Biomedical Data Analysis - Lab 4

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Libraries used in practical session:

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split
from sklearn.metrics import roc_auc_score, roc_curve, auc
from sklearn.metrics import accuracy_score, precision_score,
recall_score, f1_score, classification_report
from sklearn.metrics import confusion_matrix
from sklearn.impute import KNNImputer
from sklearn.neighbors import KNeighborsRegressor
from sklearn.model_selection import cross_val_score
from IPython.display import HTML
from scipy.stats import pearsonr
import regex as re
```

Block I - Data loading and basic description

We load the dataset using the pandas' load_csv function, remember to specify semicolon (;) as the separator

```
df=pd.read_csv("../BiomedicalDataScience_LAB04//Data/
inadvance_synth.csv",sep=";")

df.info()

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 38416 entries, 0 to 38415
Data columns (total 22 columns):
 #   Column                 Non-Null Count  Dtype
---  ------                 --------------  -----
 0   Unnamed: 0             38416 non-null  int64
 1   age                    38416 non-null  int64
 2   barthel                10218 non-null  float64
 3   charlson               38339 non-null  float64
 4   codidiagingreso        27038 non-null  object
 5   codservicioreal        38416 non-null  object
 6   creatinina             30465 non-null  float64
 7   drg                     34776 non-null  float64
 8   estancias               38416 non-null  float64
 9   glucosa                 29188 non-null  float64
 10  hematocrito             30114 non-null  float64
 11  leucocitos              30114 non-null  float64
 12  metastatic_tumor        38339 non-null  float64
 13  num_grupoact3_HOSP      17415 non-null  float64
 14  numurgenciasprevias     37864 non-null  float64
 15  potasio                 29770 non-null  float64
 16  proteina_c_reactiva     20241 non-null  float64
 17  rdw_cv                  30082 non-null  float64
 18  rdw_sd                  30082 non-null  float64
 19  sodio                   30274 non-null  float64
 20  urea                    24156 non-null  float64
 21  label                   38416 non-null  float64
dtypes: float64(18), int64(2), object(2)
memory usage: 6.4+ MB
```

1. What is the size of the dataframe?

```
# Drop the "Unnamed" column
df = df.iloc[:,1:]

df.shape

(38416, 21)
```

2. What is the mean age?

```
mean = df.age.mean()
print(mean)

79.4033215326947
```

3. What is the age standard deviation (std)?

```
std=df.age.std()
print(std)

8.361737254115944
```

4. Which is the variable with the most amount of missing values? Can you list the name of the variables, sorting them by number of missing values?

```
def nullvalues(df=df):
    nullvalues = df.isnull().sum()
    features_sorted = nullvalues.sort_values(ascending=False)
    return features_sorted
print(nullvalues())
```

```
barthel                  28198
num_grupoact3_HOSP       21001
proteina_c_reactiva      18175
urea                     14260
codidiagingreso          11378
glucosa                   9228
potasio                   8646
rdw_sd                    8334
rdw_cv                    8334
hematocrito               8302
leucocitos                8302
sodio                     8142
creatinina                7951
drg                       3640
numurgenciasprevias        552
metastatic_tumor            77
charlson                    77
age                          0
estancias                    0
codservicioreal              0
label                        0
dtype: int64
```

5. Name which are the categorical variables.

```
categorical_variables = df.select_dtypes(include=['object'])
categorical_variables_names = categorical_variables.columns.tolist()
print(categorical_variables_names)
```

```
['codidiagingreso', 'codservicioreal']
```

```
def find_cat(x):
    if isinstance(x,str):
        pattern = r'[0-9]+.?[0-9]*'
        test = not (re.match(pattern, x))
        # print(f"{x}: {test}")  # Add this line for debugging
        return test
    # print(f"{x}: False")  # Add this line for debugging
    return False

def
categorical_enumeration(cat,categorical_variables=categorical_variable
s, printing=True):

  if printing:
    print('Evaluation of categorical variable "' + cat + '"')
  categories =
categorical_variables[categorical_variables[cat].apply(find_cat)]
  if cat == categorical_variables_names[0]:
    categories =
categorical_variables[categorical_variables[cat].apply(find_cat)]
  else:
    categories = categorical_variables[cat].astype(str)


  unique, count = np.unique(categories, return_counts=True)


  if printing:
    print('Number of categories for "'+ cat + '":', len(unique))

  combined = np.column_stack((unique, count))
  sorted_combined = combined[combined[:, 1].argsort()[::-1]]

  if printing:
    for i in sorted_combined:
      if isinstance(i[0],float):
        print("Class %f has %d samples" % (i[0],i[1]))
      else:
        print("Class " + str(i[0]) + " has %d samples" % i[1])

  return np.array(sorted_combined)

categories_codidiagingreso =
categorical_enumeration(categorical_variables_names[0])
```

```
Evaluation of categorical variable "codidiagingreso"
Number of categories for "codidiagingreso": 299
Class HMUR has 507 samples
Class HNEM has 382 samples
Class HCAR has 375 samples
Class V14.8 has 245 samples
Class HMIN has 215 samples
Class HONC has 214 samples
Class V15.82 has 195 samples
Class HNER has 183 samples
Class V14.0 has 181 samples
Class V58.61 has 121 samples
Class V14.1 has 105 samples
Class HHEM has 78 samples
Class M81403 has 76 samples
Class V58.67 has 71 samples
Class HURO has 65 samples
Class V14.6 has 63 samples
Class HMDG has 54 samples
Class V45.01 has 42 samples
Class M96923 has 1 samples
Class M98233 has 1 samples
Class M97313 has 1 samples
Class M98003 has 1 samples
Class M98013 has 1 samples
Class M84416 has 1 samples
Class M83233 has 1 samples
Class V18.8 has 1 samples
Class V10.82 has 1 samples
Class V17.1 has 1 samples
Class M98103 has 1 samples
Class HSEP has 1 samples
Class HUEG has 1 samples
Class HUML has 1 samples
Class V13.29 has 1 samples
Class V13.09 has 1 samples
Class V12.50 has 1 samples
Class M80203 has 1 samples
Class M80206 has 1 samples
Class V12.41 has 1 samples
Class V12.02 has 1 samples
Class V10.44 has 1 samples
Class V10.04 has 1 samples
Class V10.43 has 1 samples
Class M80906 has 1 samples
Class V10.41 has 1 samples
Class M81303 has 1 samples
Class V10.09 has 1 samples
Class V10.07 has 1 samples
Class M81703 has 1 samples
Class M82103 has 1 samples
Class M82403 has 1 samples
Class M82606 has 1 samples
Class M82613 has 1 samples
Class M82630 has 1 samples
Class E812.1 has 1 samples
```

```
categories_codservicioreal =
categorical_enumeration(categorical_variables_names[1])
```

