3. Machine Learning Interpretability for Heart Disease Prediction

It's time to get rid of the black boxes and cultivate trust in Machine Learning

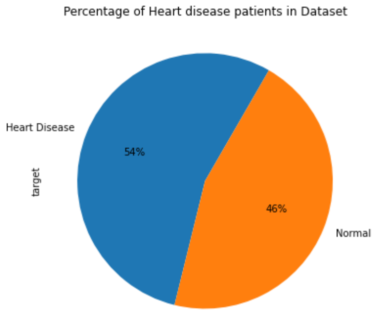
Dataset

Heart Disease UCI | link : https://www.kaggle.com/ronitf/heart-disease-uci

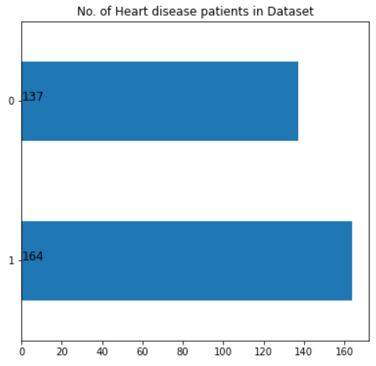
Dataset features description

This dataset consists of 13 features and a target variable. The detailed description of all the features are as follows:

1. **Age :** Patients Age in years (Numeric)
2. **Sex :** Gender of patient [Male - 1, Female - 0] (Nominal)
3. **Chest Pain Type :** Type of chest pain experienced by patient categorized into [0 typical, 1 typical angina, 2 non- anginal pain, 3 asymptomatic] (Nominal)
   understanding :(https://www.harringtonhospital.org/typical-and-atypical-angina-what-to-look-for/)
4. **resting bps :** Level of blood pressure at resting mode in mm/HG (Numerical)
   understanding :(https://www.healthline.com/health/high-blood-pressure-hypertension/blood-pressure-reading-explained#normal) / https://www.hcs.gr/artiriaki-piesi.aspx
5. **cholestrol :** Serum cholestrol in mg/dl (Numeric)
   understanding :(https://www.mikroviologos.gr/arthra/cholesterol)
6. **fasting blood sugar :** Blood sugar levels on fasting > 120 mg/dl represents as 1 in case of true and 0 as false (Nominal)
7. **resting ecg :** Result of electrocardiogram while at rest are represented in 3 distinct values 0 : Normal 1: Abnormality in ST-T wave 2: Left ventricular hypertrophy (Nominal)
8. **max heart rate :** Maximum heart rate achieved (Numeric)
9. **exercise angina :** Angina induced by exercise 0 depicting NO 1 depicting Yes (Nominal)
10. **oldpeak :** Exercise induced ST-depression in comparison with the state of rest (Numeric)
11. **ST slope :** ST segment measured in terms of slope during peak exercise [0 = Normal, 1 = Upsloping, 2 = Flat 3: Downsloping] (Nominal)
12. **ca :** The number of major vessels [0-4]
13. **thal :** A blood disorder called thalassemia [1 = normal, 2 = fixed defect, 3 = reversable defect]
    understanding :(https://bioiatriki.gr/index.php/thalassoaimies)
14. **target :** Heart disease [0 = no, 1 = yes]

