classic-pred

May 31, 2025

[1]:
```python
import pandas as pd
import numpy as np
import os
import warnings
from sklearn.model_selection import KFold
from sklearn.ensemble import RandomForestClassifier
from sklearn.model_selection import GridSearchCV
import matplotlib.pyplot as plt
from xgboost import XGBClassifier
from tqdm import tqdm
from sklearn.model_selection import LeaveOneGroupOut
from sklearn.utils.class_weight import compute_class_weight
from sklearn.metrics import (
    f1_score, accuracy_score, recall_score, precision_score,
    precision_recall_curve, confusion_matrix, roc_auc_score,
    matthews_corrcoef, roc_curve
)

warnings.filterwarnings("ignore")
```

0.0.1 Metric Calculation Utilities

[2]:
```python
def get_aupr(pre, rec):
    pr_value = 0.0
    for ii in range(len(rec[:-1])):
        x_r, x_l = rec[ii], rec[ii+1]
        y_t, y_b = pre[ii], pre[ii+1]
        tempo = abs(x_r - x_l) * (y_t + y_b) * 0.5
        pr_value += tempo
    return pr_value

def scores(y_test, y_pred, th=0.5):
    y_predlabel = [(0. if item < th else 1.) for item in y_pred]
    tn, fp, fn, tp = confusion_matrix(y_test, y_predlabel).flatten()
    SPE = tn / (tn + fp)
    MCC = matthews_corrcoef(y_test, y_predlabel)
    fpr, tpr, _ = roc_curve(y_test, y_pred)
    sen, spe, pre, f1, mcc, acc, auc, tn, fp, fn, tp = np.array([
        recall_score(y_test, y_predlabel), SPE, precision_score(y_test,␣
↪y_predlabel),
        f1_score(y_test, y_predlabel), MCC, accuracy_score(y_test, y_predlabel),
        roc_auc_score(y_test, y_pred), tn, fp, fn, tp
    ])
    precision, recall, _ = precision_recall_curve(y_test, y_pred)
    aupr = get_aupr(precision, recall)
    return [aupr, auc, f1, acc, sen, spe, pre, fpr, tpr, precision, recall]
```

1 — Utility Functions —

[3]:
```
def combine_features(phage_dna, host_dna, phage_pro, host_pro):
    combined = np.concatenate([phage_dna, host_dna, phage_pro, host_pro],␣
↪axis=1)
    return combined
```

[4]:
```
def load_feature_vector(file_path):
    return np.loadtxt(file_path)
```

[5]:
```
def obtain_features(phage_list, host_list, labels, dna_base, pro_base):
    X_phage_dna, X_host_dna = [], []
    X_phage_pro, X_host_pro = [], []
    for p, h in zip(phage_list, host_list):
        X_phage_dna.append(load_feature_vector(os.path.join(dna_base,␣
↪'phage_dna_norm_features', f'{p}.txt')))
        X_host_dna.append(load_feature_vector(os.path.join(dna_base,␣
↪'host_dna_norm_features', f'{h}.txt')))
        X_phage_pro.append(load_feature_vector(os.path.join(pro_base, 'phage',␣
↪f'{p}.txt')))
        X_host_pro.append(load_feature_vector(os.path.join(pro_base,␣
↪'bacteria', f'{h}.txt')))
    return (np.array(X_phage_dna), np.array(X_host_dna),
            np.array(X_phage_pro), np.array(X_host_pro),
            np.array(labels))
```

2 — Load interaction matrix —

[6]:
```
interaction_matrix_path = "./phage_host_interactions (1).csv"
dna_base = './dna_features'
pro_base = './protein_features'

# Get list of phages and hosts based on files present
df = pd.read_csv(interaction_matrix_path, index_col=0)
```

```
valid_phages = set([f.split('.')[0] for f in os.listdir(dna_base+"/
 ↪phage_dna_norm_features") if f.endswith('.txt')])
valid_hosts = set([f.split('.')[0] for f in os.listdir(pro_base+"/bacteria") if␣
 ↪f.endswith('.txt')])

df = df.loc[df.index.intersection(valid_hosts), df.columns.
 ↪intersection(valid_phages)]
#TODO: filter unused interaction since matrix to large

phages = df.columns.tolist()
hosts = df.index.tolist()
print(len(phages))
print(len(hosts))
```

```
105
200
```

3 Prepare data as list of (phage, host, label)

[7]:
```
all_data = []

for p in phages:
    for h in hosts:
        label = df.loc[h, p]  # Corrected access
        if pd.isna(label):
            continue  # Skip missing values
        all_data.append([p, h, int(label)])
```