```
Evaluation of categorical variable "codservicioreal"
Number of categories for "codservicioreal": 53
Class HMUR has 8233 samples
Class HNEM has 5422 samples
Class HCAR has 5124 samples
Class HMIN has 3633 samples
Class HNER has 2341 samples
Class HMDG has 2222 samples
Class HONC has 2041 samples
Class HUHP has 1159 samples
Class HURO has 1112 samples
Class HCDG has 1007 samples
Class HCOT has 741 samples
Class HHEM has 546 samples
Class HNEF has 522 samples
Class HCVA has 502 samples
Class HMDH has 472 samples
Class HCEP has 420 samples
Class HNCG has 381 samples
Class HUMI has 351 samples
Class HUEI has 332 samples
Class HCCV has 308 samples
Class HREU has 252 samples
Class HORL has 179 samples
Class HREA has 157 samples
Class HCTO has 154 samples
Class HCIR has 146 samples
Class HECR has 126 samples
Class HCLP has 71 samples
Class HSEP has 60 samples
Class HGIN has 55 samples
Class HUTP has 50 samples
Class HCMX has 49 samples
Class HUML has 44 samples
Class HCPL has 43 samples
Class HUMM has 31 samples
Class HUEM has 28 samples
Class HOFT has 22 samples
Class HRHB has 16 samples
Class HTRE has 15 samples
Class HULM has 13 samples
Class HRXD has 8 samples
Class HQUE has 5 samples
Class HALE has 4 samples
Class HDER has 4 samples
Class HUEG has 4 samples
Class HURQ has 2 samples
Class HTRA has 2 samples
Class HREM has 1 samples
Class HRER has 1 samples
Class HRQU has 1 samples
Class HRTE has 1 samples
Class HUDO has 1 samples
Class HUHT has 1 samples
Class HONG has 1 samples
```

In addition to the existing `codidiagingreso` and `codservicioreal` categorical variables including codes in the format

```
str
```

is `metastatic_tumor`, since its only values are 0 and 1.

6. Extract the 'label' column to another variable. How many positive cases there are? And negatives?

```
label_var = df['label']
positive = df[label_var==1].shape[0]
negative = df[label_var==0].shape[0]
print(f"Positive cases: {positive}")
print(f"Negative cases: {negative}")

Positive cases: 13431
Negative cases: 24985
```

Block II. Data preprocessing

1. Train-Test Split

How many samples have each set after the split?

Split the dataset in two: train (80%) and test (20%). Use a seed to allow replication.

```
seed = 42

X = df.drop('label', axis=1)
y = df['label']
X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.2, random_state=seed)

rows_train = X_train.shape[0]
rows_test = X_test.shape[0]
cols = X_train.shape[1]

print(f"Train samples: {rows_train}")
print(f"Test samples: {rows_test}")
print(f"Features: {cols}")

Train samples: 30732
Test samples: 7684
Features: 20
```

2. Categorical Variables

Implement the method to deal with categorical variables. Briefly explain the chosen alternative. What would happen if a variable in the test set contains a category that doesn't exist on the train set? How would you deal with this situation?

Categories: `codidiagingreso` and `codservicioreal`

Is required to have numerical values only in order to let a *Machine Learning Model* perform the training phase and, subsequently, the inference procedure.

It is possible to deal with categorical variables through a conversion to scalar numerical variables or create a vector *One hot encoded* substituting each `string` variable, that will be *unwinded* into the dataframe creating a new feature for each of them.

The first approach is followed in the previous defined function `categorical_enumeration` and the following `categorical_evaluation`, accordingly to the name, it is based on frequency (enumeration) of the appearing variables.

Furthermore, this approach will be abandoned in favour of the second one.

```
def categorical_evaluation(df,alpha=10):

    #
    # alpha variable represents how much weight the feature
"metastatic tumor"
    # has on the categorical variable.
    # This choice is given by the fact that features might need to be
more spread out.
    #
    # NOTE: alpha is not an tunable hyperparameter, but might need to
be suggested by a
    # medic or someone who has knowledge in the field.
    # It has been set to 10 by default to spread more the low
frequency variables,
    # but might be not a  correct assumption

    dataset = df.copy()
    cv = dataset.select_dtypes(include=['object'])
    for cat in cv.columns.tolist():
        enum =
categorical_enumeration(cat=cat,categorical_variables=cv,printing=Fals
e)

        # The ranking process starts here
        mapping = {}
        for i,e in enumerate(enum[:,0]):

            # Increase the feature "importance rank" by a slight
correlation with metastatic tumor variable
            # only for low frequency variables
            if enum[i,1]<5:
                increase =
np.sum(np.logical_and(dataset['metastatic_tumor']==1,dataset[cat]==e))

                # This increase is regulate by the aforementioned
```

```
alpha parameter
                enum[i,1] += enum[i,1]*(alpha*increase)

            enum[i,1] /= np.sum(enum[:,1]) # Represent the percentage
of appearance in the given dataset (instead of the frequency)
            mapping[e] = enum[i,1]
        dataset[cat] = dataset[cat].map(mapping)
        dataset[cat] = dataset[cat].astype(float,errors='ignore')  #
'coerce' will handle non-convertible values
        # filter =
np.logical_and(dataset.isnull(),np.logical_not(df.isnull()))
        # print(df[filter])






    #nullvalues(dataset)
    return dataset

X_train_categorical_mapped = categorical_evaluation(X_train)
X_test_categorical_mapped = categorical_evaluation(X_test)

X_train_categorical_mapped.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Index: 30732 entries, 29147 to 15795
Data columns (total 20 columns):
 #   Column                Non-Null Count  Dtype
---  ------                --------------  -----
 0   age                   30732 non-null  int64
 1   barthel               8222 non-null   float64
 2   charlson              30673 non-null  float64
 3   codidiagingreso       1905 non-null   float64
 4   codservicioreal       30732 non-null  float64
 5   creatinina            24410 non-null  float64
 6   drg                   27841 non-null  float64
 7   estancias             30732 non-null  float64
 8   glucosa               23372 non-null  float64
 9   hematocrito           24144 non-null  float64
 10  leucocitos            24144 non-null  float64
 11  metastatic_tumor      30673 non-null  float64
 12  num_grupoact3_HOSP    13964 non-null  float64
 13  numurgenciasprevias   30284 non-null  float64
 14  potasio               23860 non-null  float64
 15  proteina_c_reactiva   16210 non-null  float64
 16  rdw_cv                24120 non-null  float64
 17  rdw_sd                24120 non-null  float64
 18  sodio                 24269 non-null  float64
 19  urea                  19388 non-null  float64
```

```
dtypes: float64(19), int64(1)
memory usage: 4.9 MB
```

3.1 Dealing with Categorical Variables missing

Here we have decided to discard the categorical mapping approach in favour of an **encoding approach**, that let us achieve better results

and is more robust with respect to data acquired.