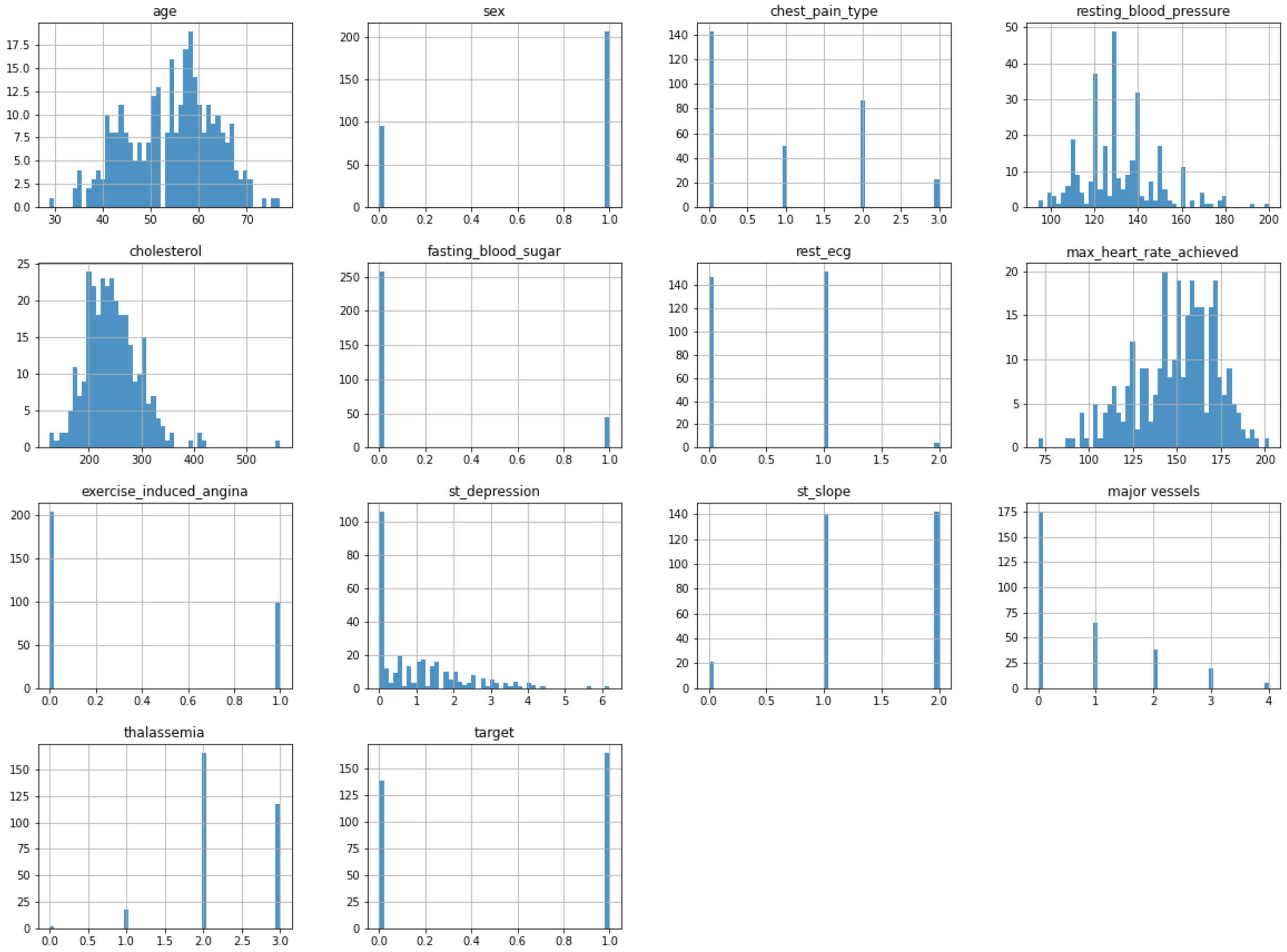


Percentage of Heart disease patients in Dataset



No. of Heart disease patients in Dataset

Dataset features



Training the models

We will train a random forest and logistic regression model.

Logistic regression is a readily interpretable model which allows us to determine the linear relationship between the features and the target. A random forest is a 'black box' model, which will require a little more work to interpret, but which will allow us to view the non-linear relationships between the features and the model predictions. As we can see from the above result random forest has equal F1 score, Precision, ROC and Recall with Logistic Regression but has lesser accuracy in comparison to Logistic Regression. But apart from that, we will be using Random forest for applying machine learning interpretation strategies. the major reason for selecting random forest is it is tree based algorithm which supports and compatible with most of the interpretation techniques.

Model	Recall	Accuracy	F1 Score	Precision	ROC
Base - Logistic Regression	0.878	0.802	0.878	0.878	0.867
Random Forest	0.878	0.788	0.865	0.852	0.850

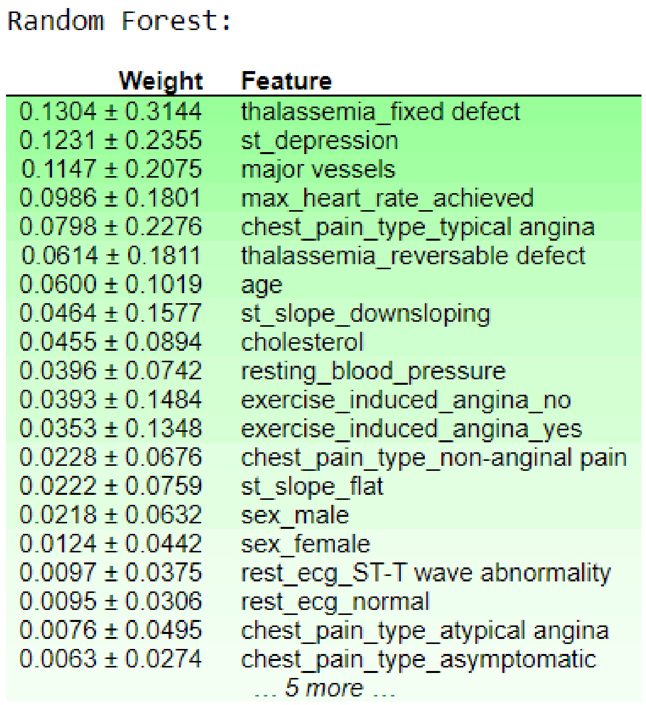
Feature Importance

Native methods

Global importance measures. i.e they answer the question 'On average, how important is feature i for making a prediction'.

