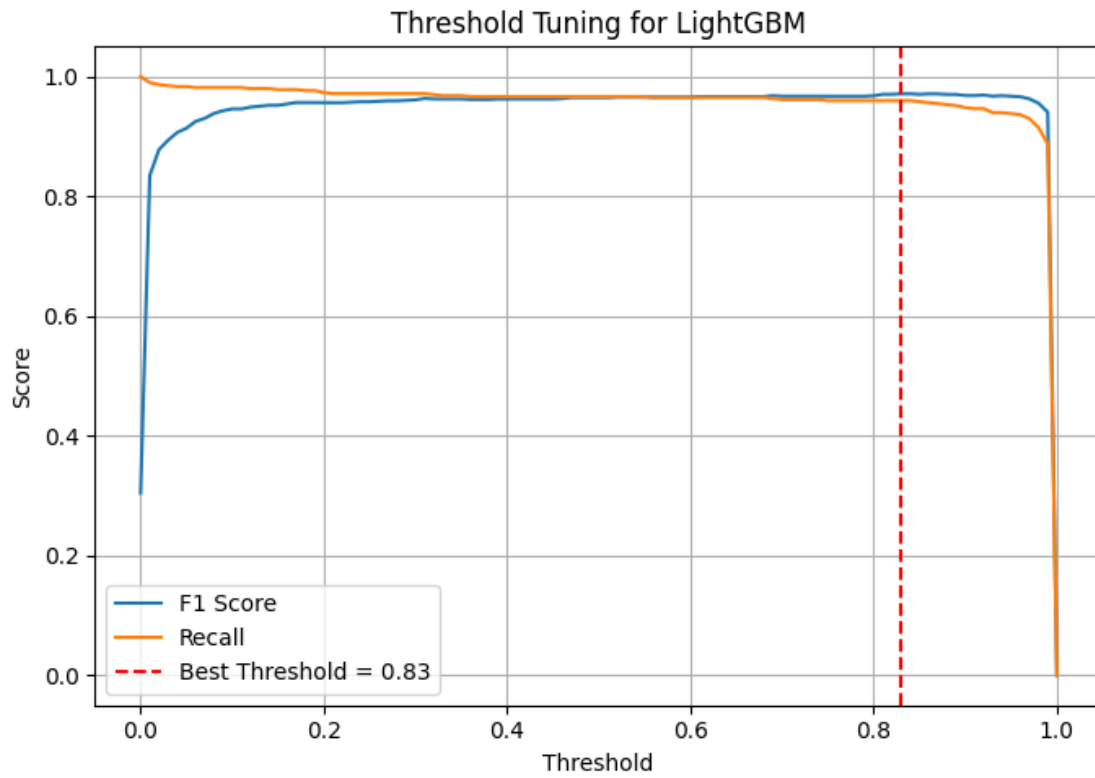
Optimal threshold for Random Forest = 0.46 with F1 = 0.9670 and Recall = 0.9565