```
median_train = X_train['codidiagingreso'].apply(pd.to_numeric,
errors='coerce').median()

X_train['codidiagingreso'].fillna(median_train, inplace=True)

X_test['codidiagingreso'].fillna(median_train, inplace=True)

X_train.info()

<class 'pandas.core.frame.DataFrame'>
Index: 30732 entries, 29147 to 15795
Data columns (total 20 columns):
 #   Column                Non-Null Count  Dtype  
---  ------                --------------  -----  
 0   age                   30732 non-null  int64  
 1   barthel               8222 non-null   float64
 2   charlson              30673 non-null  float64
 3   codidiagingreso       30732 non-null  object 
 4   codservicioreal       30732 non-null  object 
 5   creatinina            24410 non-null  float64
 6   drg                   27841 non-null  float64
 7   estancias             30732 non-null  float64
 8   glucosa               23372 non-null  float64
 9   hematocrito           24144 non-null  float64
 10  leucocitos            24144 non-null  float64
 11  metastatic_tumor      30673 non-null  float64
 12  num_grupoact3_HOSP    13964 non-null  float64
 13  numurgenciasprevias   30284 non-null  float64
 14  potasio               23860 non-null  float64
 15  proteina_c_reactiva   16210 non-null  float64
 16  rdw_cv                24120 non-null  float64
 17  rdw_sd                24120 non-null  float64
 18  sodio                 24269 non-null  float64
 19  urea                  19388 non-null  float64
dtypes: float64(17), int64(1), object(2)
memory usage: 4.9+ MB

print(f"X_train codidiagingreso null values:
{X_train['codidiagingreso'].isnull().sum()} \n\
X_test codidiagingreso null values:
{X_test['codidiagingreso'].isnull().sum()}")

X_train codidiagingreso null values: 0
X_test codidiagingreso null values: 0
```

We have used the function `pd.to_numeric` to convert the values in the `codidiagingreso` column to numbers. The `errors='coerce'` option causes non-numeric values to be replaced with NaN (Not a Number) during the conversion. At the end of this operation, we get a Series of numeric values and NaN.

After converting the values to numbers (and replacing the non-numeric values with NaN), we calculate the median of the Train Set.

The median is calculated by ignoring NaN values, so you get the median only from the valid numeric values in the `codidiagingreso` column.

Then we applied this median obtained in the Training Set on the Test Set, as it was.

Category: `metastatic_tumor`

```
k_values = list(range(1, 11))


mean_scores = []
for k in k_values:
    imputer = KNNImputer(n_neighbors=k)
    imputed_data =
imputer.fit_transform(X_train[['metastatic_tumor']])


    knn_regressor = KNeighborsRegressor(n_neighbors=k)
    scores = cross_val_score(knn_regressor, imputed_data, y_train,
cv=10, scoring='neg_mean_squared_error')
    mean_scores.append(np.mean(scores))


best_k = k_values[np.argmin(mean_scores)]
print("The best number of neighbors is", best_k)

The best number of neighbors is 1
```

The code performs a search for the best value of `k` for a KNN-based regression model.

It uses `cross_val_score` to evaluate the performance of the model on training data.

The process helps select the best k value for the KNN model based on the data provided.

```
imputer = KNNImputer(n_neighbors=1)
metastatic_tumor_train = X_train[['metastatic_tumor']]

X_train_imputed = imputer.fit_transform(metastatic_tumor_train)
```

```
X_train['metastatic_tumor'] = X_train_imputed

X_test['metastatic_tumor'].astype('object')
X_test['metastatic_tumor'].fillna('Unknown', inplace=True)
```

In this part it has been used `KNNImputer().fit_transform` to impute the data in the Training Set.

Whereas in the Test Set the data has been filled with `Unknown` label, that does not appear in the Training Set, a more detailed discussion will be held in the *sub-section* number 4.

3.2 Dealing with Numerical Values missing

Implement the method to deal with the missing values. Briefly explain the chosen alternative. What would happen if a variable without missing on the train set appears to have been missing in the test set? How would you deal with them?

```
# Test to verify consistency of flatten and reshape functions
# heavily used in the SVT algorithm later defined

# mat = X_full.shape
# vect = X_full.shape[0]*X_full.shape[1]
# mask = (X_full.copy().flatten().reshape(mat) == X_full).flatten()
# (X_full.flatten()[mask]-
X_full.copy().flatten().reshape(mat).flatten()[mask]).sum()

(X_train['age'] == 65).sum()

748

avoid_categoricals = X_test.columns.to_list()
categorical_variables_names.append('metastatic_tumor')
for i in categorical_variables_names:
    avoid_categoricals.remove(i)
avoid_categoricals

