CARDIOVASCULAR DISEASE PREDICTION WITH EXPLAINABLE AI (XAI)

FARIS HAIKAL FIRDAUS

Table of Contents

Background	2
Problem Statement	2
Dataset description	3
Import Libraries and Load the data	4
Exploratory Data Analysis (EDA)	7
Separate the Input and Target Features of the Data	9
Split the data into Train and Test Sets	10
Scaling data	10
Applying machine learning model on train set	11
Evaluation using F1-score	12
Using SHAP explainer to derive SHAP Values for the Machine Learning model	13
SHAP force plot for the first row of test data	14
SHAP force plot for all the rows in the data	15
SHAP summary plot using all features in the data	16
SHAP dependence plot to show the effect of 'chol' across the whole dataset	18
Explanations and more visualizations with SHAP	20
Waterfall plot	20

Background

Heart disease encompasses a spectrum of medical conditions that impact the functioning of the heart. The incidence of heart disease is on the rise, primarily due to escalating stress levels.

As per data from the World Health Organisation (WHO), cardiovascular diseases (CVDs) have emerged as the leading global cause of mortality. These diseases claim a staggering 17.9 million lives annually, accounting for approximately 31% of all worldwide fatalities.

Problem Statement

The healthcare team at XYZ's Doctor of Health is keen on integrating Data Science into their operations. Given the alarming surge in heart disease cases, their primary focus lies in leveraging existing data to predict the likelihood of an individual having heart disease.

Dataset description:

- id: Unique id for each patient
- age: Age of the patient in years
- origin: place of study
- sex: Gender (Male of Female)
- cp chest pain type: (typical angina, atypical angina, non-anginal, asymptomatic)
- trestbps resting blood pressure: resting blood pressure (in mm Hg on admission to the hospital)
- chol: serum cholesterol in mg/dl
- fbs: if fasting blood sugar > 120 mg/dl
- restecg: resting electrocardiographic results (normal, stt abnormality, lv hypertrophy)
- thalach: maximum heart rate achieved
- exang: exercise-induced angina (True or False)
- oldpeak: ST depression induced by exercise relative to rest
- slope: the slope of the peak exercise ST segment
- ca: number of major vessels (0-3) colored by fluoroscopy
- thal: (normal, fixed defect, reversible defect)
- num: predicted attribute

Import Libraries and Load the data

```
#Install SHAP
     !pip install shap
     Requirement already satisfied: shap in /usr/local/lib/python3.10/dist-packages (0.44.0)
     Requirement already satisfied: numpy in /usr/local/lib/python3.10/dist-packages (from shap) (1.23.5)
     Requirement already satisfied: scipy in /usr/local/lib/python3.10/dist-packages (from shap) (1.11.4)
     Requirement already satisfied: scikit-learn in /usr/local/lib/python3.10/dist-packages (from shap) (1.2.2)
     Requirement already satisfied: pandas in /usr/local/lib/python3.10/dist-packages (from shap) (1.5.3)
     Requirement already satisfied: tqdm>=4.27.0 in /usr/local/lib/python3.10/dist-packages (from shap) (4.66.1)
     Requirement already satisfied: packaging>20.9 in /usr/local/lib/python3.10/dist-packages (from shap) (23.2)
     Requirement already satisfied: slicer==0.0.7 in /usr/local/lib/python3.10/dist-packages (from shap) (0.0.7)
     Requirement already satisfied: numba in /usr/local/lib/python3.10/dist-packages (from shap) (0.58.1)
     Requirement already satisfied: cloudpickle in /usr/local/lib/python3.10/dist-packages (from shap) (2.2.1)
     Requirement already satisfied: llvmlite<0.42,>=0.41.0dev0 in /usr/local/lib/python3.10/dist-packages (from numba->shap) (0.41.1)
     Requirement already satisfied: python-dateutil>=2.8.1 in /usr/local/lib/python3.10/dist-packages (from pandas->shap) (2.8.2)
     Requirement already satisfied: pytz>=2020.1 in /usr/local/lib/python3.10/dist-packages (from pandas->shap) (2023.3.post1)
     Requirement already satisfied: joblib>=1.1.1 in /usr/local/lib/python3.10/dist-packages (from scikit-learn->shap) (1.3.2)
     Requirement already satisfied: threadpoolctl>=2.0.0 in /usr/local/lib/python3.10/dist-packages (from scikit-learn->shap) (3.2.0)
     Requirement already satisfied: six>=1.5 in /usr/local/lib/python3.10/dist-packages (from python-dateutil>=2.8.1->pandas->shap) (1.16.0)
#Import libraries
     import shap
     import matplotlib.pyplot as plt
     import numpy as np
     import seaborn as sns
     import pandas as pd
     from sklearn.metrics import confusion_matrix
     from sklearn.tree import DecisionTreeClassifier
     from \ sklearn.linear\_model \ import \ Logistic Regression
     from sklearn.model_selection import GridSearchCV, train_test_split
     from sklearn.metrics import accuracy_score, classification_report
     from sklearn.preprocessing import LabelEncoder, StandardScaler
     from \ sklearn.utils.class\_weight \ import \ compute\_class\_weight
[47] #Mount with Google Drive
     from google.colab import drive
     drive.mount('/content/drive')
     Drive already mounted at /content/drive; to attempt to forcibly remount, call drive.mount("/content/drive", force_remount=True).
[48] #Import the training and testing dataset
     import pandas as pd
     training_data = pd.read_csv('/content/drive/MyDrive/XAI Final Assessment/Training_set_heart.csv')
     testing_data = pd.read_csv('/content/drive/MyDrive/XAI Final Assessment/Testing_set_heart.csv')
```