3.0.1 Model Training and Evaluation (with Metrics)

[21]:
```
results_all = []
fprs, tprs, precisions, recalls = [], [], [], []
# Your cross-validation setup:
kf = KFold(n_splits=5, random_state=1, shuffle=True)

for fold, (train_idx, val_idx) in enumerate(kf.split(all_data)):
    print(f"Fold {fold+1}")

    train_set = [all_data[i] for i in train_idx]
    val_set = [all_data[i] for i in val_idx]

    train_phages = [x[0] for x in train_set]
    train_hosts = [x[1] for x in train_set]
    train_labels = [x[2] for x in train_set]

    val_phages = [x[0] for x in val_set]
    val_hosts = [x[1] for x in val_set]
    val_labels = [x[2] for x in val_set]

    X_phage_dna_tr, X_host_dna_tr, X_phage_pro_tr, X_host_pro_tr, y_train =␣
↪obtain_features(
        train_phages, train_hosts, train_labels, dna_base, pro_base)
    X_phage_dna_val, X_host_dna_val, X_phage_pro_val, X_host_pro_val, y_val =␣
↪obtain_features(
        val_phages, val_hosts, val_labels, dna_base, pro_base)

    X_train_combined = combine_features(X_phage_dna_tr, X_host_dna_tr,␣
↪X_phage_pro_tr, X_host_pro_tr)
    X_val_combined = combine_features(X_phage_dna_val, X_host_dna_val,␣
↪X_phage_pro_val, X_host_pro_val)

    imbalance = sum([1 for i in y_train if i==1]) / sum([1 for i in y_train if␣
↪i==0])


    model = XGBClassifier(
        scale_pos_weight=1/imbalance,
        learning_rate=0.3,
        n_estimators=250,
        max_depth=7,
        use_label_encoder=False,
        eval_metric='logloss',
        n_jobs=8
    )
    model.fit(X_train_combined, y_train)
    y_pred_prob = model.predict_proba(X_val_combined)[:,1]

    fold_metrics = scores(y_val, y_pred_prob)
    results_all.append(fold_metrics[:7])  # Save base metrics
    fprs.append(fold_metrics[7])
    tprs.append(fold_metrics[8])
    precisions.append(fold_metrics[9])
    recalls.append(fold_metrics[10])

    print(f"Fold {fold+1} | AUPR: {fold_metrics[0]:.4f}, AUC: {fold_metrics[1]:.
↪4f}, F1: {fold_metrics[2]:.4f}, Acc: {fold_metrics[3]:.4f}")
```

```
Fold 1

Exception ignored on calling ctypes callback function: <bound method
DataIter._next_wrapper of <xgboost.data.SingleBatchInternalIter object at
0x0000025422D01480>>
Traceback (most recent call last):
  File "D:\Bachelorarbeit\Prediction Notebooks\.venv2\lib\site-
```

