classic-pred

June 6, 2025

```
[13]: import pandas as pd
      import numpy as np
      import os
      import warnings
      from sklearn.model_selection import KFold
      from sklearn.model selection import StratifiedKFold
      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

```
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
```

1 — Utility Functions —

```
[15]: 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

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

2 — Load interaction matrix —

```
[6]: interaction_matrix_path = "../ordinal_dataset_features/interaction_matrix.xlsx"
    csv_output_path = "../ordinal_dataset_features/interaction_matrix.csv"

dna_base = '../ordinal_dataset_features/dna_features_ordinal_data'
    pro_base = '../ordinal_dataset_features/prot_features_ordinal_data'
```

```
[18]: interaction_matrix_path = "../phl_dataset_features/phage_host_interactions (1).
       ⇔csv"
      csv_output_path = "../phl_dataset_features/phage_host_interactions (1).csv"
      dna_base = '../phl_dataset_features/dna_features'
      pro_base = '../phl_dataset_features/protein_features'
[19]: # Get list of phages and hosts based on files present
      if interaction_matrix_path.endswith('.xlsx'):
          #Transposed because this dataset has another the wrong shape
          df = pd.read_excel(interaction_matrix_path, index_col=0).T
          df.to_csv(csv_output_path)
          interaction_matrix_path = csv_output_path # Update path to CSV
      else:
          df = pd.read_csv(interaction_matrix_path, index_col=0)
      valid_phages = set([f.split('.')[0] for f in os.listdir(dna_base+"/phage") if f.
       ⇔endswith('.txt')])
      valid_hosts = set([f.split('.')[0] for f in os.listdir(pro_base+"/bacteria") if__

¬f.endswith('.txt')])
      #filter unused interaction since matrix to large
      df = df.loc[df.index.intersection(valid_hosts), df.columns.
       →intersection(valid_phages)]
      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)

```
[20]: all_data = []

for p in phages:
    for h in hosts:
        label = df.loc[h, p]
        if pd.isna(label):
            continue # Skip missing values
        binary_label = 1 if label >= 1 else 0
        all_data.append([p, h, binary_label])
```

3.0.1 Model Training and Evaluation (with Metrics)

```
[22]: results_all = []
      fprs, tprs, precisions, recalls = [], [], []
      # Your cross-validation setup:
      kf = StratifiedKFold(n_splits=5, random_state=1, shuffle=True)
      labels = [row[2] for row in all_data]
      for fold, (train_idx, val_idx) in enumerate(kf.split(all_data, labels)):
          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])
          xgb = XGBClassifier(use_label_encoder=False, eval_metric='logloss')
          # Define hyperparameter grid
          param_grid = {
              'n_estimators': [100, 200, 250],
              'max_depth': [5, 7, None],
              'learning_rate': [0.1, 0.3],
              'scale_pos_weight': [1, 2, 1/imbalance]
          }
```

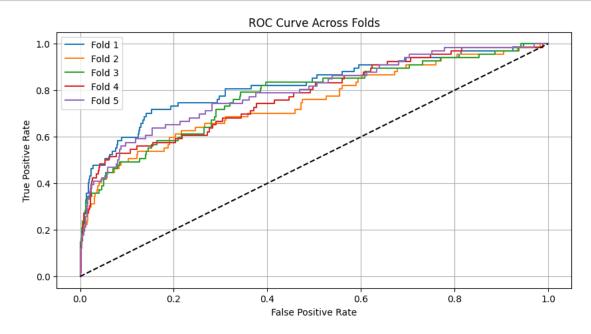
```
# Grid search
    grid_search = GridSearchCV(estimator=xgb, param_grid=param_grid,__
  ⇒scoring='average_precision', cv=5, n_jobs=-1, verbose=1)
    grid search.fit(X train combined, y train)
    best_model = grid_search.best_estimator_
    y pred prob = best model.predict proba(X val combined)[:, 1]
     #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]:.