['age',
 'barthel',
 'charlson',
 'creatinina',
 'drg',
 'estancias',
 'glucosa',
 'hematocrito',
 'leucocitos',
 'num_grupoact3_HOSP',
 'numurgenciasprevias',
 'potasio',
 'proteina_c_reactiva',
 'rdw_cv',
 'rdw_sd',
 'sodio',
 'urea']
```

SVT is a technique used in signal processing and matrix completion problems. It's primarily employed in scenarios where you have a matrix with missing or corrupted data, and you want to estimate the missing values based on the available information.

First of all we divide into two sets *Test* and *Train* the dataset in input.

Let us denote by Ω_{train} the set of observations in the train set, i.e. the values appearing in the original dataset corresponding to the train set,

similarly Ω_{test} is the set of observation in the test set. Let us denote by r_{ij} the corresponding rating.

Create a full matrix $X \in R^{n \times p}$, such that:

$$X_{i,j} = \begin{Bmatrix} r_{ij} & \text{if} \, (i,j) \in \Omega \\ 0 & \text{otherwise} \end{Bmatrix}$$

Then the algorithm is based on a iterative procedure for `n_max_iter`,

A *Singular Value Decomposition*, using `np.linalg.svd`,

a thresholding on the singular values based on `threshold`,

a `tolerance` that at each iteration is compared to the norm of the difference of the old matrix and the reconstructed new one,

the error is evaluated through:

the RMSE (root mean square error)

$$\text{RMSE} = \sqrt{\frac{1}{card\left(\Omega_{\text{test}}\right)} \sum_{(i,j) \in \Omega_{\text{test}}} \left(r_{ij} - r_{ij}^{\text{pred}}\right)^2}$$

and the Pearson correlation coefficient ρ, using `scipy.stats.pearsonr`:

$$\rho = \frac{\sum_{(i,j) \in \Omega_{\text{test}}} \left(r_{ij} - \bar{r}\right)\left(r_{ij}^{\text{pred}} - \bar{r}^{\text{pred}}\right)}{\sqrt{\sum_{(i,j) \in \Omega_{\text{test}}} \left(r_{ij} - \bar{r}\right)^2} \sqrt{\sum_{(i,j) \in \Omega_{\text{test}}} \left(r_{ij}^{\text{pred}} - \bar{r}^{\text{pred}}\right)^2}}$$

where

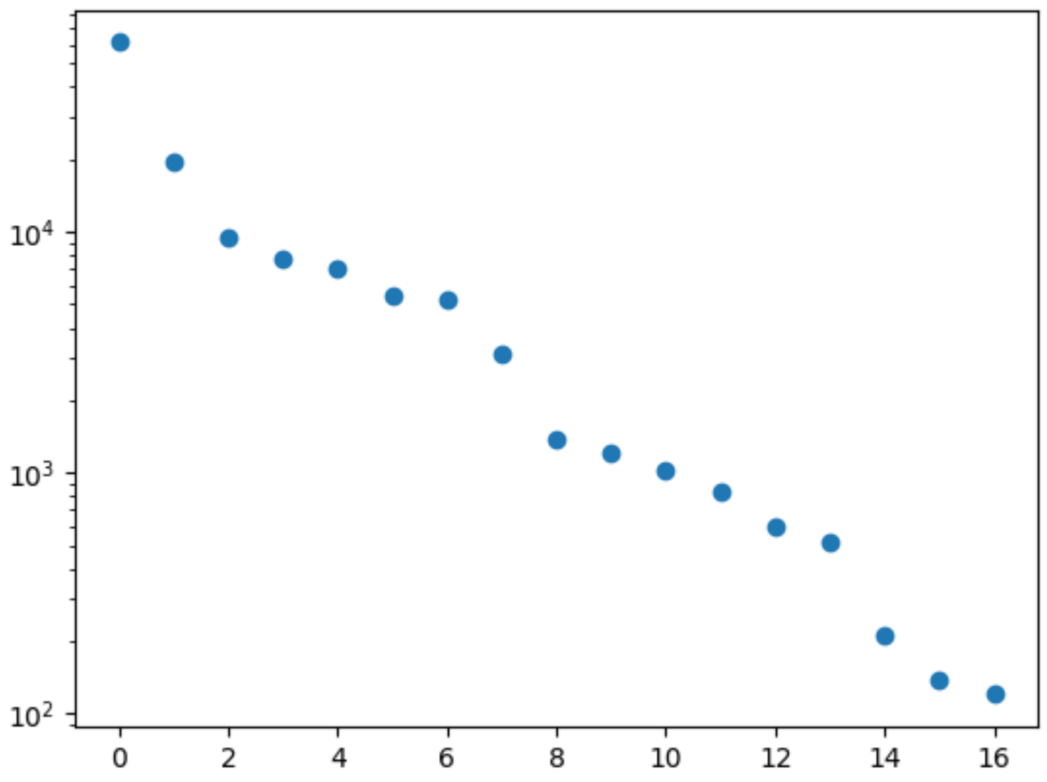
$$\begin{aligned} \bar{r} \quad & ¿ \frac{1}{card\left(\Omega_{\text{test}}\right)} \sum_{(i,j) \in \Omega_{\text{test}}} r_{ij} \\ \bar{r}^{\text{pred}} \quad & ¿ \frac{1}{card\left(\Omega_{\text{test}}\right)} \sum_{(i,j) \in \Omega_{\text{test}}} r_{ij}^{\text{pred}} \end{aligned}$$

```python
def SVT(X_input, \
        n_max_iter = 100, \
        threshold = 1000, \
        show=True, \
        tt_split = 0.2,
        tolerance = 1e-5, \
        seed=seed):

  X_input = X_input.to_numpy()
  mat = X_input.shape

  np.random.seed(seed) # for reproducibility
  indexes = np.random.permutation(mat[0])



  X = X_input.copy()[indexes]


  split = round(tt_split*mat[0])
  X_train = X[split:] # with non-null values
  X_test = X[:split] # with null values


  X_train = X_train.flatten()
  X_test = X_test.flatten()

  train_valid = ~np.isnan(X_train)
  vals_train = X_train[train_valid]

  test_valid = ~np.isnan(X_test)
  vals_test = X_test[test_valid]


  RMSE_SVT_history = []
  pearson_SVT_history = []

  X = np.append(X_train,X_test)
  X[np.isnan(X)] = 0

  X_hat = X.copy()
  for k in range(n_max_iter):
    X_hat_old = X_hat.copy()
    X_hat = X_hat.reshape(mat)
    U,s,VT = np.linalg.svd(X_hat, full_matrices = False)
    s[s < threshold] = 0
    X_hat = U @ np.diag(s) @ VT

    X_hat_train = X_hat[split:].flatten()
    X_hat_test = X_hat[:split].flatten()
    X_hat_train[train_valid] = vals_train
    X_hat = np.append(X_hat_train,X_hat_test)
    increment = np.linalg.norm(X_hat - X_hat_old)


    vals_test_SVT = X_hat_test[test_valid]
    RMSE_SVT = np.sqrt(np.mean((vals_test - vals_test_SVT)**2))
    pearson_SVT = pearsonr(vals_test, vals_test_SVT)[0]

    RMSE_SVT_history.append(RMSE_SVT)
    pearson_SVT_history.append(pearson_SVT)

    if show:
      print('======= iteration %d (increment %1.2e)' % (k, increment))
      print('RMSE = %f' % RMSE_SVT)
      print('rho = %f' % pearson_SVT)

    if tolerance > increment:
      break


  X_hat = X_hat.reshape(mat)
  X_hat_train = X_hat[split:].flatten()
  X_hat_test = X_hat[:split].flatten()

  X_hat_train[train_valid] = vals_train
  X_hat_test[test_valid] = vals_test

  X_hat = np.append(X_hat_train,X_hat_test)
  X_hat = X_hat.reshape(mat)


  X_hat = X_hat[-indexes]
  X_hat = pd.DataFrame(data=X_hat,columns=avoid_categoricals)
  X_hat['age'] = X_hat['age'].astype(int)

  if show:
    fig, axs = plt.subplots(2,1,figsize = (8,8))
    axs[0].loglog(RMSE_SVT_history, 'o-')
    axs[1].semilogx(pearson_SVT_history, 'o-')

  return X_hat

X_train_cat = X_train[categorical_variables_names]
X_train_avoid = X_train[avoid_categoricals]
```

In order to determine a value for `threshold` is recommended to plot the *singular values* first, to better understand the order of magnitude for the thresholding.