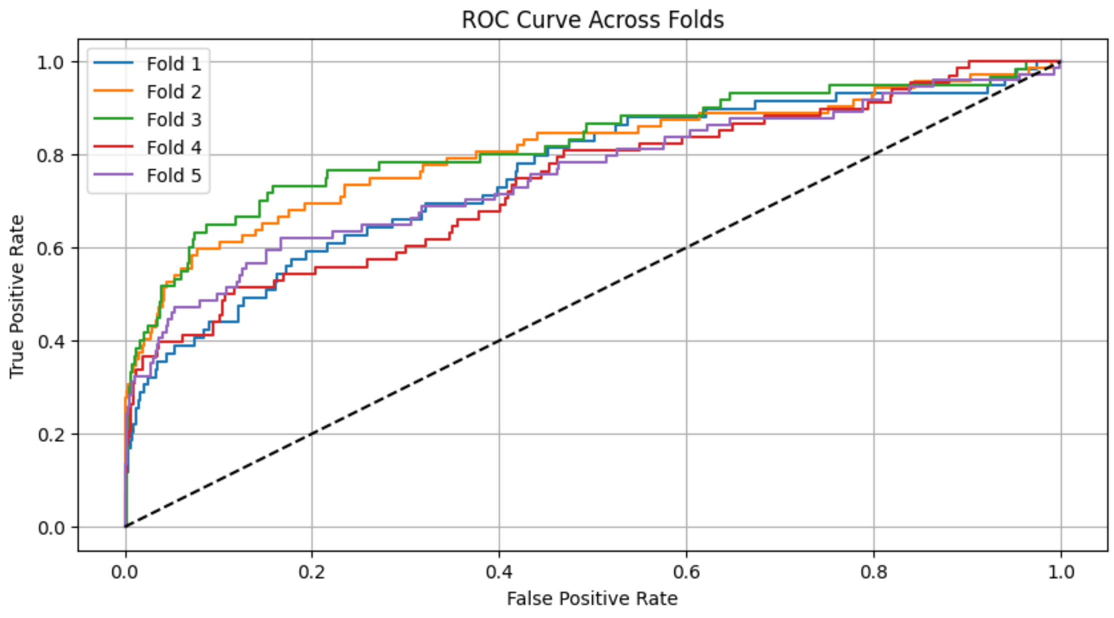
```
packages\xgboost\core.py", line 640, in _next_wrapper
    return self._handle_exception(lambda: int(self.next(input_data)), 0)
  File "D:\Bachelorarbeit\Prediction Notebooks\.venv2\lib\site-
packages\xgboost\core.py", line 553, in _handle_exception
    return fn()
  File "D:\Bachelorarbeit\Prediction Notebooks\.venv2\lib\site-
packages\xgboost\core.py", line 640, in <lambda>
    return self._handle_exception(lambda: int(self.next(input_data)), 0)
  File "D:\Bachelorarbeit\Prediction Notebooks\.venv2\lib\site-
packages\xgboost\data.py", line 1654, in next
    input_data(**self.kwargs)
  File "D:\Bachelorarbeit\Prediction Notebooks\.venv2\lib\site-
packages\xgboost\core.py", line 729, in inner_f
    return func(**kwargs)
  File "D:\Bachelorarbeit\Prediction Notebooks\.venv2\lib\site-
packages\xgboost\core.py", line 628, in input_data
    dispatch_proxy_set_data(self.proxy, new, cat_codes)
  File "D:\Bachelorarbeit\Prediction Notebooks\.venv2\lib\site-
packages\xgboost\data.py", line 1753, in dispatch_proxy_set_data
    proxy._ref_data_from_array(data)  # pylint: disable=W0212
  File "D:\Bachelorarbeit\Prediction Notebooks\.venv2\lib\site-
packages\xgboost\core.py", line 1462, in _ref_data_from_array
    _check_call(_LIB.XGProxyDMatrixSetDataDense(self.handle,
array_interface(data)))
KeyboardInterrupt:
```

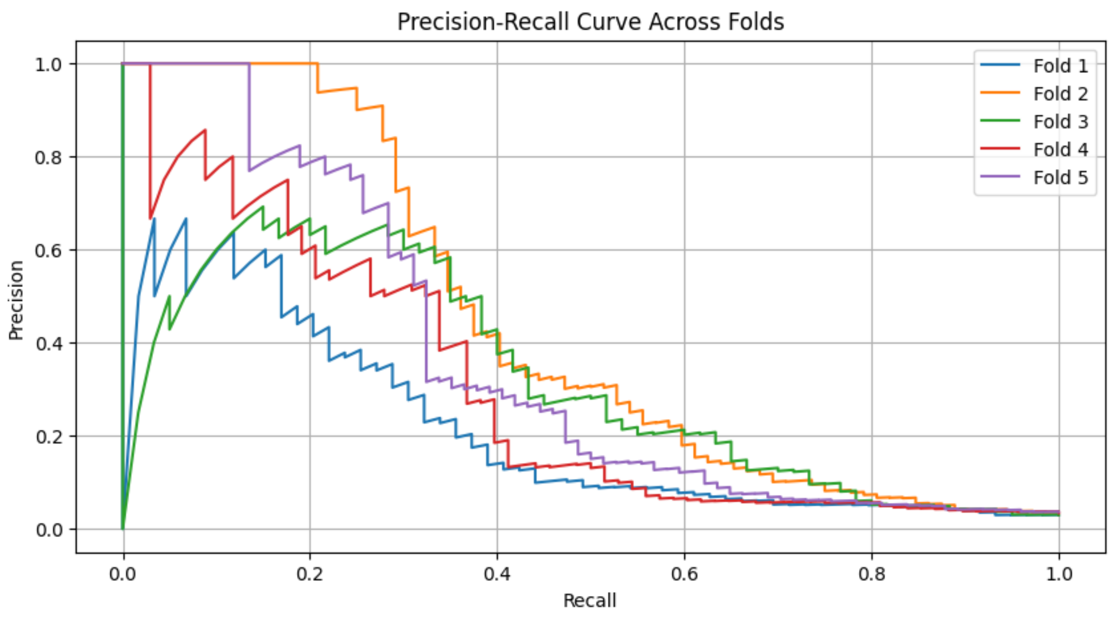
```
Fold 1 | AUPR: 0.2053, AUC: 0.7564, F1: 0.2737, Acc: 0.9655
Fold 2
Fold 2 | AUPR: 0.4361, AUC: 0.8058, F1: 0.4272, Acc: 0.9705
Fold 3
Fold 3 | AUPR: 0.3103, AUC: 0.8227, F1: 0.4330, Acc: 0.9725
Fold 4
Fold 4 | AUPR: 0.2924, AUC: 0.7381, F1: 0.3469, Acc: 0.9680
Fold 5
Fold 5 | AUPR: 0.3579, AUC: 0.7549, F1: 0.4000, Acc: 0.9685
```

