A Genes-Only Random Forest Classifier for CRC Anatomical Side

August 24, 2022

[7]:
```
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#March 27, 2022

# Description:
#This code is for evaluating and finalizing a random forest model after using␣
 ↪grid search cv to find the best parameters
#Includes scoring and validation

# Import required packages and functions
import sklearn
import numpy as np
import pandas as pd
import rpy2.robjects as robjects
import pickle
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.ensemble import RandomForestClassifier
from sklearn.model_selection import train_test_split
from sklearn import metrics
from rpy2.robjects import pandas2ri
from sklearn.metrics import confusion_matrix, make_scorer
from sklearn.metrics import classification_report
from sklearn.metrics import roc_curve
from matplotlib import pyplot


# Increase output plot resolution
plt.rcParams['figure.dpi'] = 300
plt.rcParams['savefig.dpi'] = 300
sns.set(rc={"figure.dpi":300, 'savefig.dpi':300})
sns.set_context('notebook')
sns.set_style("whitegrid")


# Import the training set data (278 samples)
pandas2ri.activate()
readRDS = robjects.r['readRDS']
```

```
ml_data=readRDS('/Volumes/FryShareNVME/Preprocessing_Workflow/2022-05-23␣
 ↪preprocessing workflow_SIDE_SPLIT/output_data/
 ↪2022-03-25-ML-VALUES-discovery-set-side-278samples.rds')
tpmdata=ml_data[0]
tpmdata2=tpmdata.transpose()
targetdata=np.ravel(ml_data[1]).astype(int)
targetlabels=np.ravel(ml_data[2])
```

[8]:
```
# Create the classifier from the best parameter set found in the grid search CV
rforest_finalparamset = RandomForestClassifier(
    bootstrap=True,
    class_weight=None,
    criterion='gini',
    max_depth=5,
    max_features=0.1,
    max_leaf_nodes=4,
    min_impurity_decrease=0.0,
    min_samples_leaf=1,
    min_samples_split=2,
    min_weight_fraction_leaf=0.0,
    n_estimators=25,
    n_jobs=2,
    oob_score=True,
    random_state=2,
    verbose=0,
    warm_start=False
)
```

[9]:
```
# Split the dataset into training and testing
#Test Size = 0.25 instructs the model to fit on 75% of the data and test on 25%
#Stratify ensures an even distribution of samples
#Fixing random state allows for reproducibility of results
X_train, X_test, y_train, y_test = train_test_split(tpmdata2, targetdata,
                                                    test_size=0.
 ↪25,random_state=1,
                                                    ␣
 ↪stratify=targetdata,shuffle=True)

# Fit (train) the classifier to our dataset
#alternatively import this from a file if you have already saved the model (.
 ↪pkl)
#rforest_finalparamset.fit(X_train,y_train)

# Load the model from disk
#filename = '/Volumes/FryShareNVME/2022-03-25-ML-Results-Side/
 ↪2022-03-26-ML-paramset-analysis/crc-side-random-forest-model.pkl'
```