```
X_train_singular = X_train_avoid.to_numpy().copy()
X_train_singular[np.isnan(X_train_avoid)] = 0

_,s,_ = np.linalg.svd(X_train_singular,full_matrices=False)
plt.semilogy(s,'o')
```

```
[<matplotlib.lines.Line2D at 0x31c9e59d0>]
```



```
# Train Dataset SVT
X_train_prev = X_train_avoid
X_train_avoid = SVT(X_train_avoid,threshold=2e3,show=False)

print(f"Values for \"age\" previous to SVT: {(X_train_prev['age'] ==
65).sum()}")
print(f"Values for \"age\" posterior to SVT: {(X_train_avoid['age'] ==
65).sum()}")
```

```
Values for "age" previous to SVT: 748
Values for "age" posterior to SVT: 748
```

```
for i in X_train_prev.columns.tolist():
    print(f"Variable {i}: \n \
        Previous nulls: {X_train_prev[i].isnull().sum()}\n \
        Posterior nulls: {X_train_avoid[i].isnull().sum()}\n\n")
```

```
Variable age:
	Previous nulls: 0
	Posterior nulls: 0


Variable barthel:
	Previous nulls: 22510
	Posterior nulls: 0


Variable charlson:
	Previous nulls: 59
	Posterior nulls: 0


Variable creatinina:
	Previous nulls: 6322
	Posterior nulls: 0


Variable drg:
	Previous nulls: 2891
	Posterior nulls: 0


Variable estancias:
	Previous nulls: 0
	Posterior nulls: 0


Variable glucosa:
	Previous nulls: 7360
	Posterior nulls: 0


Variable hematocrito:
	Previous nulls: 6588
	Posterior nulls: 0


Variable leucocitos:
	Previous nulls: 6588
	Posterior nulls: 0


Variable num_grupoact3_HOSP:
	Previous nulls: 16768
	Posterior nulls: 0


Variable numurgenciasprevias:
	Previous nulls: 448
```

```
         Posterior nulls: 0


Variable potasio:
         Previous nulls: 6872
         Posterior nulls: 0


Variable proteina_c_reactiva:
         Previous nulls: 14522
         Posterior nulls: 0


Variable rdw_cv:
         Previous nulls: 6612
         Posterior nulls: 0


Variable rdw_sd:
         Previous nulls: 6612
         Posterior nulls: 0


Variable sodio:
         Previous nulls: 6463
         Posterior nulls: 0


Variable urea:
         Previous nulls: 11344
         Posterior nulls: 0
```

```
X_train =
pd.DataFrame(data=X_train_cat.to_numpy(),columns=X_train_cat.columns)
X_train =
pd.concat([X_train,pd.DataFrame(data=X_train_avoid.to_numpy(),columns=
X_train_avoid.columns)],axis=1)
print(X_train.isnull().sum())
```

```
codidiagingreso        0
codservicioreal        0
metastatic_tumor       0
age                    0
barthel                0
charlson               0
creatinina             0
drg                    0
estancias              0
glucosa                0
```

```
hematocrito             0
leucocitos              0
num_grupoact3_HOSP      0
numurgenciasprevias     0
potasio                 0
proteina_c_reactiva     0
rdw_cv                  0
rdw_sd                  0
sodio                   0
urea                    0
dtype: int64
```

```
for c in X_train.columns.tolist():
    median_train_c = X_train[c].apply(pd.to_numeric,
errors='coerce').median()

    X_test[c].fillna(median_train_c, inplace=True)
```

```
/Users/ermarinellone/Library/Mobile
Documents/com~apple~CloudDocs/BDS/myenv/lib/python3.11/site-packages/
numpy/lib/nanfunctions.py:1215: RuntimeWarning: Mean of empty slice
  return np.nanmean(a, axis, out=out, keepdims=keepdims)
```

```
X_test.isnull().sum()
```

```
age                     0
barthel                 0
charlson                0
codidiagingreso         0
codservicioreal         0
creatinina              0
drg                     0
estancias               0
glucosa                 0
hematocrito             0
leucocitos              0
metastatic_tumor        0
num_grupoact3_HOSP      0
numurgenciasprevias     0
potasio                 0
proteina_c_reactiva     0
rdw_cv                  0
rdw_sd                  0
sodio                   0
urea                    0
dtype: int64
```

To fill continous variables only we opted for an optimal approach, the SVT algorithm, described in the Markdown above.

We used the dataset selecting to avoid the categorical variables, already filled in the previous section, not employed in the matrix given as argument to the function `SVT`.

```
categorical_cols = ['codidiagingreso',
'codservicioreal','metastatic_tumor']

combined_data = pd.concat([X_train, X_test], axis=0)

combined_data_encoded = pd.get_dummies(combined_data,
columns=categorical_cols, prefix=categorical_cols)


X_train_encoded = combined_data_encoded.iloc[:len(X_train),:]
X_test_encoded = combined_data_encoded.iloc[len(X_train):,:]
```

To manage numerically the string values, we have used an *encoding-like* approach, thanks to the function `pd.get_dummies`.

Merging X_train and X_test into a single combined_data dataset ensures that the one-hot encoding takes into account all categories present in both sets, without having `np.shape` inconsistencies between Train Set and Test Set, otherwise issues could occur during prediction of the values. In this way all the features are represented both in the Train and Test Set, this will be discussed in *sub-section* 4.

NOTE: The previous cell should be in the *sub-section* 3.2, but for semplicity of coding we have left it as the last cell of the pre-processing phase.

4. Categorical Test-Train Dilemma

With our *features extension* approach we have proved that at most one of the new features generated by `pd.get_dummies` have a positive binary value (1), and the rest is set to negative (0).

This is particularly useful when it comes to the Test Set, indeed the unseen features in the Training Set will have the default weight (usually 0, but could be random) applied by the specific *Machine Learning Model* to features constantly null.

Therefore it does not try to improve it from the default weight and it will be kept constantly default until the end of the training!

Hence it is possible to say that the added value will not modify the behaviour of the algorithm, and in the inference phase the weight applied to the unseen feature is nothing but the default weight, since the original model has not been trained on it having a value different from 0.

Block III: Random Forest

```
from sklearn.ensemble import RandomForestClassifier

rf_classifier = RandomForestClassifier()
```

```
print("Default parameters of RandomForestClassifier:")
print(rf_classifier.get_params())
```

```
Default parameters of RandomForestClassifier:
{'bootstrap': True, 'ccp_alpha': 0.0, 'class_weight': None,
'criterion': 'gini', 'max_depth': None, 'max_features': 'sqrt',
'max_leaf_nodes': None, 'max_samples': None, 'min_impurity_decrease':
0.0, 'min_samples_leaf': 1, 'min_samples_split': 2,
'min_weight_fraction_leaf': 0.0, 'n_estimators': 100, 'n_jobs': None,
'oob_score': False, 'random_state': None, 'verbose': 0, 'warm_start':
False}
```

```
rf_classifier.fit(X_train_encoded, y_train)
```

```
RandomForestClassifier()
```

```
probabilities = rf_classifier.predict_proba(X_test_encoded)
```

```
positive_class_probabilities = probabilities[:, 1]
```

```
print(positive_class_probabilities)
```

```
[0.25 0.75 0.16 ... 0.24 0.42 0.23]
```

```
positive_probs = rf_classifier.predict_proba(X_test_encoded)[:, 1]


auc_roc_rf = round(roc_auc_score(y_test, positive_probs),4)
print("AUC-ROC Score:", auc_roc_rf)
```

```
AUC-ROC Score: 0.7543
```

The AUC-ROC score (Area Under the Receiver Operating Characteristic Curve) is a numerical measure of the area under the ROC curve. This value represents the ability of a classification model to distinguish between positive and negative classes.

In other words, the AUC-ROC score quantifies how well the model is able to separate positive and negative instances without being affected by the specific choice of classification threshold.

The AUC-ROC score is particularly useful when comparing binary classification models and wanting an overall assessment of their performance without having to choose a specific decision threshold.

A higher AUC-ROC value generally indicates a better model in distinguishing between positive and negative classes.

AUC-ROC = 1: Indicates a perfect model that is able to distinguish perfectly between positive and negative classes while AUC-ROC < 0.5: Indicates that the model is performing worse than a random case.