3.0.2 Plotting Metrics Across Folds

[9]:
```
# Plot ROC Curves
plt.figure(figsize=(10, 5))
for i in range(len(fprs)):
    plt.plot(fprs[i], tprs[i], label=f'Fold {i+1}')
plt.plot([0, 1], [0, 1], 'k--')
plt.title("ROC Curve Across Folds")
plt.xlabel("False Positive Rate")
plt.ylabel("True Positive Rate")
plt.legend()
plt.grid()
plt.show()

# Plot PR Curves
plt.figure(figsize=(10, 5))
for i in range(len(precisions)):
    plt.plot(recalls[i], precisions[i], label=f'Fold {i+1}')
plt.title("Precision-Recall Curve Across Folds")
plt.xlabel("Recall")
plt.ylabel("Precision")
plt.legend()
plt.grid()
plt.show()
```

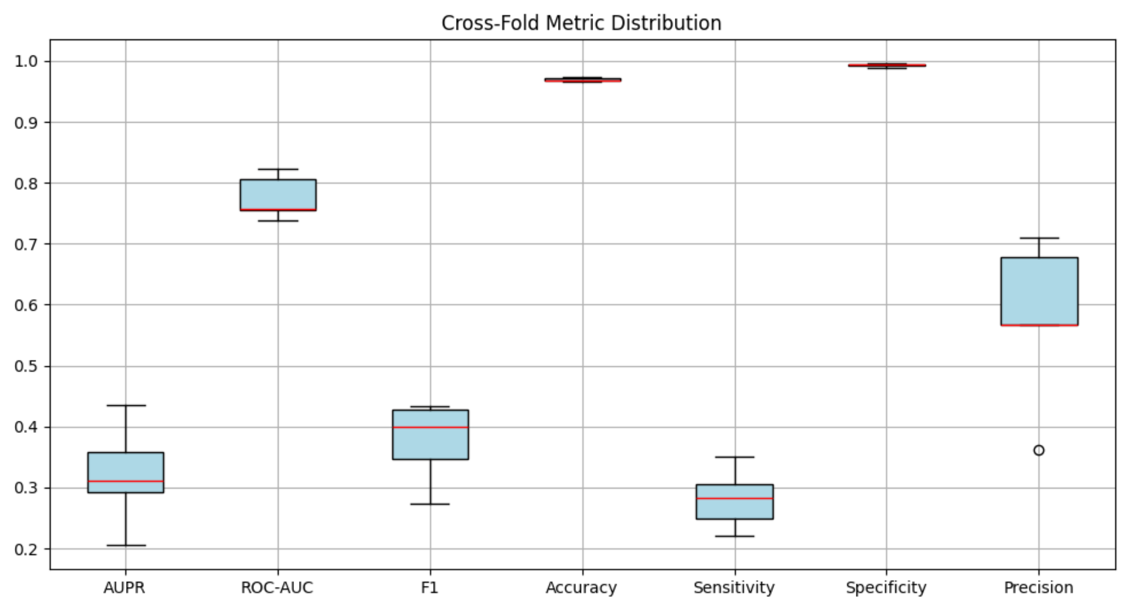




3.0.3 Summary Boxplot of All Metrics

```
[10]: metric_names = ["AUPR", "ROC-AUC", "F1", "Accuracy", "Sensitivity",␣
       ↪"Specificity", "Precision"]
      results_array = np.array(results_all)

      plt.figure(figsize=(12, 6))
      plt.boxplot(results_array, labels=metric_names, patch_artist=True,
                  boxprops=dict(facecolor='lightblue', color='black'),
                  medianprops=dict(color='red'),
                  whiskerprops=dict(color='black'))
      plt.title("Cross-Fold Metric Distribution")
      plt.grid()
      plt.show()
```