=== Tuning XGBoost Threshold ===



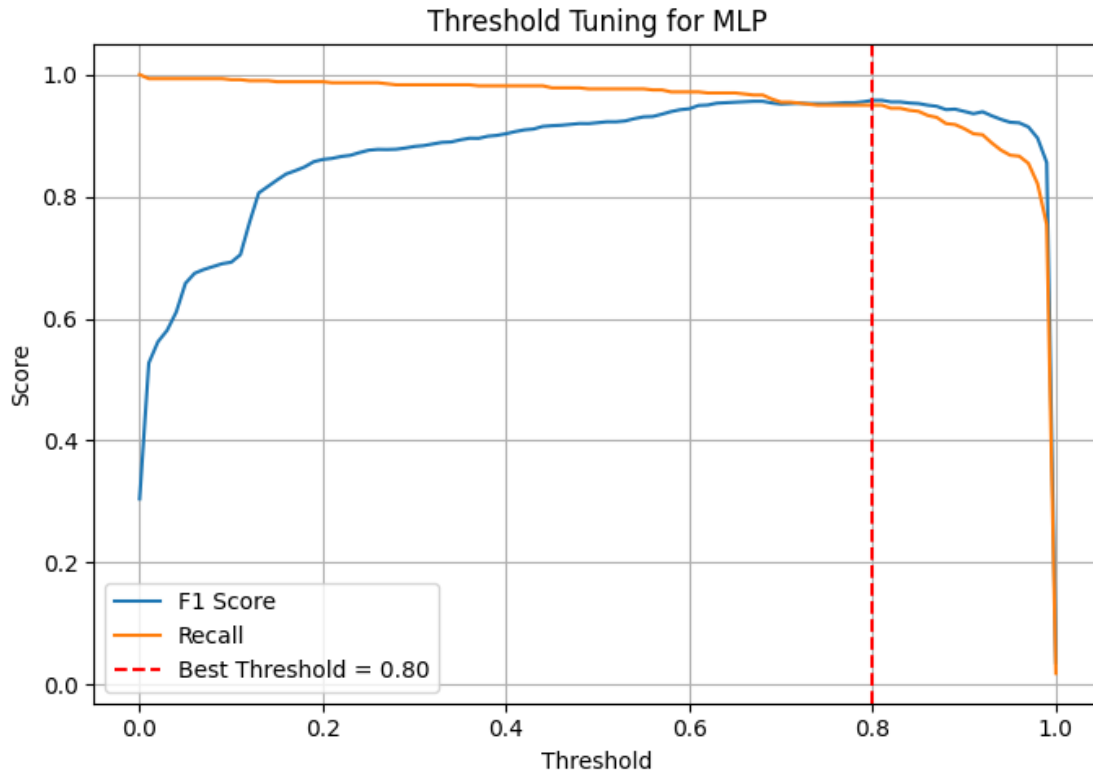
Optimal threshold for XGBoost = 0.66 with F1 = 0.9740 and Recall = 0.9699

=== Tuning LightGBM Threshold ===



Optimal threshold for LightGBM = 0.83 with F1 = 0.9712 and Recall = 0.9599

=== Tuning MLP Threshold ===



Optimal threshold for MLP = 0.80 with F1 = 0.9578 and Recall = 0.9498

=== Summary of Optimal Thresholds ===

SVM: 0.59

Random Forest: 0.46

XGBoost: 0.66

LightGBM: 0.83

MLP: 0.80

```
[32]: # === 6. Evaluate and Plot ROC Curves ===
from sklearn.metrics import roc_curve
import matplotlib.pyplot as plt

def evaluate_model(model, X_test, y_test, name, is_pytorch=False, threshold=0.
    ↪5):
    if is_pytorch:
        preds, probs = get_pytorch_predictions(model, X_test, threshold)
    else:
        probs = model.predict_proba(X_test)[: , 1]
        preds = (probs > threshold).astype(int)
```



```

cm = confusion_matrix(y_test, preds)
auc_val = roc_auc_score(y_test, probs)
print(f"\n--- {name} ---")
print("Confusion Matrix:\n", cm)
print(f"TP: {cm[1, 1]} | FN: {cm[1, 0]} | FP: {cm[0, 1]} | TN: {cm[0, 0]}")
print(f"Recall (Malicious): {cm[1, 1] / (cm[1, 1] + cm[1, 0]):.4f}")
print(f"F1 (Malicious): {f1_score(y_test, preds):.4f}")
print(f"ROC AUC: {auc_val:.4f}")
fpr, tpr, _ = roc_curve(y_test, probs)
plt.plot(fpr, tpr, label=f"{name} (AUC={auc_val:.2f})")

print("\n--- Malware Detection Focused Evaluation ---")
plt.figure(figsize=(8,6))
evaluate_model(svm_model, X_test_scaled, y_test, name="SVM", threshold=0.4)
evaluate_model(rf_model, X_test_df, y_test, name="Random Forest", threshold=0.4)
evaluate_model(xgb_model, X_test_df, y_test, name="XGBoost", threshold=0.4)
evaluate_model(lgb_model, X_test_df, y_test, name="LightGBM", threshold=0.4)
evaluate_model(mlp_model, X_test_scaled, y_test, name="MLP", is_pytorch=True,
    ↪threshold=0.4)

plt.plot([0, 1], [0, 1], 'k--')
plt.title("ROC Curves for Malware Detection")
plt.xlabel("False Positive Rate")
plt.ylabel("True Positive Rate")
plt.legend()
plt.grid(True)
plt.tight_layout()
plt.show()

# === 7. Save the Optimized Thresholds ===
# Save the threshold values for future inference
thresholds_dict = {
    'svm': svm_best_threshold,
    'random_forest': rf_best_threshold,
    'xgboost': xgb_best_threshold,
    'lightgbm': lgb_best_threshold,
    'mlp': mlp_best_threshold
}

# Save thresholds as a joblib file
joblib.dump(thresholds_dict, "/home/nhat/projectcuoiky/models/
    ↪optimal_thresholds.joblib")
print("Optimal thresholds saved to /home/nhat/projectcuoiky/models/
    ↪optimal_thresholds.joblib")