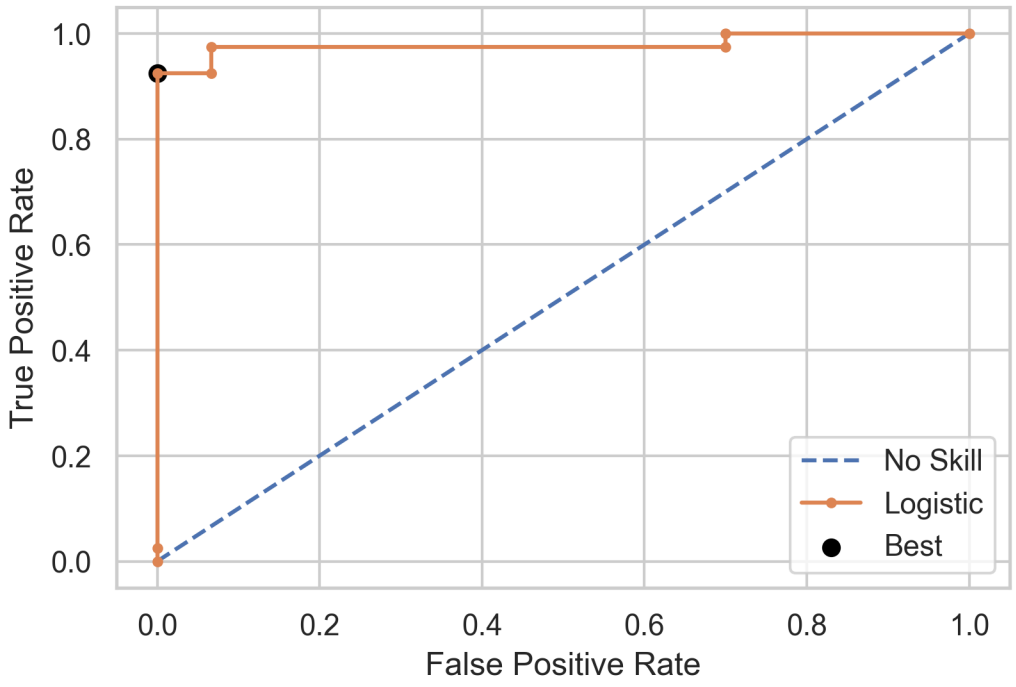
```
filename = '/Volumes/FryShareNVME/2022-03-25-ML-Results-Side/
 ↪2022-03-27-finalized-paper-data/genes-rf-exploration/
 ↪crc-side-random-forest-model.pkl'
rforest_finalparamset = pickle.load(open(filename, 'rb'))
#rforest_finalparamset2.score(X_test, Y_test)
# Save the model to disk
#filename = '/Volumes/FryShareNVME/2022-03-25-ML-Results-Side/
 ↪2022-03-26-ML-paramset-analysis/crc-side-random-forest-model.pkl'
#pickle.dump(rforest_finalparamset, open(filename, 'wb'))


# Make predictions from the training data
rfpredictions=rforest_finalparamset.predict(X_test)
print("Model Accuracy:",metrics.accuracy_score(y_test,rfpredictions))
```

```
Model Accuracy: 0.9428571428571428
```

[12]:
```
# Threshold hyperparameter optimization
#The default threshold for a binary variable is 0.5
#Checking the threshold allows for the optimization of the sensitivity and␣
 ↪specificity
#and a correction for imbalanced datasets
#If a new threshold is set then you must nolonger use .predict, and must use .
 ↪predict_proba



# Generate prediction probabilities (necessary for AUROC/AUPRC and thresholds)
yhat = rforest_finalparamset.predict_proba(X_test)
# keep probabilities for the positive outcome only
yhat = yhat[:, 1]
# calculate roc curves
fpr, tpr, thresholds = roc_curve(y_test, yhat)
# calculate the g-mean for each threshold
gmeans = np.sqrt(tpr * (1-fpr))
# locate the index of the largest g-mean
ix = np.argmax(gmeans)
print('Best Threshold=%f, G-Mean=%.3f' % (thresholds[ix], gmeans[ix]))
# plot the roc curve for the model
pyplot.plot([0,1], [0,1], linestyle='--', label='No Skill')
pyplot.plot(fpr, tpr, marker='.', label='Logistic')
pyplot.scatter(fpr[ix], tpr[ix], marker='o', color='black', label='Best')
# axis labels
pyplot.xlabel('False Positive Rate')
pyplot.ylabel('True Positive Rate')
pyplot.legend()
# show the plot
```

```
pyplot.show()

#With Code Adapted From: https://machinelearningmastery.com/
 ↪threshold-moving-for-imbalanced-classification/
```

```
Best Threshold=0.539077, G-Mean=0.962
```



[13]:
```
# See how a threshold adjustment affects the training set
#I ultimately chose to just keep the 0.5 threshold as the scores are close␣
 ↪enough
#and it is not of utmost importance in this model to prioritize
#precision(specificity) or recall(sensitivity) over the other

threshold = 0.539077
thresholdpredictions = rforest_finalparamset.predict_proba(X_test)
discpreds2 = thresholdpredictions[:, 1]
test_predictions=rforest_finalparamset.predict(X_test)

preds = [1 if thresholdpredictions[i][1]> threshold else 0 for i in␣
 ↪range(len(thresholdpredictions))]

print("0.539077 Threshold:")
pd.DataFrame(classification_report(y_test,preds,output_dict=True)).T
```

```
0.539077 Threshold:
```