```
predictions = rf_classifier.predict(X_test_encoded)
```

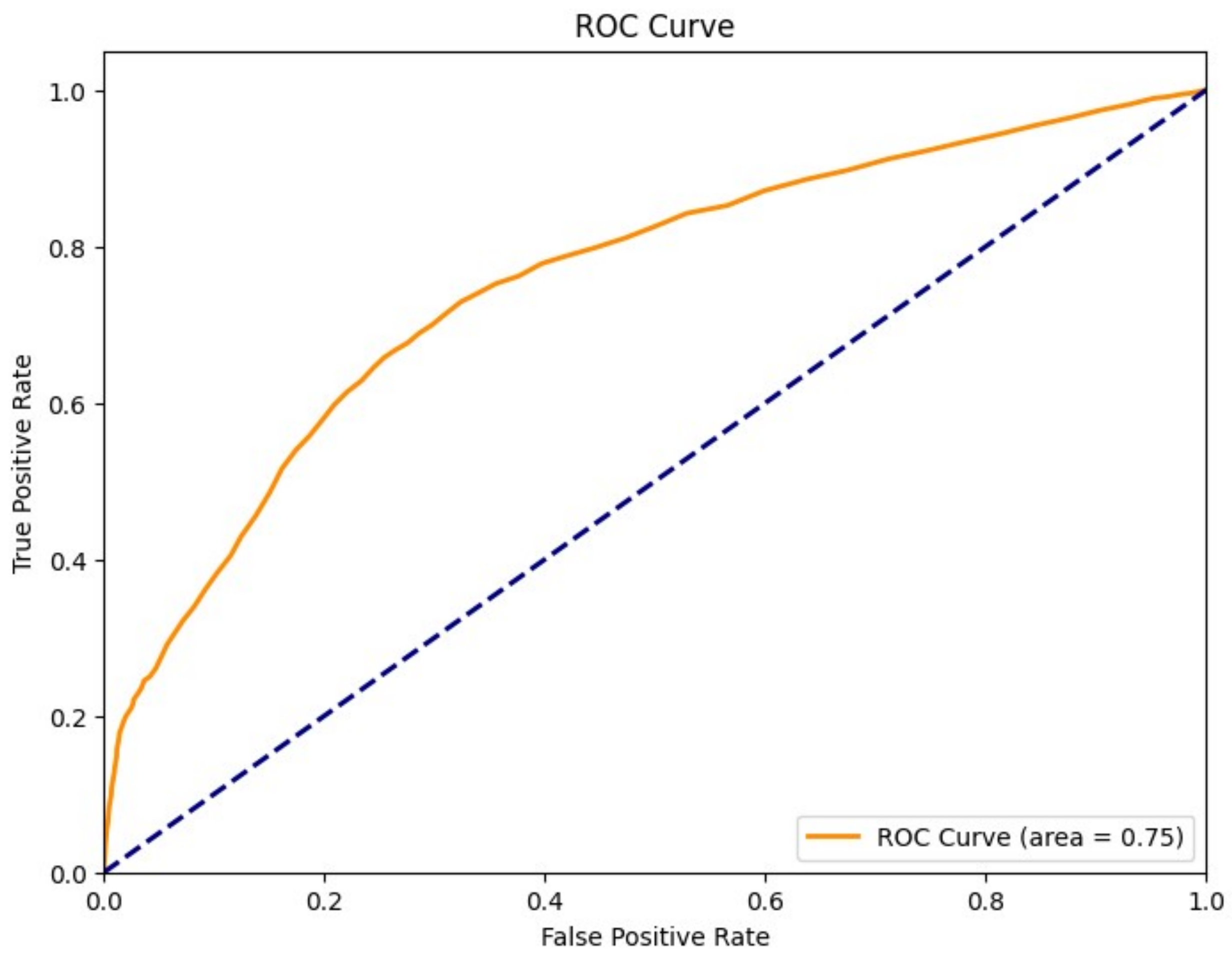
```
accuracy_rf = round(accuracy_score(y_test, predictions),4)
print("Accuracy:", accuracy_rf)

conf_matrix = confusion_matrix(y_test, predictions)

true_negative, false_positive, false_negative, true_positive =
conf_matrix.ravel()


sensitivity = round(true_positive / (true_positive +
false_negative),4)
specificity = round(true_negative / (true_negative +
false_positive),4)

print("Sensitivity (True Positive Rate):", sensitivity)
print("Specificity (True Negative Rate):", specificity)
```

```
Accuracy: 0.7185
Sensitivity (True Positive Rate): 0.3835
Specificity (True Negative Rate): 0.8969
```

1) Sensitivity measures the proportion of true positives (correctly classified positive instances) to the total number of true positive instances in the dataset. In other words, it indicates the model's ability to correctly identify instances of the positive class. Sensitivity (TPR) = $TP/TP+FN$ Sensitivity is important when the cost of a false negative (a negative prediction for an actually positive instance) is high, for example, in a diagnostic test where missing a positive condition is serious.

2) Specificity measures the proportion of true negatives (correctly classified negative instances) to the total number of true negative instances in the dataset. It indicates the model's ability to correctly identify instances of the negative class. Specificity (TNR) = $TN/TF+FP$ Specificity is important when the cost of a false positive (a positive prediction for an actually negative instance) is high, for example, in a test to identify dangerous behavior or safety situations.