Figure 1: import libraries and data loading

Figure 1 above shows the procedure of importing libraries and loading the dataset. As this project is using SHAP as XAI model, hence it needs to be installed. Upon installing SHAP, import all related libraries such as NumPy, Pandas and sklearn. For data loading, the datasets are loaded from Google Drive. training_data is for importing training dataset and testing_data for importing testing dataset. The provided training and testing are in two separate CSV files.

```
[49] print(training_data.head())
                                  chol
                                        fbs
                                                       thalach
                                                                exang oldpeak
                                                                                 slope \
                       trestbps
                                             restecg
     0
                                                           175
                                                                     0
                                                                            0.0
         48
                            124
                                                                                      2
                0
                            120
                                   211
                                          0
                                                    0
                                                           115
                                                                     0
                                                                            1.5
     1
                    0
                            120
                                   249
                                          0
                                                   0
                                                           144
                                                                     0
                                                                            0.8
         46
                                                                                      2
         60
                    0
                            130
                                   253
                                          0
                                                           144
                                                                            1.4
     4
                    0
                            115
                                   303
                                          0
                                                           181
                                                                     0
                                                                            1.2
            thal
                  target
     0
         0
     2
         0
                        0
                        0
         0
     print(testing_data.head())
                                                                                 slope
        age
                  ср
                       trestbps
                                  chol
                                        fbs restecg
                                                      thalach exang oldpeak
                                                                            0.0
         46
               0
                    0
                            138
                                   243
                                          0
                                                           152
                                                   0
               0
                                   236
                                          0
                                                   0
                                                           152
     1
         45
                    0
                            138
                                                                            0.2
     2
         59
                                                    0
                                                                     0
                            160
                                   273
                                          0
                                                           125
                                                                            0.0
                            108
                                          0
                                                           175
                                                                     0
                                                                            0.6
         44
                0
                                   141
         47
                            108
                                   243
                                          0
                                                           152
                                                                     0
                                                                            0.0
            thal
        ca
     0
         0
     1
         0
         0
         0
         0
```