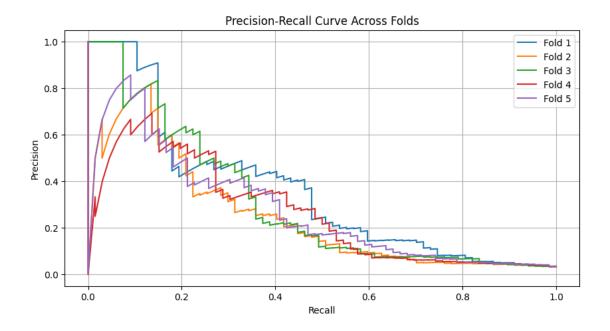
    -4f}, F1: {fold_metrics[2]:.4f}, Acc: {fold_metrics[3]:.4f}")

Fold 1
Fitting 5 folds for each of 54 candidates, totalling 270 fits
Fold 1 | AUPR: 0.3544, AUC: 0.8206, F1: 0.2558, Acc: 0.9680
Fold 2
Fitting 5 folds for each of 54 candidates, totalling 270 fits
Fold 2 | AUPR: 0.2418, AUC: 0.7489, F1: 0.2410, Acc: 0.9685
Fitting 5 folds for each of 54 candidates, totalling 270 fits
Fold 3 | AUPR: 0.3068, AUC: 0.7775, F1: 0.2588, Acc: 0.9685
Fitting 5 folds for each of 54 candidates, totalling 270 fits
Fold 4 | AUPR: 0.2543, AUC: 0.7754, F1: 0.2439, Acc: 0.9690
Fold 5
Fitting 5 folds for each of 54 candidates, totalling 270 fits
Fold 5 | AUPR: 0.2694, AUC: 0.7963, F1: 0.2727, Acc: 0.9680
```

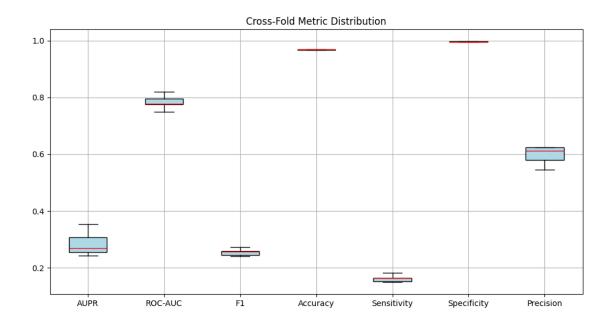
3.0.2 Plotting Metrics Across Folds

```
[23]: # 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



3.0.4 Fold-wise Metric Table

```
[25]: 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	0.354439	0.820641	0.255814	0.968032	0.164179	0.995866	
Fold 2	0.241840	0.748893	0.240964	0.968516	0.149254	0.996898	
Fold 3	0.306834	0.777524	0.258824	0.968516	0.164179	0.996381	
Fold 4	0.254304	0.775429	0.243902	0.969015	0.151515	0.996899	
Fold 5	0.269388	0.796320	0.272727	0.968016	0.181818	0.994832	

Precision

Fold 1 0.578947 Fold 2 0.625000 Fold 3 0.611111 Fold 4 0.625000 Fold 5 0.545455

Mean Metrics:

AUPR 0.285361 ROC-AUC 0.783761 F1 0.254446 Accuracy 0.968419 Sensitivity 0.162189 Specificity 0.996175 Precision 0.597103 dtype: float64

3.1 Random Forest Model with Grid SearchCV

```
[27]: rf_results_all = []
      rf_fprs, rf_tprs, rf_precisions, rf_recalls = [], [], [], []
      kf = StratifiedKFold(n_splits=5, random_state=1, shuffle=True)
      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]
      labels = [row[2] for row in all data]
      for fold, (train_idx, val_idx) in enumerate(kf.split(all_data, labels)):
          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] \text{ for } x \text{ 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:__