```

--- Malware Detection Focused Evaluation ---

--- SVM ---

Confusion Matrix:

[[2707 26]

[74 524]]

TP: 524 | FN: 74 | FP: 26 | TN: 2707

Recall (Malicious): 0.8763

F1 (Malicious): 0.9129

ROC AUC: 0.9776

--- Random Forest ---

Confusion Matrix:

[[2717 16]

[25 573]]

TP: 573 | FN: 25 | FP: 16 | TN: 2717

Recall (Malicious): 0.9582

F1 (Malicious): 0.9655

ROC AUC: 0.9970

--- XGBoost ---

Confusion Matrix:

[[2707 26]

[15 583]]

TP: 583 | FN: 15 | FP: 26 | TN: 2707

Recall (Malicious): 0.9749

F1 (Malicious): 0.9660

ROC AUC: 0.9981

--- LightGBM ---

Confusion Matrix:

[[2708 25]

[20 578]]

TP: 578 | FN: 20 | FP: 25 | TN: 2708

Recall (Malicious): 0.9666

F1 (Malicious): 0.9625

ROC AUC: 0.9979

--- MLP ---

Confusion Matrix:

[[2618 115]

[11 587]]

TP: 587 | FN: 11 | FP: 115 | TN: 2618

Recall (Malicious): 0.9816

F1 (Malicious): 0.9031

ROC AUC: 0.9923

--- SVM ---

Confusion Matrix:

```
[[2707  26]
 [ 74 524]]
TP: 524 | FN: 74 | FP: 26 | TN: 2707
Recall (Malicious): 0.8763
F1 (Malicious): 0.9129
ROC AUC: 0.9776
```

--- Random Forest ---

```
Confusion Matrix:
[[2717  16]
 [ 25 573]]
TP: 573 | FN: 25 | FP: 16 | TN: 2717
Recall (Malicious): 0.9582
F1 (Malicious): 0.9655
ROC AUC: 0.9970
```