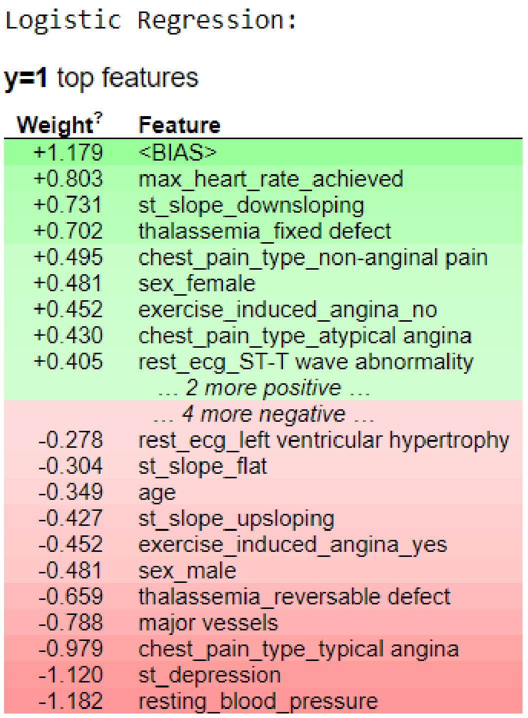
Both random forests and logistic regression have native methods of formulating the relative importance of features.

- Decision trees come with a method for measuring the importance of a feature which works by adding up the total decrease in the gini coefficient from nodes that depend on that feature. For a random forest, we can average this value across all trees to get an estimate of festure importance. This is called the mean decrease in gini.
- For logistic regression, the importances of a feature is just given by the absolute value of its weight. Note that this is only true since we have standardised the variables. Of course the weights themselves have a straightforward interpretation in terms of how the associated feature affects the predicted outcome.



Random Forest:

Weight	Feature
0.1304 ± 0.3144	thalassemia_fixed defect
0.1231 ± 0.2355	st_depression
0.1147 ± 0.2075	major vessels
0.0986 ± 0.1801	max_heart_rate_achieved
0.0798 ± 0.2276	chest_pain_type_typical angina
0.0614 ± 0.1811	thalassemia_reversable defect
0.0600 ± 0.1019	age
0.0464 ± 0.1577	st_slope_downsloping
0.0455 ± 0.0894	cholesterol
0.0396 ± 0.0742	resting_blood_pressure
0.0393 ± 0.1484	exercise_induced_angina_no
0.0353 ± 0.1348	exercise_induced_angina_yes
0.0228 ± 0.0676	chest_pain_type_non-anginal pain
0.0222 ± 0.0759	st_slope_flat
0.0218 ± 0.0632	sex_male
0.0124 ± 0.0442	sex_female
0.0097 ± 0.0375	rest_ecg_ST-T wave abnormality
0.0095 ± 0.0306	rest_ecg_normal
0.0076 ± 0.0495	chest_pain_type_atypical angina
0.0063 ± 0.0274	chest_pain_type_asymptomatic
	… 5 more …



Logistic Regression:

y=1 top features

Weight?	Feature
+1.179	<BIAS>
+0.803	max_heart_rate_achieved
+0.731	st_slope_downsloping
+0.702	thalassemia_fixed defect
+0.495	chest_pain_type_non-anginal pain
+0.481	sex_female
+0.452	exercise_induced_angina_no
+0.430	chest_pain_type_atypical angina
+0.405	rest_ecg_ST-T wave abnormality
	… 2 more positive …
	… 4 more negative …
-0.278	rest_ecg_left ventricular hypertrophy
-0.304	st_slope_flat
-0.349	age
-0.427	st_slope_upsloping
-0.452	exercise_induced_angina_yes
-0.481	sex_male
-0.659	thalassemia_reversable defect
-0.788	major vessels
-0.979	chest_pain_type_typical angina
-1.120	st_depression
-1.182	resting_blood_pressure

One thing that both methods have in common is that they examine which features play the biggest role in fitting to the training set, not which features are most useful for generalization. If we want to know which risk factors are the most impactful on one's chance of developing heart disease, it is really this second kind of feature importance that we want.

There are other drawbacks that are specific to each model:

- Random forest: Mean decrease in gini tends to overestimate the importance of continuous and high cardinality categorical data. It also underestimates the importance of highly correlated features.
- Logistic regression: By its nature, logistic regression can only model linear relationships between the features and target, and this obviously limits its ability to demonstrate the importance of features which have a non-linear effect on the target.

The primary advantage of both is that they are trivial to compute once you have fitted the model.

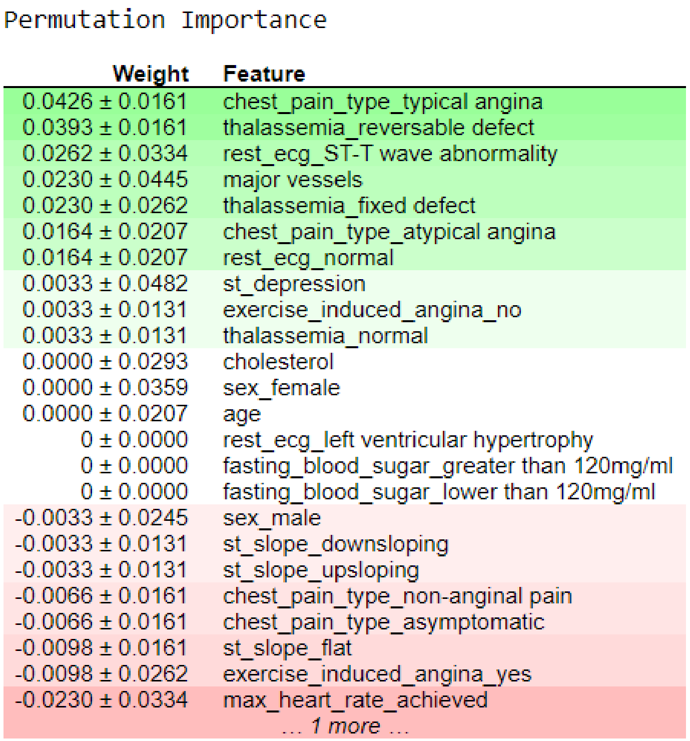
First Technique - Permutation Importance

What features does a model think are important ? Which features might have a greater impact on the model predictions than the others ?