```
fpr, tpr, thresholds = roc_curve(y_test, positive_probs)
roc_auc = auc(fpr, tpr)


plt.figure(figsize=(8, 6))
plt.plot(fpr, tpr, color='darkorange', lw=2, label='ROC Curve (area =
%0.2f)' % roc_auc)
plt.plot([0, 1], [0, 1], color='navy', lw=2, linestyle='--')
plt.xlim([0.0, 1.0])
plt.ylim([0.0, 1.05])
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('ROC Curve')
plt.legend(loc='lower right')
plt.show()
```



This code is used to visualize the ROC curve (Receiver Operating Characteristic curve) and calculate the AUC-ROC score for a binary classification model.

First the true positive and false positive rates are calculated for the classes predicted by the model, and then these quantities are used to calculate the Area Under the Curve (AUC) using false positive rates (fpr) and true positive rates (tpr).

Gradient Boosting & SVM (Optional)

Gradient Boosting

```
from sklearn.ensemble import GradientBoostingClassifier
from sklearn.model_selection import GridSearchCV

gb_clf = GradientBoostingClassifier()
print("Default parameters of Gradient Boosting:")
print(gb_clf.get_params())
```

```
Default parameters of Gradient Boosting:
{'ccp_alpha': 0.0, 'criterion': 'friedman_mse', 'init': None,
'learning_rate': 0.1, 'loss': 'log_loss', 'max_depth': 3,
'max_features': None, 'max_leaf_nodes': None, 'min_impurity_decrease':
```

```
0.0, 'min_samples_leaf': 1, 'min_samples_split': 2,
'min_weight_fraction_leaf': 0.0, 'n_estimators': 100,
'n_iter_no_change': None, 'random_state': None, 'subsample': 1.0,
'tol': 0.0001, 'validation_fraction': 0.1, 'verbose': 0, 'warm_start':
False}
```

```
gb_clf.fit(X_train_encoded, y_train)
```

```
GradientBoostingClassifier()
```

```
positive_probs = gb_clf.predict_proba(X_test_encoded)[:, 1]
```

```
auc_roc_gb = round(roc_auc_score(y_test, positive_probs),4)
print("AUC-ROC Score:", auc_roc_gb)
```

```
AUC-ROC Score: 0.7506
```

```
predictions = gb_clf.predict(X_test_encoded)
```

```
conf_matrix = confusion_matrix(y_test, predictions)
```

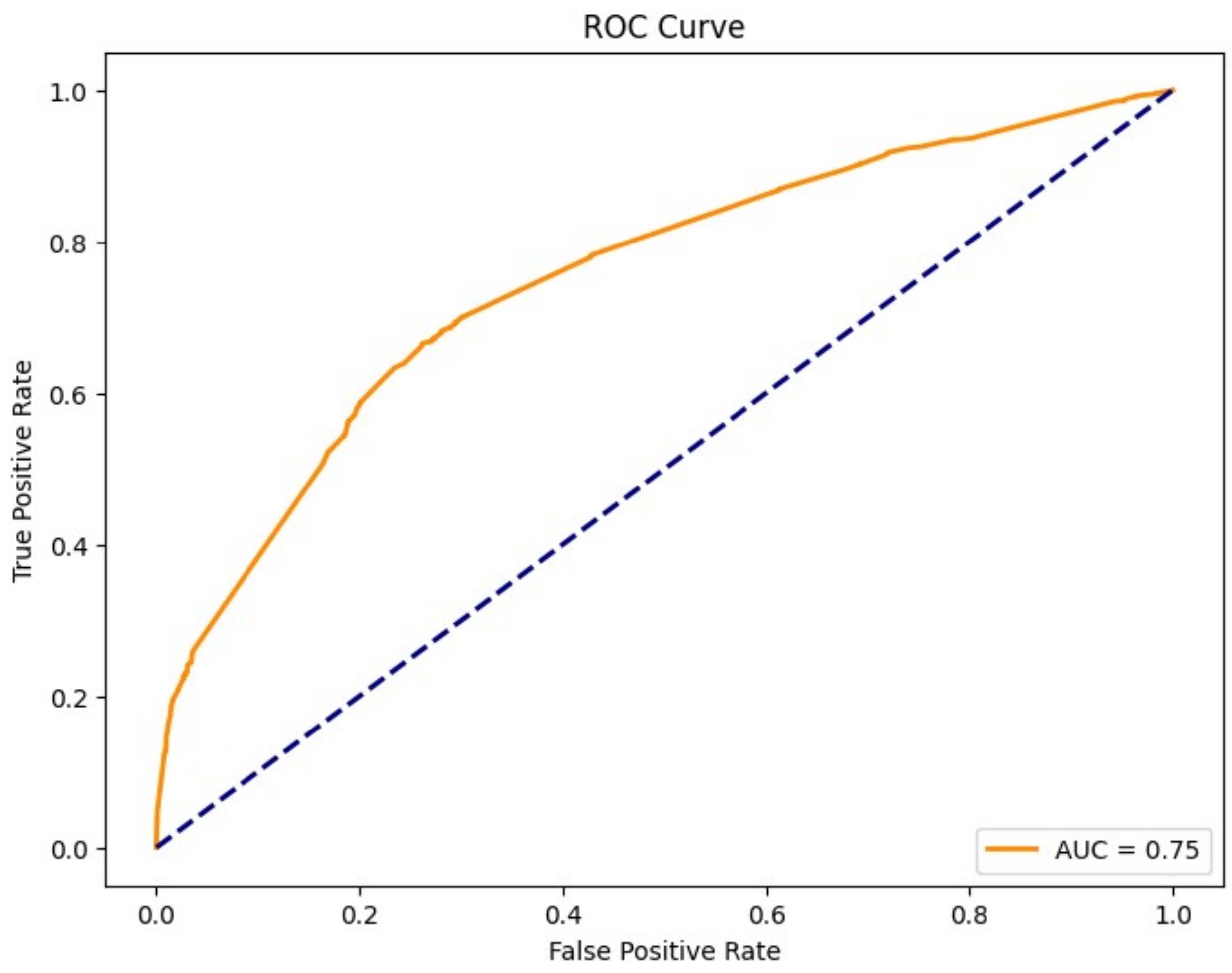
```
true_negative, false_positive, false_negative, true_positive =
conf_matrix.ravel()


sensitivity = round(true_positive / (true_positive +
false_negative),4)
specificity = round(true_negative / (true_negative +
false_positive),4)

print("Sensitivity (True Positive Rate):", sensitivity)
print("Specificity (True Negative Rate):", specificity)
```

```
Sensitivity (True Positive Rate): 0.261
Specificity (True Negative Rate): 0.9631
```

```
predictions = gb_clf.predict(X_test_encoded)
```

```
accuracy_gb = round(accuracy_score(y_test, predictions),4)
print(f'Accuracy of model: {accuracy_gb}')


class_names = ["Negative", "Positive"]
print(classification_report(y_test, predictions,
target_names=class_names))
```

```
Accuracy of model: 0.7192
              precision    recall  f1-score   support

    Negative       0.71      0.96      0.82      5014
    Positive       0.79      0.26      0.39      2670
    accuracy                           0.72      7684
   macro avg       0.75      0.61      0.60      7684
weighted avg       0.74      0.72      0.67      7684


probabilities = gb_clf.decision_function(X_test_encoded)
fpr, tpr, thresholds = roc_curve(y_test, probabilities)
auc = roc_auc_score(y_test, probabilities)

plt.figure(figsize=(8, 6))
plt.plot(fpr, tpr, color='darkorange', lw=2, label=f'AUC = {auc:.2f}')
plt.plot([0, 1], [0, 1], color='navy', lw=2, linestyle='--')
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('ROC Curve')
plt.legend(loc='lower right')
plt.show()
```



SVM