--- XGBoost ---

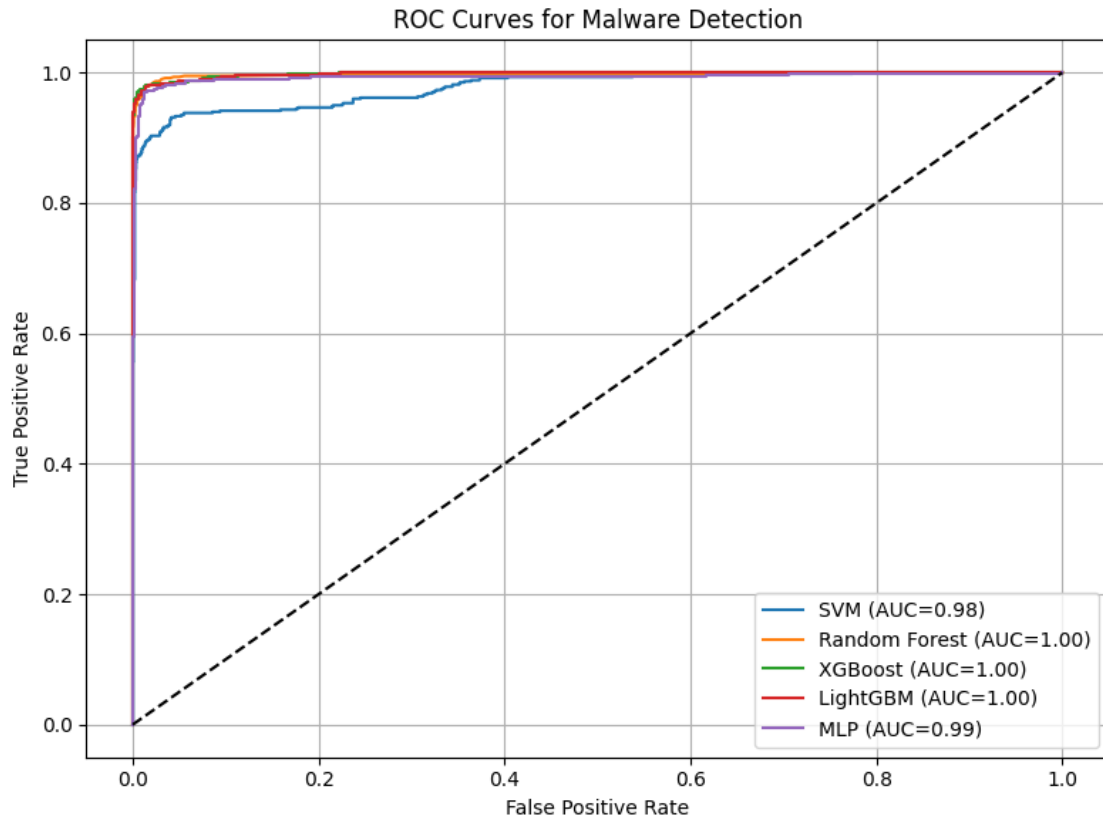
```
Confusion Matrix:
[[2707  26]
 [ 15 583]]
TP: 583 | FN: 15 | FP: 26 | TN: 2707
Recall (Malicious): 0.9749
F1 (Malicious): 0.9660
ROC AUC: 0.9981
```

--- LightGBM ---

```
Confusion Matrix:
[[2708  25]
 [ 20 578]]
TP: 578 | FN: 20 | FP: 25 | TN: 2708
Recall (Malicious): 0.9666
F1 (Malicious): 0.9625
ROC AUC: 0.9979
```

--- MLP ---

```
Confusion Matrix:
[[2618 115]
 [ 11 587]]
TP: 587 | FN: 11 | FP: 115 | TN: 2618
Recall (Malicious): 0.9816
F1 (Malicious): 0.9031
ROC AUC: 0.9923
```