This concept is called feature importance and Permutation Importance is a technique used widely for calculating feature importance. It helps us to see when our model produces counterintuitive results, and it helps to show the others when our model is working as we'd hope.

Permutation Importance works for many scikit-learn estimators. The idea is simple: Randomly permutate or shuffle a single column in the validation dataset leaving all the other columns intact. A feature is considered "important" if the model's accuracy drops a lot and causes an increase in error. On the other hand, a feature is considered 'unimportant' if shuffling its values doesn't affect the model's accuracy.

Permutation importance is calculated after a model has been fitted!



Permutation Importance

Weight	Feature
0.0426 ± 0.0161	chest_pain_type_typical angina
0.0393 ± 0.0161	thalassemia_reversable defect
0.0262 ± 0.0334	rest_ecg_ST-T wave abnormality
0.0230 ± 0.0445	major vessels
0.0230 ± 0.0262	thalassemia_fixed defect
0.0164 ± 0.0207	chest_pain_type_atypical angina
0.0164 ± 0.0207	rest_ecg_normal
0.0033 ± 0.0482	st_depression
0.0033 ± 0.0131	exercise_induced_angina_no
0.0033 ± 0.0131	thalassemia_normal
0.0000 ± 0.0293	cholesterol
0.0000 ± 0.0359	sex_female
0.0000 ± 0.0207	age
0 ± 0.0000	rest_ecg_left ventricular hypertrophy
0 ± 0.0000	fasting_blood_sugar_greater than 120mg/ml
0 ± 0.0000	fasting_blood_sugar_lower than 120mg/ml
-0.0033 ± 0.0245	sex_male
-0.0033 ± 0.0131	st_slope_downsloping
-0.0033 ± 0.0131	st_slope_upsloping
-0.0066 ± 0.0161	chest_pain_type_non-anginal pain
-0.0066 ± 0.0161	chest_pain_type_asymptomatic
-0.0098 ± 0.0161	st_slope_flat
-0.0098 ± 0.0262	exercise_induced_angina_yes
-0.0230 ± 0.0334	max_heart_rate_achieved
	… 1 more …

Interpretation :

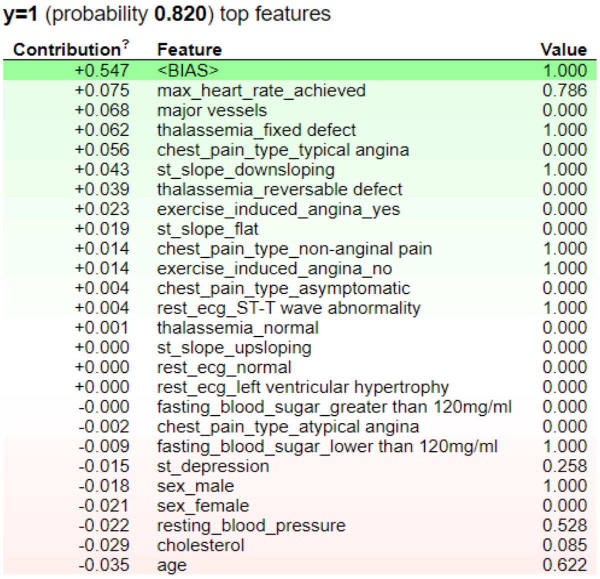
- The features at the top are most important and at the bottom, the least.
- The number after the ± measures how performance varied from one-reshuffling to the next.
- Some weights are negative. This is because in those cases predictions on the shuffled data were found to be more accurate than the real data.

Here top 5 important features :

- **chest_pain_type_typical angina**
- **thalassemia_reversable defect**
- **rest_ecg_ST-T wave abnormality**
- **major vessels**
- **thalassemia_fixed defect**

Next, to explain individual prediction by random forest model there is a method in eli5 library called show_prediction().

- We explain the the 10th record of test set having following prediction as shown in below figure.