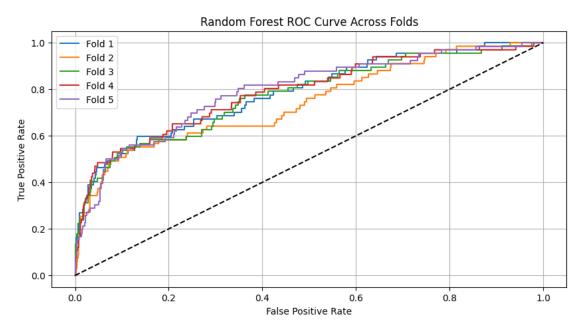
¬{rf_fold_metrics[1]:.4f}, "
        f"F1: {rf_fold_metrics[2]:.4f}, Acc: {rf_fold_metrics[3]:.4f}")
```

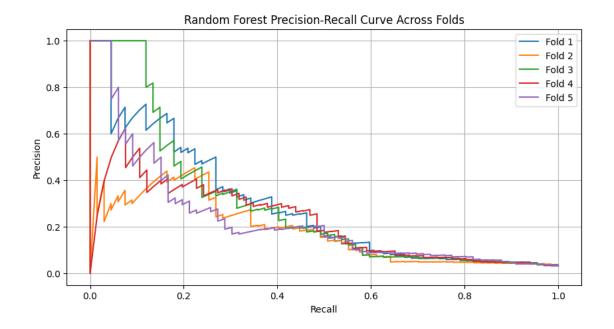
```
RF Fold 1
Fold 1 | AUPR: 0.2833, AUC: 0.7858, F1: 0.3146, Acc: 0.9391
RF Fold 2
Fold 2 | AUPR: 0.1777, AUC: 0.7437, F1: 0.2703, Acc: 0.9460
RF Fold 3
Fold 3 | AUPR: 0.2907, AUC: 0.7751, F1: 0.3000, Acc: 0.9510
RF Fold 4
Fold 4 | AUPR: 0.2140, AUC: 0.7885, F1: 0.3452, Acc: 0.9450
RF Fold 5
Fold 5 | AUPR: 0.2258, AUC: 0.7930, F1: 0.2414, Acc: 0.9560
```

3.1.1 Random Forest ROC & PR Curves

```
[28]: 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))
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()
```



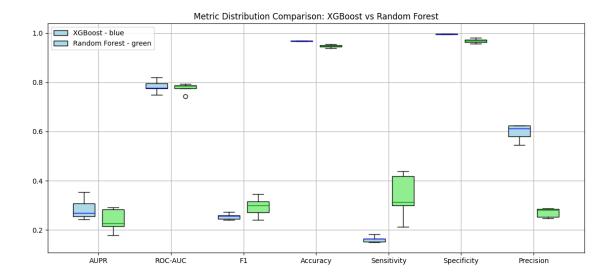


3.1.2 Metric Boxplot: XGBoost vs Random Forest

```
[29]: 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'), u
       →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()
```



Random Forest Fold-wise Metrics 3.1.3

```
[30]: 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	0.283325	0.785815	0.314607	0.939061	0.417910	0.957106	
Fold 2	0.177674	0.743683	0.270270	0.946027	0.298507	0.968459	
Fold 3	0.290701	0.775147	0.300000	0.951024	0.313433	0.973113	
Fold 4	0.214031	0.788474	0.345238	0.945027	0.439394	0.962274	
Fold 5	0.225815	0.793015	0.241379	0.956022	0.212121	0.981395	

Precision

Fold 1 0.252252 Fold 2 0.246914

Fold 3 0.287671

Fold 4

0.284314

Fold 5 0.280000

Random Forest - Mean Metrics:

AUPR 0.238309 ROC-AUC 0.777227 F1 0.294299 Accuracy 0.947432 Sensitivity 0.336273 Specificity 0.968469

Precision 0.270230

dtype: float64

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

```
[31]: 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
                                                  Accuracy Sensitivity \
                                              F1
     XGBoost
                    0.285361 0.783761 0.254446
                                                  0.968419
                                                               0.162189
     Random Forest 0.238309 0.777227 0.294299 0.947432
                                                               0.336273
                    Specificity Precision
                       0.996175
     XGBoost
                                  0.597103
     Random Forest
                       0.968469
                                  0.270230
```