Figure 2: displaying first 5 rows

Upon loading the dataset, display first 5 rows of training and testing dataset using data.head. This provide the structure of the dataset such as the columns and data type.

```
[51] #Summary of the training dataset
    print(training data.info())
    <class 'pandas.core.frame.DataFrame'>
    RangeIndex: 212 entries, 0 to 211
    Data columns (total 14 columns):
     # Column
                Non-Null Count Dtype
        age
                  212 non-null
                                int64
                212 non-null int64
                 212 non-null int64
     3 trestbps 212 non-null int64
     4 chol
                212 non-null int64
     5 fbs
                 212 non-null int64
     6 restecg 212 non-null int64
     7 thalach 212 non-null int64
                               int64
     8 exang
                 212 non-null
     9 oldpeak 212 non-null float64
     10 slope
                 212 non-null
                                int64
                  212 non-null
                                int64
     12 thal
                212 non-null int64
                212 non-null
                                int64
     13 target
    dtypes: float64(1), int64(13)
    memory usage: 23.3 KB
    None
#Summary of the testing dataset
    print(testing_data.info())
<class 'pandas.core.frame.DataFrame'>
    RangeIndex: 91 entries, 0 to 90
    Data columns (total 13 columns):
     # Column
                Non-Null Count Dtype
     0
                 91 non-null
                                int64
        age
                91 non-null
                               int64
                91 non-null
                               int64
     3 trestbps 91 non-null
                               int64
     4 chol
                91 non-null
                               int64
     5 fbs
                 91 non-null
                               int64
     6 restecg 91 non-null
                               int64
       thalach 91 non-null
                               int64
                  91 non-null
                                int64
        exang
        oldpeak
                 91 non-null
                                float64
     10 slope
                 91 non-null
                                int64
                  91 non-null
                                int64
     12 thal
                  91 non-null
                                int64
    dtypes: float64(1), int64(12)
    memory usage: 9.4 KB
    None
```

Figure 3: summary of the dataset

Exploratory Data Analysis (EDA)

```
[55] #Check for missing values on training dataset
    print(training_data.isnull().sum())
               0
    age
    sex
               0
               0
    cр
    trestbps
               0
    chol
               0
    fbs
               0
              0
    restecg
    thalach
              0
    exang
              0
    oldpeak 0
    ca
               0
    thal
    target
    dtype: int64
[56] #Check for missing values on testing dataset
    print(testing_data.isnull().sum())
               0
    age
    sex
               0
               0
    ср
    trestbps
               0
    chol
               0
    fbs
               0
    restecg
              0
    thalach
               0
               0
    exang
    oldpeak
              0
    slope
               0
    ca
               0
    thal
    dtype: int64
```

Figure 4: check for missing values

Figure 4 is the procedure of checking for any missing values on both datasets. Based on the outcome shown, there are no missing values.

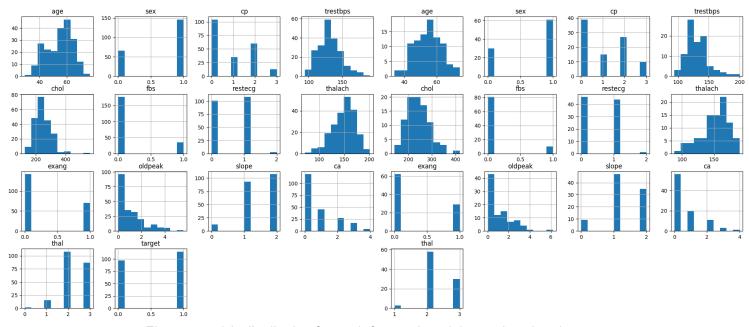


Figure 5 and 6: distribution for each feature in training and testing dataset

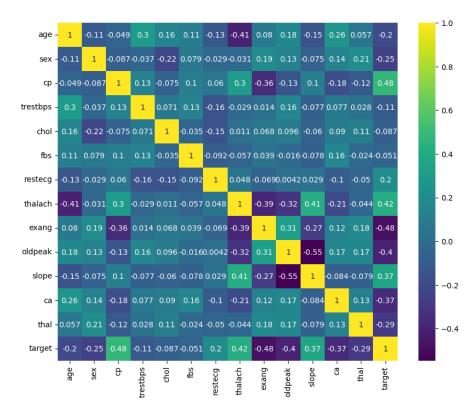


Figure 7: correlation matrix on training dataset

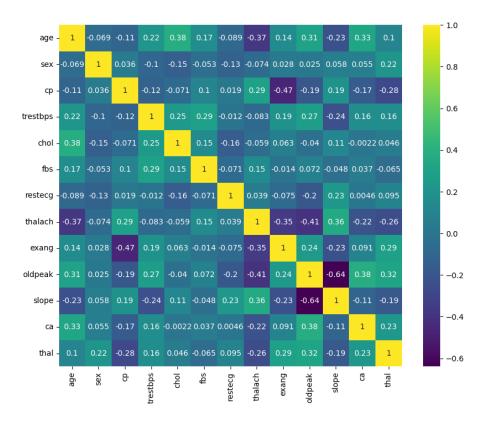


Figure 8: correlation matrix on testing dataset

Figure 5 to Figure 8 is the visualization for both datasets. Figure 5 and Figure 6 are the histograms that shows the distribution of each feature within training (Figure 5) and testing dataset (Figure 6). Figure 7 and Figure 8 is the heatmap that shows the correlation between each feature in training (Figure 7) and testing dataset (Figure 8).