y=1 (probability **0.820**) top features

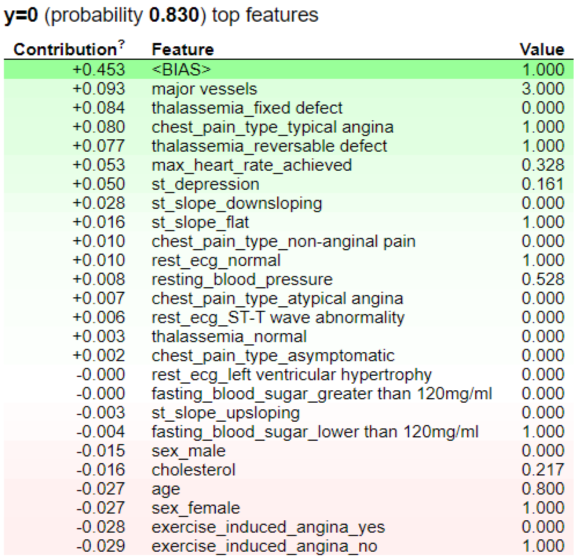
Contribution?	Feature	Value
+0.547	<BIAS>	1.000
+0.075	max_heart_rate_achieved	0.786
+0.068	major vessels	0.000
+0.062	thalassemia_fixed defect	1.000
+0.056	chest_pain_type_typical angina	0.000
+0.043	st_slope_downsloping	1.000
+0.039	thalassemia_reversable defect	0.000
+0.023	exercise_induced_angina_yes	0.000
+0.019	st_slope_flat	0.000
+0.014	chest_pain_type_non-anginal pain	1.000
+0.014	exercise_induced_angina_no	1.000
+0.004	chest_pain_type_asymptomatic	0.000
+0.004	rest_ecg_ST-T wave abnormality	1.000
+0.001	thalassemia_normal	0.000
+0.000	st_slope_upsloping	0.000
+0.000	rest_ecg_normal	0.000
+0.000	rest_ecg_left ventricular hypertrophy	0.000
-0.000	fasting_blood_sugar_greater than 120mg/ml	0.000
-0.002	chest_pain_type_atypical angina	0.000
-0.009	fasting_blood_sugar_lower than 120mg/ml	1.000
-0.015	st_depression	0.258
-0.018	sex_male	1.000
-0.021	sex_female	0.000
-0.022	resting_blood_pressure	0.528
-0.029	cholesterol	0.085
-0.035	age	0.622

To make random forest predictions more interpretable, every prediction of the model can be presented as a sum of feature contributions (plus the bias), showing how the features lead to a particular prediction. In above plot, ELI5 does it by showing weights for each feature with their actual value depicting how influential it might have been in contributing to the final prediction decision across all trees.

In the above individual prediction, the top 3 influential features seems to be, after the bias,

- the major vessels,
- thalassemia_fixed defect
- max_heart_rate_achieved.

- 42th record of test set having following prediction as shown in below figure :



y=0 (probability **0.830**) top features

Contribution?	Feature	Value
+0.453	<BIAS>	1.000
+0.093	major vessels	3.000
+0.084	thalassemia_fixed defect	0.000
+0.080	chest_pain_type_typical angina	1.000
+0.077	thalassemia_reversable defect	1.000
+0.053	max_heart_rate_achieved	0.328
+0.050	st_depression	0.161
+0.028	st_slope_downsloping	0.000
+0.016	st_slope_flat	1.000
+0.010	chest_pain_type_non-anginal pain	0.000
+0.010	rest_ecg_normal	1.000
+0.008	resting_blood_pressure	0.528
+0.007	chest_pain_type_atypical angina	0.000
+0.006	rest_ecg_ST-T wave abnormality	0.000
+0.003	thalassemia_normal	0.000
+0.002	chest_pain_type_asymptomatic	0.000
-0.000	rest_ecg_left ventricular hypertrophy	0.000
-0.000	fasting_blood_sugar_greater than 120mg/ml	0.000
-0.003	st_slope_upsloping	0.000
-0.004	fasting_blood_sugar_lower than 120mg/ml	1.000
-0.015	sex_male	0.000
-0.016	cholesterol	0.217
-0.027	age	0.800
-0.027	sex_female	1.000
-0.028	exercise_induced_angina_yes	0.000
-0.029	exercise_induced_angina_no	1.000

In the above individual prediction, the top 3 influential features seems to be, after the bias,

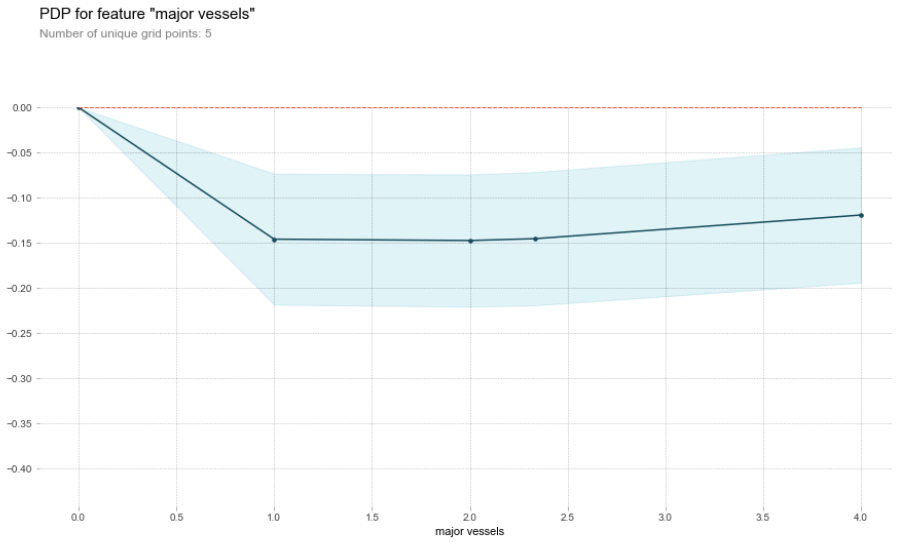
- major vessels
- thalassemia_fixed defect
- chest_pain_type_typical angina