[13]:

	precision	recall	f1-score	support
0	0.882353	1.000000	0.937500	30.000000
1	1.000000	0.900000	0.947368	40.000000
accuracy	0.942857	0.942857	0.942857	0.942857
macro avg	0.941176	0.950000	0.942434	70.000000
weighted avg	0.949580	0.942857	0.943139	70.000000

[14]:
```
print("0.5 Threshold:")
pd.DataFrame(classification_report(y_test,test_predictions,output_dict=True)).T
```

```
0.5 Threshold:
```

[14]:

	precision	recall	f1-score	support
0	0.933333	0.933333	0.933333	30.000000
1	0.950000	0.950000	0.950000	40.000000
accuracy	0.942857	0.942857	0.942857	0.942857
macro avg	0.941667	0.941667	0.941667	70.000000
weighted avg	0.942857	0.942857	0.942857	70.000000

[15]:
```
# Print Scoring Metrics for Training (Model Discovery) Set
print("Accuracy:",metrics.accuracy_score(y_test,rfpredictions))
print("Out-of-Bag Score:",rforest_finalparamset.oob_score_)
print("F1 Score:",metrics.f1_score(y_test,rfpredictions))
print("ROC AUC Score:",metrics.roc_auc_score(y_test,rfpredictions))
print("Recall Score:",metrics.recall_score(y_test,rfpredictions))
print("Precision Score:",metrics.precision_score(y_test,rfpredictions))
confmat = confusion_matrix(y_test,rfpredictions)
fp = confmat[0][1]
tn = confmat[0][0]
tp = confmat[1][1]
fn = confmat[1][0]
tprate=tp/(tp+fn)
fprate=fp/(fp+tn)

print("False Positives:",fp)
print("False Negatives:",fn)
print("True Positives:",tp)
print("True Negatives:",tn)
print("True Positive Rate:",tprate)
print("False Positive Rate:",fprate)

print(classification_report(y_test,rfpredictions))
```

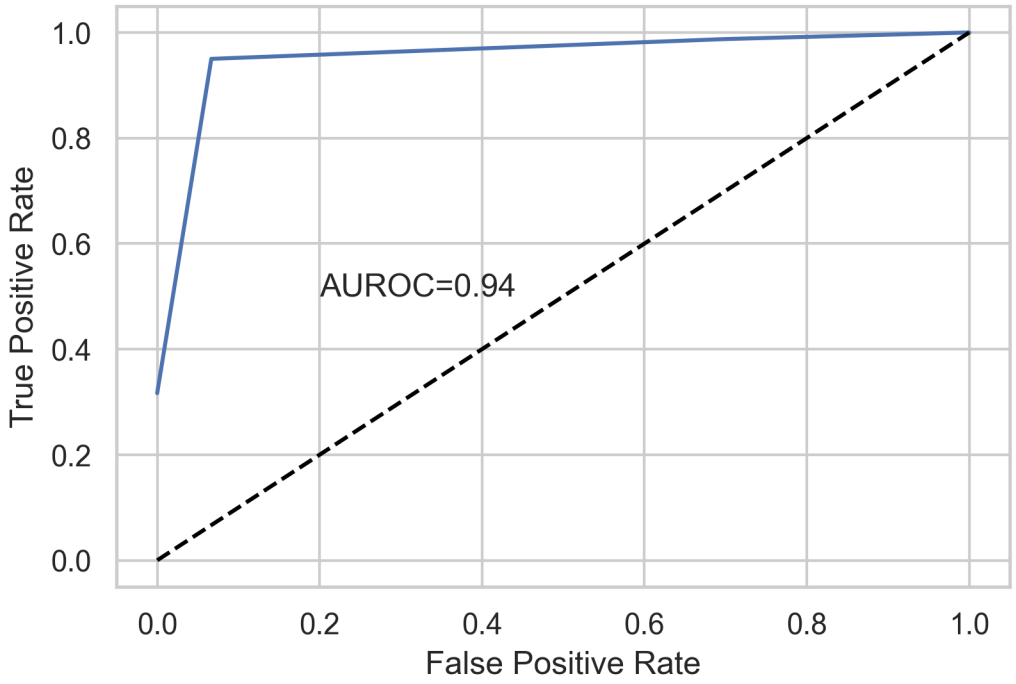
```
Accuracy: 0.9428571428571428
Out-of-Bag Score: 0.7342342342342343
F1 Score: 0.9500000000000001
ROC AUC Score: 0.9416666666666667
Recall Score: 0.95
```

```
Precision Score: 0.95
False Positives: 2
False Negatives: 2
True Positives: 38
True Negatives: 28
True Positive Rate: 0.95
False Positive Rate: 0.06666666666666667
              precision    recall  f1-score   support

           0       0.93      0.93      0.93        30
           1       0.95      0.95      0.95        40

    accuracy                           0.94        70
   macro avg       0.94      0.94      0.94        70
weighted avg       0.94      0.94      0.94        70
```