Separate the Input and Target Features of the Data

```
[59] #Training
    from sklearn.model_selection import train_test_split

X_train = training_data.drop('target', axis=1)
    y_train = training_data['target']
```

Figure 9: separate target feature

Figure 9 shows the separation of the target feature of the data from the training dataset. This feature labeled as 'target' shows the actual case whether the patient has heart attack or not. Also, this feature does not exist in the testing dataset.

Split the data into Train and Test Sets

```
[60] #Split the training set into train and validation sets
X_train, X_val, y_train, y_val = train_test_split(X_train, y_train, test_size=0.2, random_state=42)
```

Figure 10: splitting dataset

Figure 10 shows the splitting of the datasets. For this project, the training data is split on a ratio of 80:20. 80% will be training data and 20% will be validation data. The testing dataset will not be split.

Scaling data

```
[61] from sklearn.preprocessing import StandardScaler

#Feature Scaling
scaler = StandardScaler()
scaler.fit(X_train)
X_train_scaled = scaler.transform(X_train)
X_val_scaled = scaler.transform(X_val)
X_test_scaled = scaler.transform(testing_data)
[62] #Compute class weights
class_weights = compute_class_weight(class_weight='balanced', classes=np.unique(y_train), y=y_train)
class_weights_dict = dict(zip(np.unique(y_train), class_weights))
```

Figure 11: Feature Scaling and compute class weights

Figure 11: shows the employment of feature scaling and the computation of class weights, which is to balance the classes by giving more weightage on the minor class to avoid biases.

Applying machine learning model on train set

```
#Logistic Regression
from sklearn.linear model import LogisticRegression
from sklearn.metrics import accuracy_score, confusion_matrix, classification_report, f1_score
logreg_model = LogisticRegression(random_state=42, class_weight=class_weights_dict)
logreg_model.fit(X_train, y_train)
y_val_pred = logreg_model.predict(X_val)
accuracy = accuracy_score(y_val, y_val_pred)
conf_matrix = confusion_matrix(y_val, y_val_pred)
classification_rep = classification_report(y_val, y_val_pred)
f1 = f1_score(y_val, y_val_pred, average='weighted')
print(f'Accuracy on Validation Set: {accuracy * 100:.2f}%\n')
print(f'Weighted F1-score on Validation Set: {f1:.4f}')
print('Confusion Matrix:')
print(conf_matrix)
print('\nClassification Report:')
print(classification_rep)
```

Figure 12: apply logistic regression

Figure 12 shows the application of logistic regression as chosen classification model. As this project is to determine if heart disease is present and risk assessment (binary predictions, 0 or 1), logistic regression would be a suitable model.

Evaluation using F1-score

```
Accuracy: 86.05%
Weighted F1-score: 0.8606
Confusion Matrix:
[[18 2]
 [ 4 19]]
Classification Report:
             precision
                        recall f1-score
                                             support
          0
                  0.82
                            0.90
                                      0.86
                                                  20
          1
                  0.90
                            0.83
                                      0.86
                                                  23
                                                  43
   accuracy
                                      0.86
                                      0.86
                                                  43
  macro avg
                  0.86
                            0.86
weighted avg
                  0.86
                            0.86
                                      0.86
                                                  43
```

Figure 13: classification report

Figure 13 above indicates the classification report after training the logistic regression model. This classification report shows the details of evaluation metrics such as accuracy, precision, recall, F1-score, and support. This model achieved an accuracy of 86.05% and the F1-score is 0.8606.

Figure 14: predictions on testing set

Figure 14 shows the predictions made on the testing set using the trained model from the training and validation dataset. The results shows the results of each patients. There was a warning message which says "X does not have valid feature names, but LogisticRegression was fitted with feature names." This warning message is about possible feature names mismatch. Hence, Figure 15 shows that I displayed the feature names from both training and testing dataset. And the outcome did not show any feature names mismatch.