Second Technique - Partial Dependence Plots

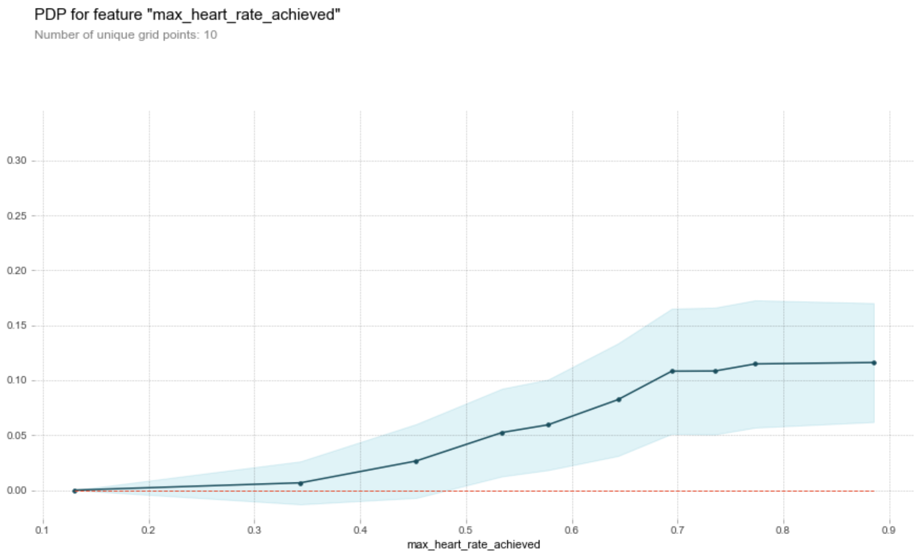
How does each feature affect your predictions ?

The partial dependence plot (short PDP or PD plot) shows the marginal effect one or two features have on the predicted outcome of a machine learning model. PDPs show how a feature affects predictions. PDP can show the relationship between the target and the selected features via 1D or 2D plots.

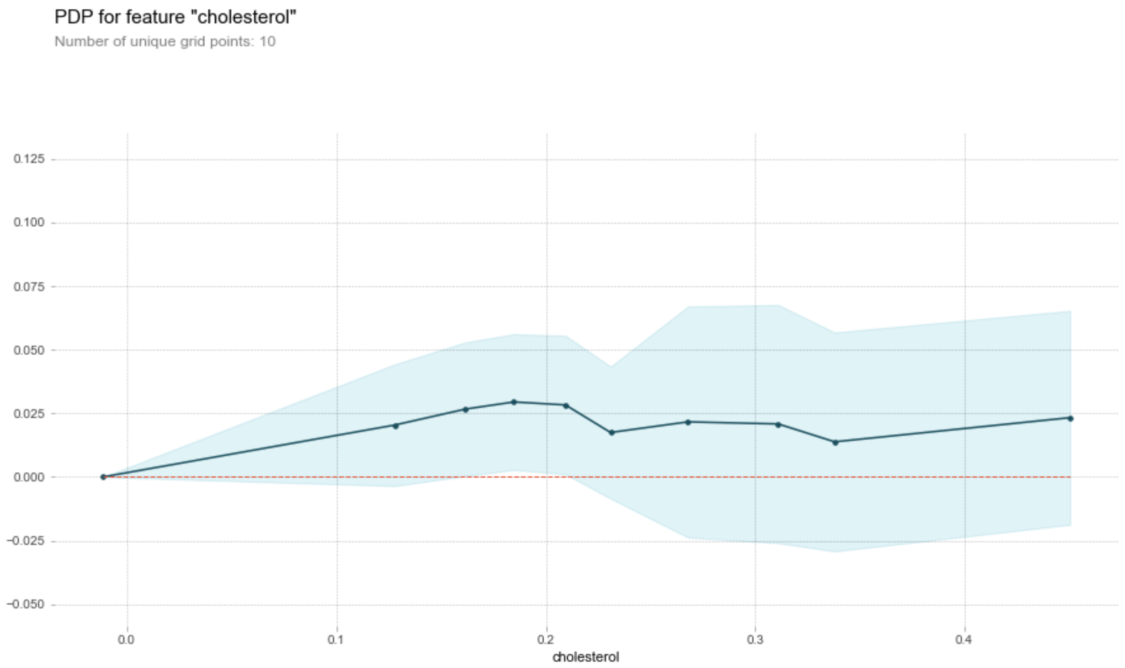
Like permutation importance, partial dependence plots are calculated after a model has been fit. The model is fit on real data that has not been artificially manipulated in any way.
A few items are worth pointing out as you interpret this plot The y axis is interpreted as change in the prediction from what it would be predicted at the baseline or leftmost value. A blue shaded area indicates level of confidence.