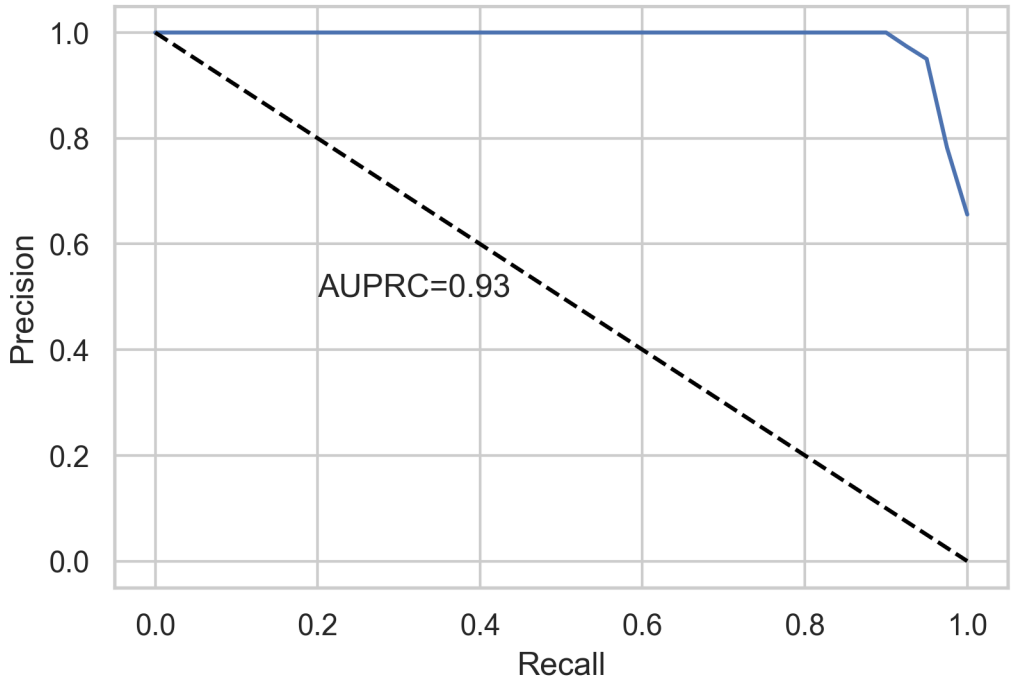
[16]:
```python
# Generate AUROC/AUPRC scores and create functions for plotting curves
val_auprc = sklearn.metrics.
 ↪average_precision_score(y_test,rfpredictions,pos_label=1)

val_auroc = sklearn.metrics.roc_auc_score(y_test,rfpredictions)
aurocscore="AUROC="+str(round(val_auroc,2))
auprcscore="AUPRC="+str(round(val_auprc,2))
print(auprcscore)
print(aurocscore)
def plot_auroc_curve(y_test,rfpredictions,aurocscore):
    data_fpr, data_tpr, data_thresholds = sklearn.metrics.
 ↪roc_curve(y_test,rfpredictions)
    data_fpr_tpr = pd.DataFrame({'fpr':data_fpr, 'tpr':data_tpr})
    p = sns.lineplot(data=data_fpr_tpr, x='fpr', y='tpr',ci=None)
    p.set(xlabel='False Positive Rate', ylabel='True Positive Rate')
    p.plot([0, 1], [0, 1], color='black', ls='--')
    p.text(0.2,0.5,aurocscore)

def plot_auprc_curve(y_test,rfpredictions,auprcscore):
    data_prcsn, data_rcll, data_thrshlds = sklearn.metrics.
 ↪precision_recall_curve(y_test,rfpredictions)
    data_prcsn_rcll = pd.DataFrame({'prcsn':data_prcsn, 'rcll':data_rcll})
    p = sns.lineplot(data=data_prcsn_rcll, x='rcll', y='prcsn',ci=None)
    p.set(xlabel='Recall', ylabel='Precision')
    p.plot([0, 1], [1, 0], color='black', ls='--')
    p.text(0.2,0.5,auprcscore)
```

```
AUPRC=0.93
AUROC=0.94
```