Figure 15: checking feature names

<u>Using SHAP explainer to derive SHAP Values for the Machine Learning model.</u>

```
[23] #SHAP explainer
import shap

explainer = shap.LinearExplainer(logreg_model, X_test_scaled)
shap_values_val = explainer.shap_values(X_val)

shap_values_test = explainer.shap_values(X_test_scaled)
```

Figure 16: applying SHAP model

Figure 16 shows the application of SHAP model as XAI model. With these calculated SHAP values, it will be used to interpret the predictions through global and local explanations.

SHAP force plot for the first row of test data.

```
#Force plot for first row of testing data
#Selecting the first row of the testing data
sample = sample.iloc[[0]]

shap_values_sample = explainer.shap_values(sample)

intercept = logreg_model.intercept_[0]
coefficients = logreg_model.coef_[0]
z = intercept + np.dot(coefficients, shap_values_sample.flatten())
probability = 1 / (1 + np.exp(-z))

#Generate force plot
shap.force_plot(explainer.expected_value, shap_values_sample, sample, matplotlib=True)

print("\n")
print(f'Probability: {probability:.4f}\n')
```

Figure 17: Force plot for first row of test data, with probability

Figure 17 shows the coding where I develop the force plot with SHAP. I also included a feature to display the probability of the patient to develop heart disease. Refer Figure 18 and Figure 19.

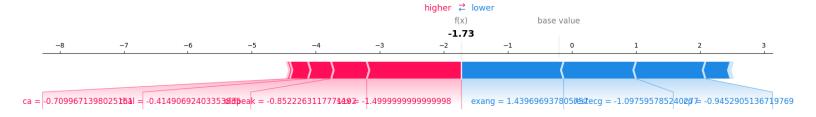


Figure 18: force plot

Figure 18 indicates the force plot for the first row of testing data. This interpretation from this plot is local explanation since I only take the first row of the testing data, which means only one patient. The bold black number in the middle shows the SHAP value. In this case, the lower the SHAP value, the lower the risk of having heart disease. The blue lines shows

what are the features that contribute to lower the risk of heart disease, while the pink line are features that raises the risk of heart disease. For this patient, the feature that contributes the most towards lowering the risk of heart disease is the 'exang' which stands for exercise-induced angina. Exercise-induced angina is a type of chest pain during physical activity. Having less angina is better for our body's health. On the other hand, the feature that contributes most towards increasing the risk of heart disease is 'sex' which stands for gender. Referring to Figure 19 shows the probability of this patient develop heart disease which is 0.0376 or 3.76%.

```
Probability: 0.0376
```

Figure 19: probability

Having a very low probability shows that this patient might be a very healthy man. In order to decrease the risk, doctors can advise this patient to maintain a healthy body by keeping fit such as taking sports and have enough rest to avoid the increasing the exercise-induced angina.

SHAP force plot for all the rows in the data.

```
# Force plot for all rows of testing data
shap_values_test = explainer.shap_values(X_test_scaled)
shap.initjs()
# Generate force plot for all rows
shap.force_plot(explainer.expected_value, shap_values_test, X_test_scaled)
```

Figure 20: force plot for all the rows

Figure 20 is the coding to display force plot for all the rows in the testing data. To display all the rows, the model loops until the end of the rows.

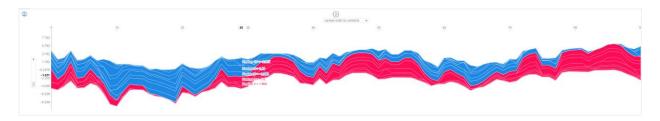


Figure 21: force plots

Figure 21 above shows the force plots from all rows. Every single waves shows every single factors in the dataset on what contributes to the risk of heart disease. *The higher the waves means the higher predicted risk of getting heart disease (in average). The red area represents what or which of the factors increases the overall risk and the blue area represents the factors that decreases the overall risk of heart disease. y-axis is the SHAP value and x-axis is the order by rows. As we hover through the plot, the force plot will show the features with SHAP values on a particular row, based on location of the mouse cursor align with x-axis.