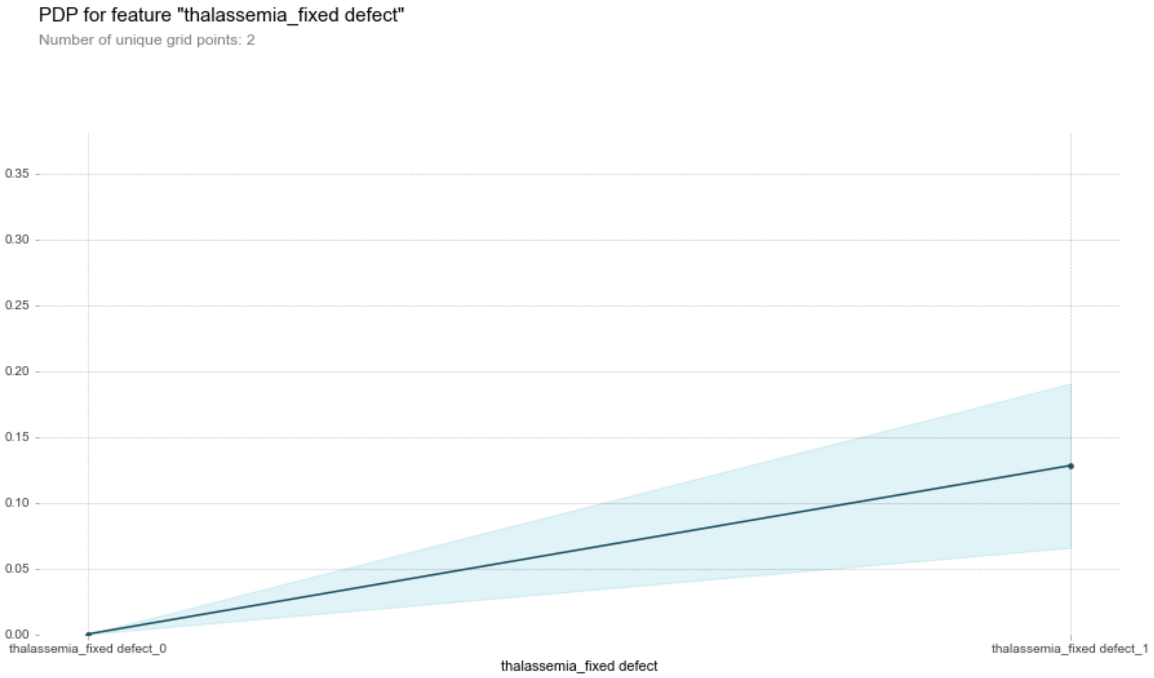
- **So, we can see that as the number of major blood vessels increases, the probability of heart disease decreases. That makes sense, as it means more blood can get to the heart.**



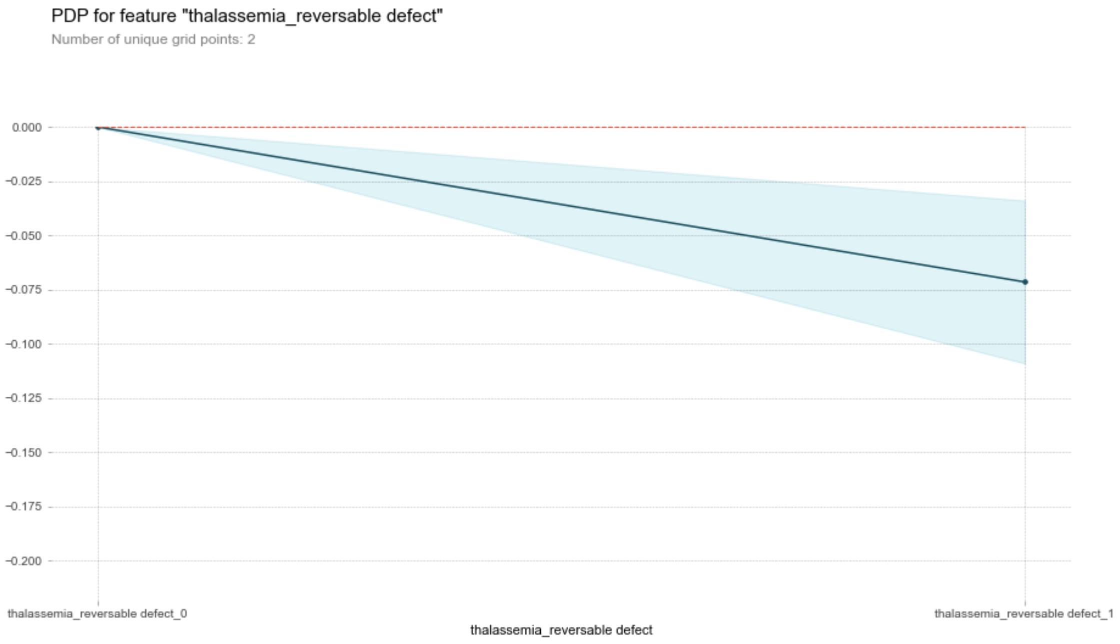
- **Here we can see when max_heart_rate_achieved increases, the probability of heart disease increases. That makes sense**