[18]:
```
# Plot AUROC Curve
plot_auroc_curve(y_test,discpreds2,aurocscore)

# Save to file
plt.savefig("/Volumes/FryShareNVME/2022-03-25-ML-Results-Side/
  ↪2022-03-27-finalized-paper-data/genes-rf-exploration/plots-for-paper/
  ↪AUROC-training-set-v2genesonly.pdf")
```



[19]:
```
# Plot AUPRC Curve
plot_auprc_curve(y_test,discpreds2,auprcscore)

# Save to file
plt.savefig("/Volumes/FryShareNVME/2022-03-25-ML-Results-Side/
  ↪2022-03-27-finalized-paper-data/genes-rf-exploration/plots-for-paper/
  ↪AUPRC-training-set-v2genesonly.pdf")
```



[20]:
```
# Import independent validation set (30 samples the model has never seen before)
pandas2ri.activate()
readRDS = robjects.r['readRDS']
val_data=readRDS('/Volumes/FryShareNVME/Preprocessing_Workflow/2022-05-23␣
 ↪preprocessing workflow_SIDE_SPLIT/output_data/
 ↪2022-03-25-ML-VALUES-validation-set-side-30samples.rds')
valdata=val_data[0]
valdata2=valdata.transpose()
valtargetdata=np.ravel(val_data[1]).astype(int)
```

[21]:
```
# Run the model on the validation set
runmodelonvaldata=rforest_finalparamset.predict(valdata2)
```

[22]:
```
# Generate prediction probabilities (necessary for AUROC/AUPRC and thresholds)
val_prob_preds = rforest_finalparamset.predict_proba(valdata2)

# Take only the positive values
val_preds = val_prob_preds[:, 1]
```

[23]:
```
# Print Scoring Metrics for Validation Set
print("Accuracy:",metrics.accuracy_score(runmodelonvaldata, valtargetdata))
print("F1 Score:",metrics.f1_score(runmodelonvaldata, valtargetdata))
print("ROC AUC Score:",metrics.roc_auc_score(runmodelonvaldata, valtargetdata))
print("Recall Score:",metrics.recall_score(runmodelonvaldata, valtargetdata))
```

```
print("Precision Score:",metrics.precision_score(runmodelonvaldata,␣
 ↪valtargetdata))
confmat = confusion_matrix(runmodelonvaldata,valtargetdata)
fp = confmat[0][1]
tn = confmat[0][0]
tp = confmat[1][1]
fn = confmat[1][0]
tprate=tp/(tp+fn)
fprate=fp/(fp+tn)

print("False Positives:",fp)
print("False Negatives:",fn)
print("True Positives:",tp)
print("True Negatives:",tn)
print("True Positive Rate:",tprate)
print("True Negative Rate:",fprate)

print(classification_report(runmodelonvaldata, valtargetdata))
```