3.0.4 Fold-wise Metric Table

```
[11]: results_df = pd.DataFrame(results_all, columns=metric_names)
results_df.index = [f"Fold {i+1}" for i in range(len(results_all))]
display(results_df)

print("Mean Metrics:")
display(results_df.mean())
```

```
            AUPR   ROC-AUC        F1  Accuracy  Sensitivity  Specificity  \
Fold 1  0.205312  0.756370  0.273684  0.965534     0.220339     0.988163
Fold 2  0.436058  0.805793  0.427184  0.970515     0.305556     0.995334
Fold 3  0.310329  0.822746  0.432990  0.972514     0.350000     0.991757
Fold 4  0.292393  0.738124  0.346939  0.968016     0.250000     0.993275
Fold 5  0.357870  0.754926  0.400000  0.968516     0.283784     0.994811

        Precision
Fold 1   0.361111
Fold 2   0.709677
Fold 3   0.567568
Fold 4   0.566667
Fold 5   0.677419

Mean Metrics:

AUPR           0.320392
ROC-AUC        0.775592
F1             0.376159
Accuracy       0.969019
```

```
Sensitivity    0.281936
Specificity    0.992668
Precision      0.576488
dtype: float64
```

3.1 Random Forest Model with Grid SearchCV

[12]:
```
rf_results_all = []
rf_fprs, rf_tprs, rf_precisions, rf_recalls = [], [], [], []

rf_param_grid = {
    'n_estimators': [50, 100, 200],
    'max_depth': [None, 10],
    'min_samples_split': [2, 5],
    'min_samples_leaf': [1, 2],
    'max_features': ['auto', 'sqrt', 'log2'],
    'bootstrap': [True, False]
}

for fold, (train_idx, val_idx) in enumerate(kf.split(all_data)):
    print(f"RF Fold {fold+1}")

    train_set = [all_data[i] for i in train_idx]
    val_set = [all_data[i] for i in val_idx]

    train_phages = [x[0] for x in train_set]
    train_hosts = [x[1] for x in train_set]
    train_labels = [x[2] for x in train_set]

    val_phages = [x[0] for x in val_set]
    val_hosts = [x[1] for x in val_set]
    val_labels = [x[2] for x in val_set]

    X_phage_dna_tr, X_host_dna_tr, X_phage_pro_tr, X_host_pro_tr, y_train =␣
↪obtain_features(
        train_phages, train_hosts, train_labels, dna_base, pro_base)
    X_phage_dna_val, X_host_dna_val, X_phage_pro_val, X_host_pro_val, y_val =␣
↪obtain_features(
        val_phages, val_hosts, val_labels, dna_base, pro_base)

    X_train_combined = combine_features(X_phage_dna_tr, X_host_dna_tr,␣
↪X_phage_pro_tr, X_host_pro_tr)
    X_val_combined = combine_features(X_phage_dna_val, X_host_dna_val,␣
↪X_phage_pro_val, X_host_pro_val)

    class_weights = compute_class_weight(class_weight='balanced', classes=np.
↪array([0, 1]), y=y_train)
```

```
    class_weight_dict = {0: class_weights[0], 1: class_weights[1]}

    rf_base = RandomForestClassifier(class_weight=class_weight_dict,␣
↪random_state=42, n_jobs=-1)
    grid_search = GridSearchCV(estimator=rf_base, param_grid=rf_param_grid,
                               scoring='f1', cv=3, n_jobs=-1, verbose=0)
    grid_search.fit(X_train_combined, y_train)
    best_rf = grid_search.best_estimator_

    y_pred_prob = best_rf.predict_proba(X_val_combined)[:, 1]

    rf_fold_metrics = scores(y_val, y_pred_prob)
    rf_results_all.append(rf_fold_metrics[:7])
    rf_fprs.append(rf_fold_metrics[7])
    rf_tprs.append(rf_fold_metrics[8])
    rf_precisions.append(rf_fold_metrics[9])
    rf_recalls.append(rf_fold_metrics[10])

    print(f"Fold {fold+1} | AUPR: {rf_fold_metrics[0]:.4f}, AUC:␣
↪{rf_fold_metrics[1]:.4f}, "
          f"F1: {rf_fold_metrics[2]:.4f}, Acc: {rf_fold_metrics[3]:.4f}")
```