SHAP summary plot using all features in the data.

```
#Summary plot using all features
X_test_df = pd.DataFrame(X_test_scaled, columns=testing_data.columns)
shap_values_test_all = explainer.shap_values(X_test_df)

feature_names = X_val.columns
shap.summary_plot(shap_values_test_all, X_test_scaled,feature_names)
```

Figure 22: develop summary plot for all features

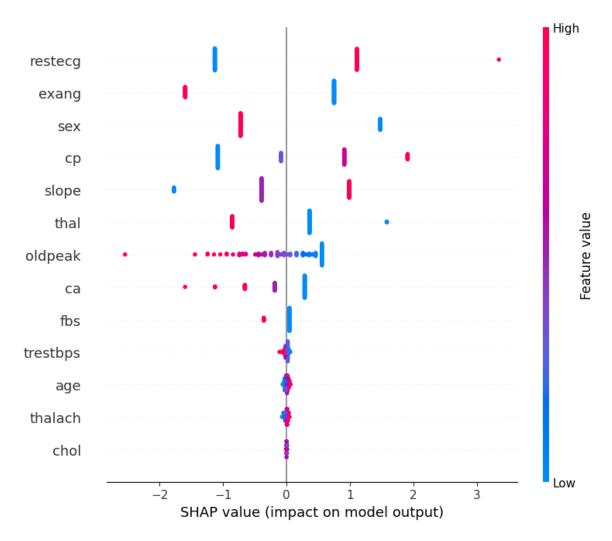


Figure 23: summary plot

Figure 22 shows the coding for develop and display the summary plot using SHAP for all the features, as shown in Figure 23 is the summary plot. This summary plot consists of all features from all the rows, which suggests global explanation.

The components in this summary plot includes:

- y-axis: List of features, ranked by importance in descending order
- x-axis: SHAP values, indicates the impact on the prediction
- Dots: each of the dots represents feature contributions
- Feature value: color that indicates feature value

According to the summary plot, top three features with the highest impact on the predictions are:

- restecg
- exang
- sex

Some details we can see from these three features from the plot are:

- They are ranked the highest in the summary plot, which arranged in descending order.
- The dots on the features have significant SHAP values as they are located further from zero, either less than or greater than zero.
 - Zero (0) SHAP values means less or no contribution towards the model's predictions.
 - Positive SHAP values (to the right) contributes to lower risk of heart disease.
 - Negative SHAP values (to the left) contributes to higher risk of heart disease.
- The dots with wider span means it has more impacts on multiple rows.
- The dots on the three features also have wider span and red in colour, which means they pose a high value in model's prediction.

SHAP dependence plot to show the effect of 'chol' across the whole dataset.

```
#Dependence plot
chol_index = X_test_df.columns.get_loc('chol')
shap.dependence_plot(chol_index, shap_values_test_all, X_test_df, interaction_index="chol", show=False)
```

Figure 24: develop dependence plot to show the effect of 'chol' feature across the dataset.

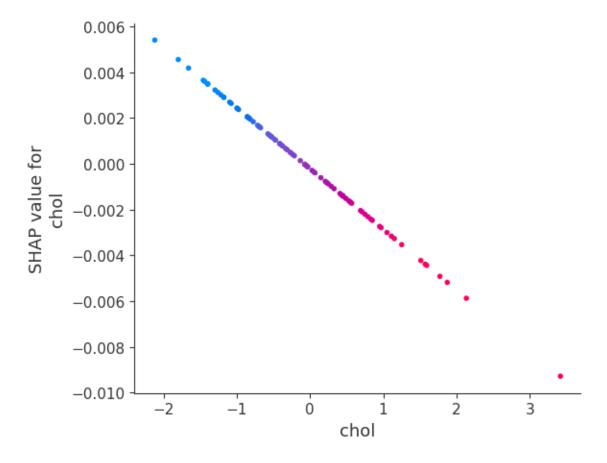


Figure 25: dependence plot

Figure 24 is the code for developing the dependence plot, which shows the effect of 'chol' feature across the dataset as shown in Figure 25. In Figure 25, we can see that:

- The higher chol value leads to lower SHAP value for chol. Which means it leads to higher risk of heart disease.
- The dots that incline towards negative SHAP values are colored pink, which means it poses a higher feature value in model's prediction.
- However, referring to summary plot (Figure 23), chol ranked last in the plot, which means it has the least overall contribution towards model's prediction.