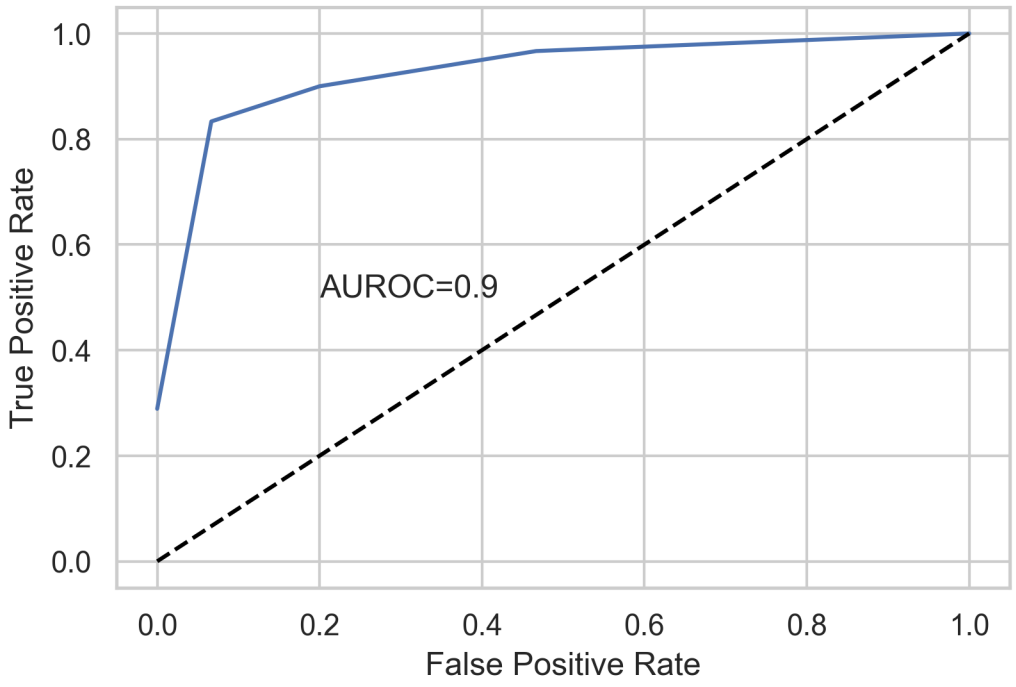
```
Accuracy: 0.9
F1 Score: 0.896551724137931
ROC AUC Score: 0.9017857142857143
Recall Score: 0.9285714285714286
Precision Score: 0.8666666666666667
False Positives: 2
False Negatives: 1
True Positives: 13
True Negatives: 14
True Positive Rate: 0.9285714285714286
True Negative Rate: 0.125
              precision    recall  f1-score   support

           0       0.93      0.88      0.90        16
           1       0.87      0.93      0.90        14

    accuracy                           0.90        30
   macro avg       0.90      0.90      0.90        30
weighted avg       0.90      0.90      0.90        30
```

[24]:
```
# Generate validation set AUROC/AUPRC scores
val_auprc = sklearn.metrics.average_precision_score(runmodelonvaldata,␣
 ↪valtargetdata,pos_label=1)

val_auroc = sklearn.metrics.roc_auc_score(runmodelonvaldata, valtargetdata)
aurocscore="AUROC="+str(round(val_auroc,2))
auprcscore="AUPRC="+str(round(val_auprc,2))
```

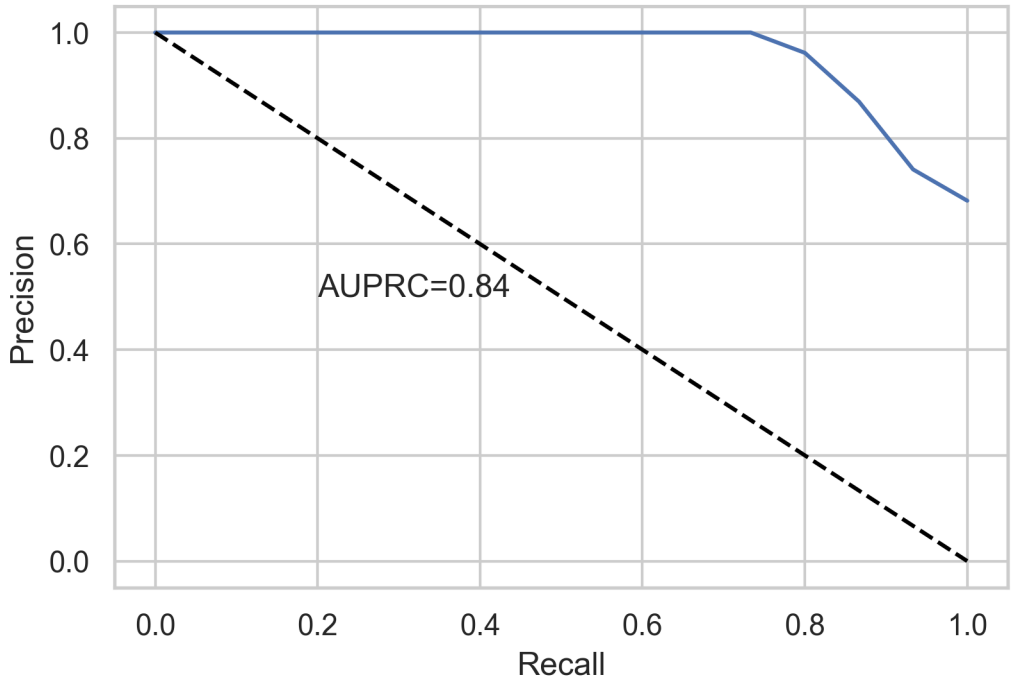
```
print(auprcscore)
print(aurocscore)
```

```
AUPRC=0.84
AUROC=0.9
```