```
from sklearn.svm import SVC

svm_classifier = SVC(probability=True)

print("Default parameters of SVM Classifier:")
print(svm_classifier.get_params())
```

```
Default parameters of SVM Classifier:
{'C': 1.0, 'break_ties': False, 'cache_size': 200, 'class_weight':
None, 'coef0': 0.0, 'decision_function_shape': 'ovr', 'degree': 3,
'gamma': 'scale', 'kernel': 'rbf', 'max_iter': -1, 'probability':
True, 'random_state': None, 'shrinking': True, 'tol': 0.001,
'verbose': False}
```

```
cut = round(X_test_encoded.shape[0]*1) # this cut (*<1) is needed to
train the dataset on a smaller Training Set size
svm_classifier.fit(X_train_encoded.iloc[:cut,:], y_train[:cut])
```

```
SVC(probability=True)
```

```
positive_probs = svm_classifier.predict_proba(X_test_encoded)[:, 1]

auc_roc_svm = round(roc_auc_score(y_test, positive_probs),4)
print("AUC-ROC Score:", auc_roc_svm)
```

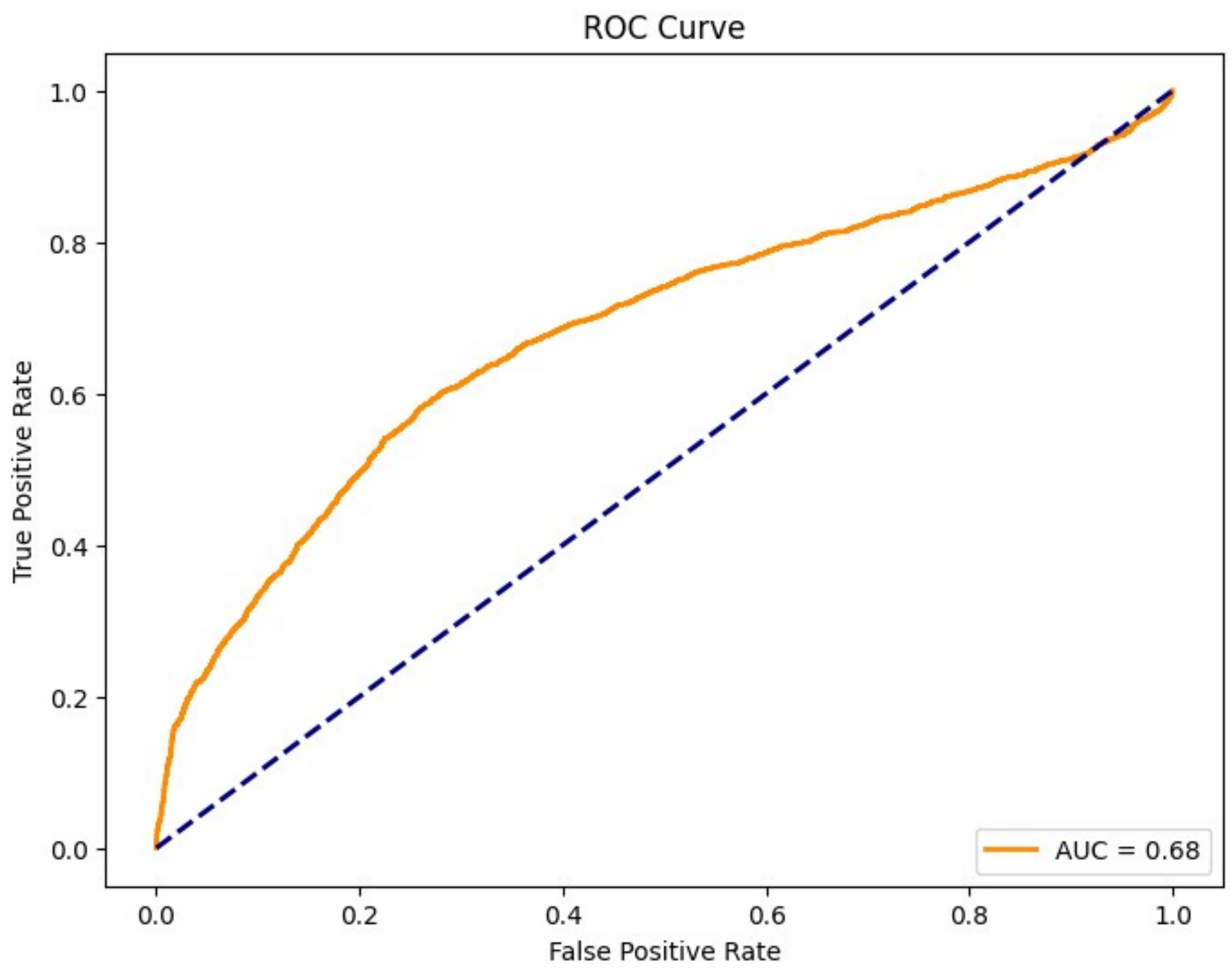
```
AUC-ROC Score: 0.6816
```

```
predictions = svm_classifier.predict(X_test_encoded)

conf_matrix = confusion_matrix(y_test, predictions)

true_negative, false_positive, false_negative, true_positive =
conf_matrix.ravel()


sensitivity = true_positive / (true_positive + false_negative)
specificity = true_negative / (true_negative + false_positive)

print("Sensitivity (True Positive Rate):", sensitivity)
print("Specificity (True Negative Rate):", specificity)
```

```
Sensitivity (True Positive Rate): 0.0
Specificity (True Negative Rate): 1.0
```

```
predictions = svm_classifier.predict(X_test_encoded)

accuracy_svm = round(accuracy_score(y_test, predictions),4)
print(f'Accuracy of model: {accuracy_svm}')

class_names = ["Negative", "Positive"]
```

```
print(classification_report(y_test, predictions,
target_names=class_names))

Accuracy of model: 0.6525

probabilities = svm_classifier.decision_function(X_test_encoded)
fpr, tpr, thresholds = roc_curve(y_test, probabilities)
auc = roc_auc_score(y_test, probabilities)

plt.figure(figsize=(8, 6))
plt.plot(fpr, tpr, color='darkorange', lw=2, label=f'AUC = {auc:.2f}')
plt.plot([0, 1], [0, 1], color='navy', lw=2, linestyle='--')
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('ROC Curve')
plt.legend(loc='lower right')
plt.show()
```



Results

```
res = {
    'Models': ['Random Forest', 'Gradient Boosting', 'Support Vector
Machine'],
    'Accuracy': [accuracy_rf,accuracy_gb,accuracy_svm],
    'AUC-ROC-Score': [auc_roc_rf, auc_roc_gb, auc_roc_svm],

}


results = pd.DataFrame(res)
display(HTML(results.to_html(index=False)))
```

```
<IPython.core.display.HTML object>
```