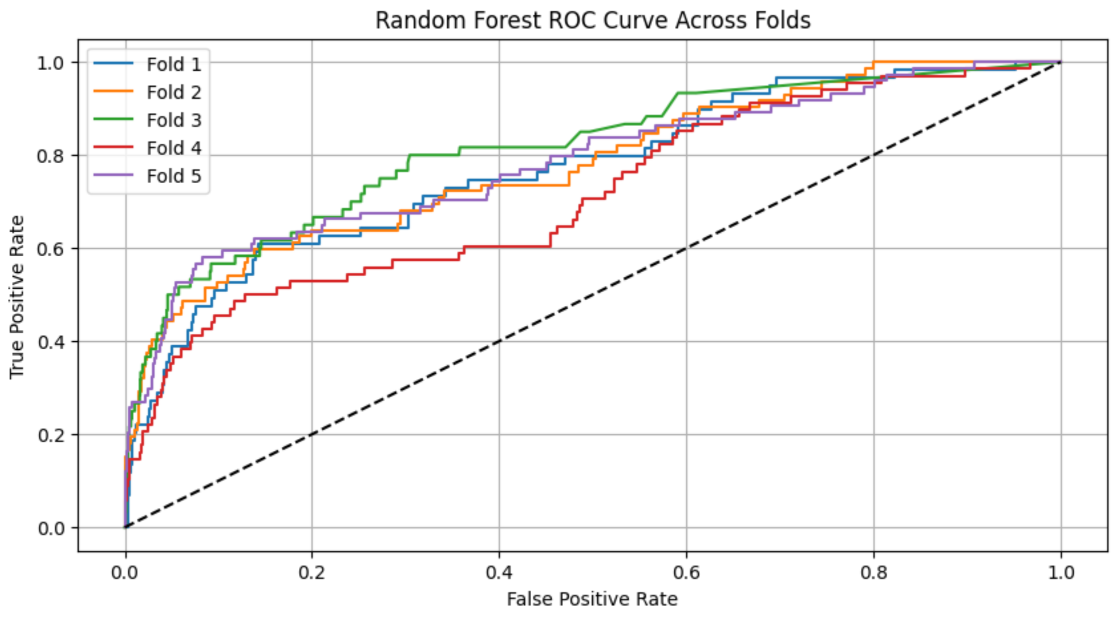
```
RF Fold 1
Fold 1 | AUPR: 0.1528, AUC: 0.7708, F1: 0.2553, Acc: 0.9650
RF Fold 2
Fold 2 | AUPR: 0.2967, AUC: 0.7781, F1: 0.3580, Acc: 0.9480
RF Fold 3
Fold 3 | AUPR: 0.2531, AUC: 0.8121, F1: 0.2597, Acc: 0.9715
RF Fold 4
Fold 4 | AUPR: 0.1722, AUC: 0.7137, F1: 0.2424, Acc: 0.9375
RF Fold 5
Fold 5 | AUPR: 0.3326, AUC: 0.7834, F1: 0.3371, Acc: 0.9410
```