[25]:
```
# Plot AUROC Curve
auroccurve=plot_auroc_curve(valtargetdata,val_preds,aurocscore)

# Save to file
plt.savefig("/Volumes/FryShareNVME/2022-03-25-ML-Results-Side/
  ↪2022-03-27-finalized-paper-data/genes-rf-exploration/plots-for-paper/
  ↪AUROC-validation-set-v2-genesonly.pdf")
```



[26]:
```
# Plot AUPRC Curve
plot_auprc_curve(valtargetdata,val_preds,auprcscore)

# Save to file
plt.savefig("/Volumes/FryShareNVME/2022-03-25-ML-Results-Side/
  ↪2022-03-27-finalized-paper-data/genes-rf-exploration/plots-for-paper/
  ↪AUPRC-validation-set-v2-genesonly.pdf")
```



[27]:
```
# See how a threshold adjustment affects the validation set (as a post-measure
 ↪of performance, not for threshold optimization)
#I ultimately chose to just keep the 0.5 threshold as the scores are close
 ↪enough
#and it is not of utmost importance in this model to prioritize
#precision(specificity) or recall(sensitivity) over the other

threshold = 0.539077 # define threshold here
thresholdpredictions = rforest_finalparamset.predict_proba(valdata2)
valpredictions=rforest_finalparamset.predict(valdata2)

preds = [1 if thresholdpredictions[i][1]> threshold else 0 for i in
 ↪range(len(thresholdpredictions))]

# Print Classification Report for New Threshold
print("0.539077 Threshold:")
pd.DataFrame(classification_report(valtargetdata,preds,output_dict=True)).T
```

```
0.539077 Threshold:
```

[27]:

	precision	recall	f1-score	support
0	0.789474	1.000000	0.882353	15.000000
1	1.000000	0.733333	0.846154	15.000000
accuracy	0.866667	0.866667	0.866667	0.866667

macro avg	0.894737	0.866667	0.864253	30.000000
weighted avg	0.894737	0.866667	0.864253	30.000000

[28]:
```
# Print Classification Report for 0.5 Threshold (Default)
print("0.5 Threshold:")
pd.
 ↪DataFrame(classification_report(valtargetdata,valpredictions,output_dict=True)).
 ↪T
```

```
0.5 Threshold:
```

[28]:

	precision	recall	f1-score	support
0	0.875000	0.933333	0.903226	15.0
1	0.928571	0.866667	0.896552	15.0
accuracy	0.900000	0.900000	0.900000	0.9
macro avg	0.901786	0.900000	0.899889	30.0
weighted avg	0.901786	0.900000	0.899889	30.0

[29]:
```
# Save the feature importance scores of the random forest model mapped to the␣
 ↪features (genes)
ftnames=rforest_finalparamset.feature_names_in_
ftimportances=rforest_finalparamset.feature_importances_
df=pd.DataFrame({ 'feature_names':ftnames,'feature_importances':ftimportances,})
#df.shape
# Save to file
#df.to_csv("/Volumes/FryShareNVME/2022-03-25-ML-Results-Side/
 ↪2022-03-26-ML-paramset-analysis/
 ↪2022-03-27-crc-rf-final-feature-importance-scores.csv")
```