This dependence plot still shows that chol feature has minimal impact towards heart disease risk. Hence to mitigate heart disease risk based on this feature, doctors can advise patients to decrease cholesterol intake. Some suggested steps include consuming more fiber-rich foods, limit processed foods, regular exercise and decrease or quit smoking.

Explorations and more visualizations with SHAP

Waterfall plot

```
[84] import shap
     import matplotlib.pyplot as plt
     import numpy as np
     shap_values_val = explainer.shap_values(X_val_scaled)
     instance index = 0
     shap_values_sample = shap_values_val[instance_index]
     feature names = X val.columns
     cumulative_shap_values = shap_values_sample.cumsum()
     # Define colors based on the direction of contribution
     colors = np.where(shap_values_sample > 0, 'blue', 'red')
     plt.figure(figsize=(8, 10))
     bars = plt.barh(feature names, cumulative shap values, color=colors)
     plt.ylabel('Features')
     plt.xlabel('Cumulative SHAP Values')
     plt.title('Vertical Waterfall Plot of Feature Contributions')
     # Add direction labels and values on each bar
     for bar, value, shap_value in zip(bars, cumulative_shap_values, shap_values_sample):
         width = bar.get_width()
         plt.text(width, bar.get_y() + bar.get_height() / 2, f"{value:.2f}\n",
                  ha='left' if shap_value > 0 else 'right', va='center', color='black')
     plt.show()
```

Figure 26: develop waterfall plot

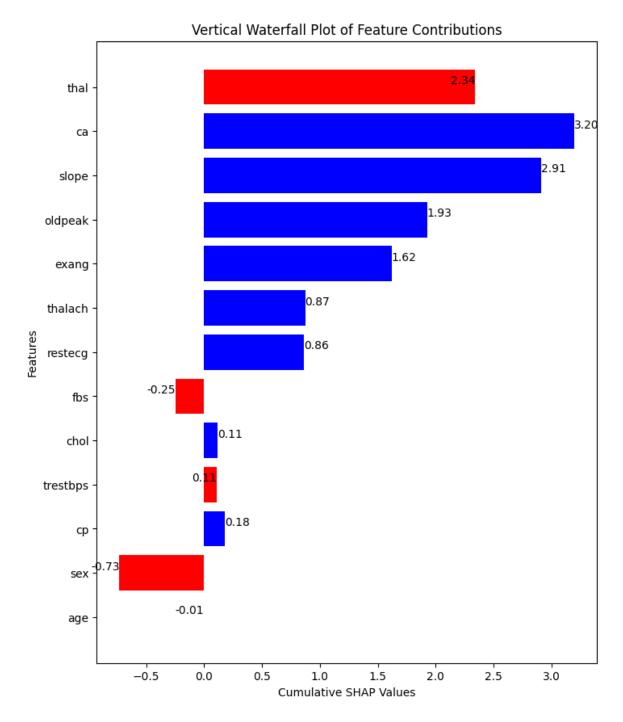


Figure 27: Waterfall plot

Figure 26 is the code to develop the waterfall plot as shown in Figure 27. Based on the code, we considered instance_index=0 which means that this waterfall plot are generated for the first row in the testing dataset, which suggests local explanation.

The characteristics of this waterfall plot are as below:

- x-axis = Cumulative SHAP values calculated on each features
- y-axis = features in the testing dataset
- Colors = features that contribute to increase the heart disease risk indicates in red, and features that contribute to decrease the heart disease risk indicates in blue.
- Bar lengths = corresponds to the cumulative SHAP values for each features
- The values shown on each bar is the cumulated SHAP values for the corresponding feature.

Analysis:

- There are 8 features that contribute towards decreasing heart disease risk, which are:
 - o ca
 - slope
 - oldpeak
 - exang
 - o thalach
 - restecg
 - o chol
 - o cp
- There are 4 features that contribute towards increasing heart disease risk, include:
 - o thal
 - o fbs
 - trestbps
 - o sex
- Since 'age' features bar cannot be seen, which means that this feature contributes least to none to the model's predictions.

As data scientists, we can show the healthcare experts that these red coded features are the ones they can plan for their patients' personalized treatment/mitigation plan.

As healthcare experts, considering some of the features that can be mitigated, we can plan on any treatment plan for the patients to manage heart disease risk such as personalized prescriptions on medications.