4 XGBoost with LOGO

```
[31]: # 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): 65

```
[32]: 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 =
 dobtain_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 =
 Gobtain 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)
```

0%| | 0/65 [00:00<?, ?it/s]

```
FileNotFoundError
                                         Traceback (most recent call last)
Cell In[32], line 25
     22 val_labels = [x[2] for x in val_set]
     24 # Obtain features
---> 25 X_phage_dna_tr, X_host_dna_tr, X_phage_pro_tr, X_host_pro_tr, y_train =
 cobtain features(train phages, train hosts, train labels, dna base, pro base)
     26 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)
     29 # Combine features for train and val
Cell In[19], line 5, in obtain_features(phage_list, host_list, labels, dna_base__
 →pro_base)
      3 X_phage_pro, X_host_pro = [], []
     4 for p, h in zip(phage_list, host_list):
           X phage dna.
 ⇒append(load_feature_vector(os.path.join(dna_base, 'phage', f'{p}.txt')))
           X_host_dna.append(load_feature_vector(os.path.join(dna_base,__
 X_phage_pro.append(load_feature_vector(os.path.join(pro_base,_

¬'phage', f'{p}.txt')))
Cell In[5], line 2, in load feature vector(file path)
     1 def load_feature_vector(file_path):
----> 2
           return np.loadtxt(file_path)
```

```
File D:\Bachelorarbeit\Prediction Notebooks\.
  ovenv2\lib\site-packages\numpy\lib\_npyio_impl.py:1395, in loadtxt(fname,udtype, comments, delimiter, converters, skiprows, usecols, unpack, ndmin, u
   ⇔encoding, max rows, quotechar, like)
       1392 if isinstance(delimiter, bytes):
                           delimiter = delimiter.decode('latin1')
       1393
-> 1395 arr = read(fname, dtype=dtype, comment-comment, delimiter=delimiter,
       1396
                                             converters=converters, skiplines=skiprows, usecols=usecols,
       1397
                                             unpack=unpack, ndmin=ndmin, encoding=encoding,
       1398
                                             max_rows=max_rows, quote=quotechar)
       1400 return arr
File D:\Bachelorarbeit\Prediction Notebooks\.
   ovenv2\lib\site-packages\numpy\lib\_npyio_impl.py:1022, in _read(fname,_
   delimiter, comment, quote, imaginary unit, usecols, skiplines, max_rows, u
   ⇔converters, ndmin, unpack, dtype, encoding)
                           fname = os.fspath(fname)
       1020
       1021 if isinstance(fname, str):
-> 1022
                           fh = np.lib._datasource.open(fname, 'rt', encoding=encoding)
                           if encoding is None:
       1023
       1024
                                    encoding = getattr(fh, 'encoding', 'latin1')
File D:\Bachelorarbeit\Prediction Notebooks\.
   ovenv2\lib\site-packages\numpy\lib\_datasource.py:192, in open(path, mode, open (path, open (pa
   ⇔destpath, encoding, newline)
         155 """
         156 Open `path` with `mode` and return the file object.
         157
       (...)
         188
         189 """
         191 ds = DataSource(destpath)
--> 192 return ds open(path, mode, encoding=encoding, newline=newline)
File D:\Bachelorarbeit\Prediction Notebooks\.
   ovenv2\lib\site-packages\numpy\lib\_datasource.py:529, in DataSource.open(self_u
   →path, mode, encoding, newline)
         526
                           return file openers[ext](found, mode=mode,
         527
                                                                                      encoding=encoding, newline=newline)
         528 else:
--> 529
                           raise FileNotFoundError(f"{path} not found.")
FileNotFoundError: ../ordina_dataset_features/
   ⇒dna_features_ordinal_data\phage\001-023.txt not found.
```