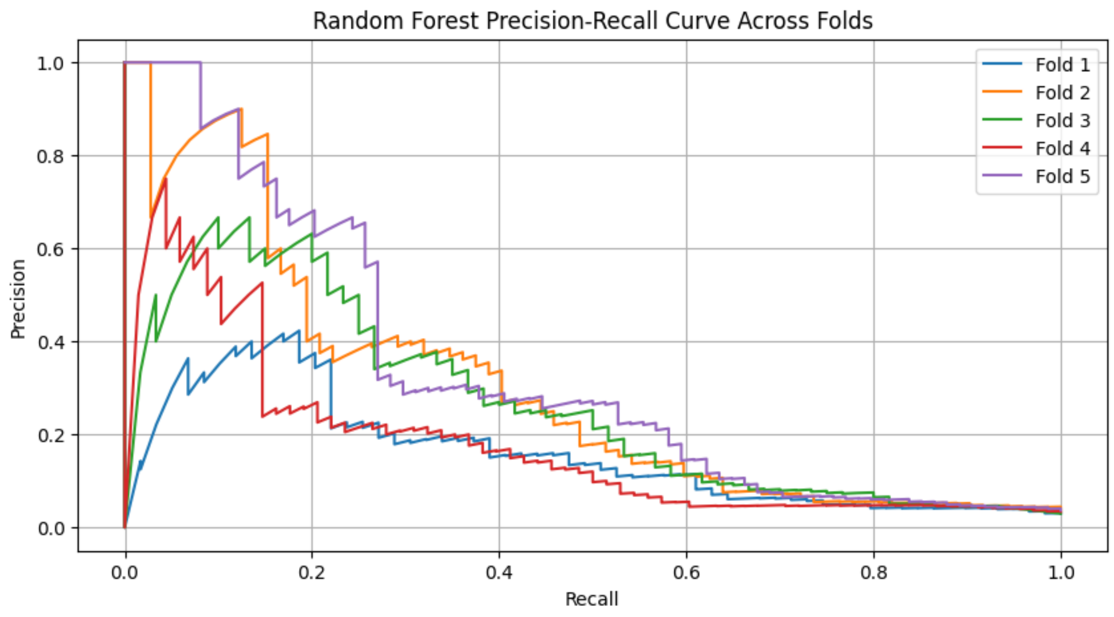
3.1.1 Random Forest ROC & PR Curves

[13]:
```
plt.figure(figsize=(10, 5))
for i in range(len(rf_fprs)):
    plt.plot(rf_fprs[i], rf_tprs[i], label=f'Fold {i+1}')
plt.plot([0, 1], [0, 1], 'k--')
plt.title("Random Forest ROC Curve Across Folds")
plt.xlabel("False Positive Rate")
plt.ylabel("True Positive Rate")
plt.legend()
plt.grid()
plt.show()

plt.figure(figsize=(10, 5))
```

```python
for i in range(len(rf_precisions)):
    plt.plot(rf_recalls[i], rf_precisions[i], label=f'Fold {i+1}')
plt.title("Random Forest Precision-Recall Curve Across Folds")
plt.xlabel("Recall")
plt.ylabel("Precision")
plt.legend()
plt.grid()
plt.show()
```





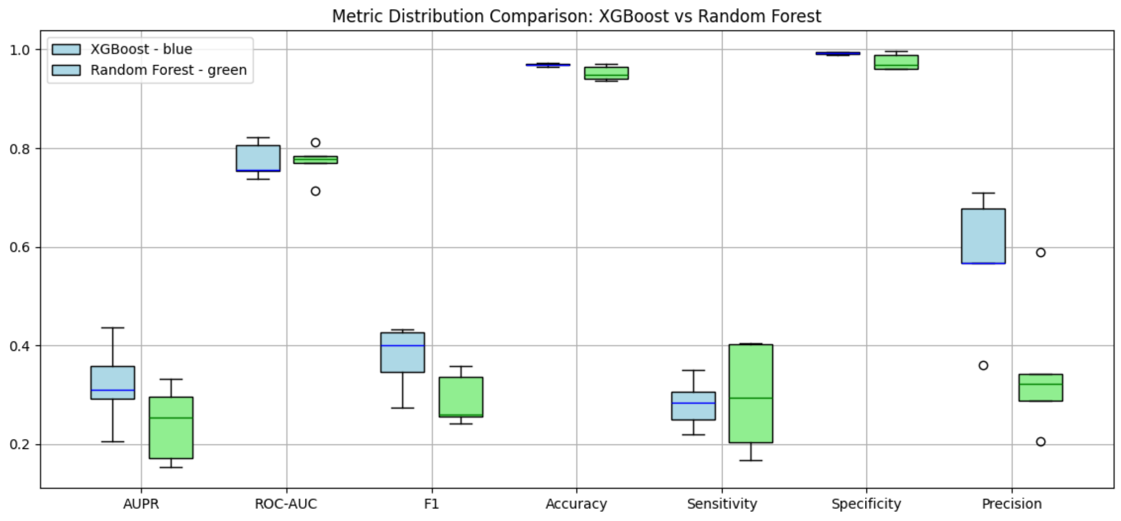
3.1.2 Metric Boxplot: XGBoost vs Random Forest

```
[14]: all_metric_names = ["AUPR", "ROC-AUC", "F1", "Accuracy", "Sensitivity",␣
      ↪"Specificity", "Precision"]

      plt.figure(figsize=(14, 6))
      plt.boxplot([np.array(results_all)[:,i] for i in range(7)],
                  positions=np.arange(1, 8) - 0.2, widths=0.3, patch_artist=True,
                  boxprops=dict(facecolor='lightblue'),␣
      ↪medianprops=dict(color='blue'), labels=all_metric_names)

      plt.boxplot([np.array(rf_results_all)[:,i] for i in range(7)],
                  positions=np.arange(1, 8) + 0.2, widths=0.3, patch_artist=True,
                  boxprops=dict(facecolor='lightgreen'),␣
      ↪medianprops=dict(color='green'))

      plt.legend(['XGBoost - blue', 'Random Forest - green'])
      plt.title("Metric Distribution Comparison: XGBoost vs Random Forest")
      plt.grid()
      plt.xticks(np.arange(1, 8), all_metric_names)
      plt.show()
```



3.1.3 Random Forest Fold-wise Metrics

```
[15]: rf_df = pd.DataFrame(rf_results_all, columns=all_metric_names)
rf_df.index = [f"Fold {i+1}" for i in range(len(rf_results_all))]
display(rf_df)

print("Random Forest - Mean Metrics:")
display(rf_df.mean())
```

```
            AUPR   ROC-AUC        F1  Accuracy  Sensitivity  Specificity  \
Fold 1  0.152843  0.770798  0.255319  0.965035     0.203390     0.988163
Fold 2  0.296718  0.778087  0.358025  0.948026     0.402778     0.968377
Fold 3  0.253124  0.812142  0.259740  0.971514     0.166667     0.996394
Fold 4  0.172177  0.713741  0.242424  0.937531     0.294118     0.960166
Fold 5  0.332612  0.783447  0.337079  0.941029     0.405405     0.961598

        Precision
Fold 1   0.342857
Fold 2   0.322222
Fold 3   0.588235
Fold 4   0.206186
Fold 5   0.288462
```

```
Random Forest - Mean Metrics:
```

```
AUPR           0.241495
ROC-AUC        0.771643
F1             0.290517
Accuracy       0.952627
Sensitivity    0.294471
Specificity    0.974940
Precision      0.349592
dtype: float64
```