Optimal thresholds saved to
/home/nhat/projectcuaiky/models/optimal_thresholds.joblib

```
[33]: # === 7. Evaluate and Plot ROC Curves ===
from sklearn.metrics import roc_curve

def evaluate_model(model, X_test, y_test, name, is_pytorch=False, threshold=0.
    ↪5):
    if is_pytorch:
        preds, probs = get_pytorch_predictions(model, X_test, threshold)
    else:
        probs = model.predict_proba(X_test)[:, 1]
        preds = (probs > threshold).astype(int)

    cm = confusion_matrix(y_test, preds)
    auc_val = roc_auc_score(y_test, probs)
    print(f"\n--- {name} ---")
    print("Confusion Matrix:\n", cm)
    print(f"TP: {cm[1, 1]} | FN: {cm[1, 0]} | FP: {cm[0, 1]} | TN: {cm[0, 0]}")
    print(f"Recall (Malicious): {cm[1, 1] / (cm[1, 1] + cm[1, 0]):.4f}")
    print(f"F1 (Malicious): {f1_score(y_test, preds):.4f}")
```

```

print(f"ROC AUC: {auc_val:.4f}")
fpr, tpr, _ = roc_curve(y_test, probs)
plt.plot(fpr, tpr, label=f"{name} (AUC={auc_val:.2f})")

print("\n--- Malware Detection Focused Evaluation ---")
plt.figure(figsize=(8,6))
evaluate_model(svm_model, X_test_scaled, y_test, name="SVM",
    ↳threshold=svm_best_threshold)
evaluate_model(rf_model, X_test_df, y_test, name="Random Forest",
    ↳threshold=rf_best_threshold)
evaluate_model(xgb_model, X_test_df, y_test, name="XGBoost",
    ↳threshold=xgb_best_threshold)
evaluate_model(lgb_model, X_test_df, y_test, name="LightGBM",
    ↳threshold=lgb_best_threshold)
evaluate_model(mlp_model, X_test_scaled, y_test, name="MLP", is_pytorch=True,
    ↳threshold=mlp_best_threshold)

plt.plot([0, 1], [0, 1], 'k--')
plt.title("ROC Curves for Malware Detection")
plt.xlabel("False Positive Rate")
plt.ylabel("True Positive Rate")
plt.legend()
plt.grid(True)
plt.tight_layout()
plt.show()

```

--- Malware Detection Focused Evaluation ---

--- SVM ---

Confusion Matrix:

```
[[2721  12]
```

```
[ 78 520]]
```

TP: 520 | FN: 78 | FP: 12 | TN: 2721

Recall (Malicious): 0.8696

F1 (Malicious): 0.9204

ROC AUC: 0.9776

--- Random Forest ---

Confusion Matrix:

```
[[2720  13]
```

```
[ 27 571]]
```

TP: 571 | FN: 27 | FP: 13 | TN: 2720

Recall (Malicious): 0.9548

F1 (Malicious): 0.9662

ROC AUC: 0.9970

--- XGBoost ---

Confusion Matrix:

[[2720 13]

[18 580]]

TP: 580 | FN: 18 | FP: 13 | TN: 2720

Recall (Malicious): 0.9699

F1 (Malicious): 0.9740

ROC AUC: 0.9981

--- LightGBM ---

Confusion Matrix:

[[2723 10]

[24 574]]

TP: 574 | FN: 24 | FP: 10 | TN: 2723

Recall (Malicious): 0.9599

F1 (Malicious): 0.9712

ROC AUC: 0.9979

--- MLP ---

Confusion Matrix:

[[2713 20]

[30 568]]

TP: 568 | FN: 30 | FP: 20 | TN: 2713

Recall (Malicious): 0.9498

F1 (Malicious): 0.9578

ROC AUC: 0.9923

--- SVM ---

Confusion Matrix:

[[2721 12]

[78 520]]

TP: 520 | FN: 78 | FP: 12 | TN: 2721

Recall (Malicious): 0.8696

F1 (Malicious): 0.9204

ROC AUC: 0.9776

--- Random Forest ---

Confusion Matrix:

[[2720 13]

[27 571]]

TP: 571 | FN: 27 | FP: 13 | TN: 2720

Recall (Malicious): 0.9548

F1 (Malicious): 0.9662

ROC AUC: 0.9970

--- XGBoost ---

Confusion Matrix:

[[2720 13]

```
[ 18 580]]
TP: 580 | FN: 18 | FP: 13 | TN: 2720
Recall (Malicious): 0.9699
F1 (Malicious): 0.9740
ROC AUC: 0.9981
```

--- LightGBM ---

Confusion Matrix:

```
[[2723  10]
```

```
[ 24 574]]
```

TP: 574 | FN: 24 | FP: 10 | TN: 2723

Recall (Malicious): 0.9599

F1 (Malicious): 0.9712

ROC AUC: 0.9979

--- MLP ---

Confusion Matrix:

```
[[2713  20]
```

```
[ 30 568]]
```

TP: 568 | FN: 30 | FP: 20 | TN: 2713

Recall (Malicious): 0.9498

F1 (Malicious): 0.9578

ROC AUC: 0.9923