3.1.4 Side-by-side Mean Metrics (XGBoost vs RF)

```
[16]: xgb_mean = pd.DataFrame([np.mean(results_all, axis=0)],␣
  ↪columns=all_metric_names, index=["XGBoost"])
rf_mean = pd.DataFrame([np.mean(rf_results_all, axis=0)],␣
  ↪columns=all_metric_names, index=["Random Forest"])

display(pd.concat([xgb_mean, rf_mean]))
```

```
                   AUPR   ROC-AUC        F1  Accuracy  Sensitivity  \
XGBoost        0.320392  0.775592  0.376159  0.969019     0.281936
Random Forest  0.241495  0.771643  0.290517  0.952627     0.294471

               Specificity  Precision
XGBoost           0.992668   0.576488
```

```
Random Forest     0.974940   0.349592
```

4 XGBoost with LOGO

[17]:
```
# Assuming:
# all_data = [(phage, host, label), ...]
# hosts = list of host IDs
# phages = list of phage IDs

# Create groups based on host for LOGO
groups = []
for sample in all_data:
    phage, host, label = sample
    group_id = hosts.index(host)  # group by host
    groups.append(group_id)

print(f"Number of unique groups (hosts): {len(set(groups))}")
```

```
Number of unique groups (hosts): 200
```

[18]:
```
logo = LeaveOneGroupOut()
cpus = 8

# For collecting predictions and labels
scores_all = []
label_list = []

# Progress bar for number of groups
pbar = tqdm(total=len(set(groups)))

for fold, (train_idx, val_idx) in enumerate(logo.split(all_data,␣
 ↪groups=groups)):
    # Prepare data
    train_set = [all_data[i] for i in train_idx]
    val_set = [all_data[i] for i in val_idx]

    train_phages = [x[0] for x in train_set]
    train_hosts = [x[1] for x in train_set]
    train_labels = [x[2] for x in train_set]

    val_phages = [x[0] for x in val_set]
    val_hosts = [x[1] for x in val_set]
    val_labels = [x[2] for x in val_set]

    # Obtain features
    X_phage_dna_tr, X_host_dna_tr, X_phage_pro_tr, X_host_pro_tr, y_train =␣
 ↪obtain_features(train_phages, train_hosts, train_labels, dna_base, pro_base)
```

```
    X_phage_dna_val, X_host_dna_val, X_phage_pro_val, X_host_pro_val, y_val =␣
 ↪obtain_features(val_phages, val_hosts, val_labels, dna_base, pro_base)


    # Combine features for train and val
    X_train_combined = combine_features(X_phage_dna_tr, X_host_dna_tr,␣
 ↪X_phage_pro_tr, X_host_pro_tr)
    X_val_combined = combine_features(X_phage_dna_val, X_host_dna_val,␣
 ↪X_phage_pro_val, X_host_pro_val,)

    # Class imbalance handling
    pos = sum(y_train)
    neg = len(y_train) - pos
    scale_pos_weight = neg / pos if pos > 0 else 1

    # Train
    model = XGBClassifier(
        scale_pos_weight=scale_pos_weight,
        learning_rate=0.3,
        n_estimators=250,
        max_depth=7,
        use_label_encoder=False,
        eval_metric='logloss',
        n_jobs=cpus
    )
    model.fit(X_train_combined, y_train)

    # Predict
    y_pred_prob = model.predict_proba(X_val_combined)[:, 1]
    scores_all.append(y_pred_prob)
    label_list.append(y_val)

    pbar.update(1)

pbar.close()

# Concatenate all predictions and labels
y_pred_all = np.concatenate(scores_all)
y_true_all = np.concatenate(label_list)

# Now evaluate final performance
final_metrics = scores(y_true_all, y_pred_all)

print("\nFinal LOGO metrics across all folds:")
print(f"AUPR: {final_metrics[0]:.4f}, AUC: {final_metrics[1]:.4f}, F1:␣
 ↪{final_metrics[2]:.4f}, Accuracy: {final_metrics[3]:.4f}")
 72%|      | 144/200 [33:41<13:39, 14.63s/it]
KeyboardInterrupt
```

[ ]:

```
```