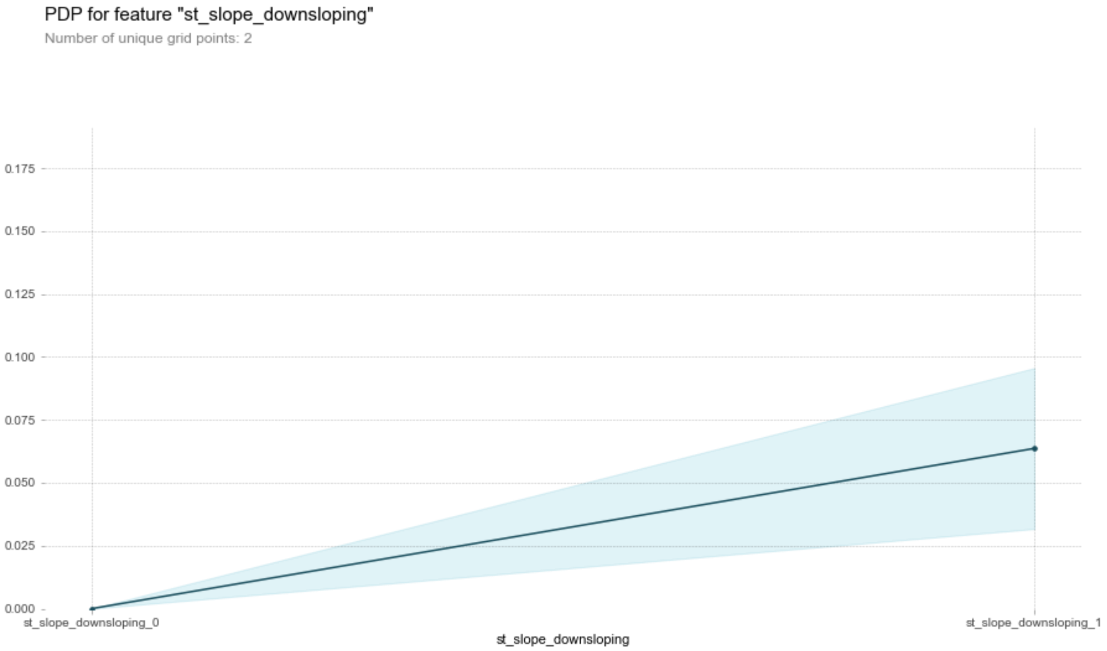
- we can see when cholesterol increases, the probability of heart disease increases. That makes sense,because high cholesterol increases the risk of cardiovascular disease due to a) an increase in blood pressure and b) the extra load that the heart has to face.



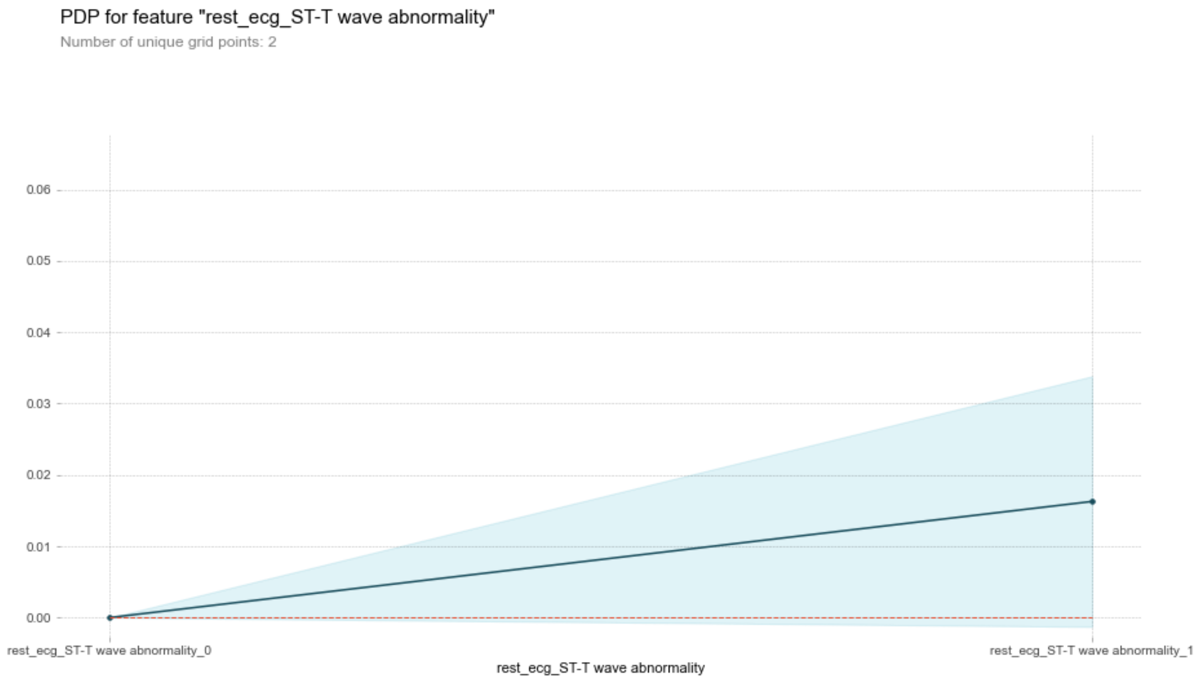
- So, we can see when thalassemia_fixed defect increases, the probability of heart disease increases. That makes sense



- **So, we can see when thalassemia_reversable defect increases, the probability of heart disease decreases. That makes sense**



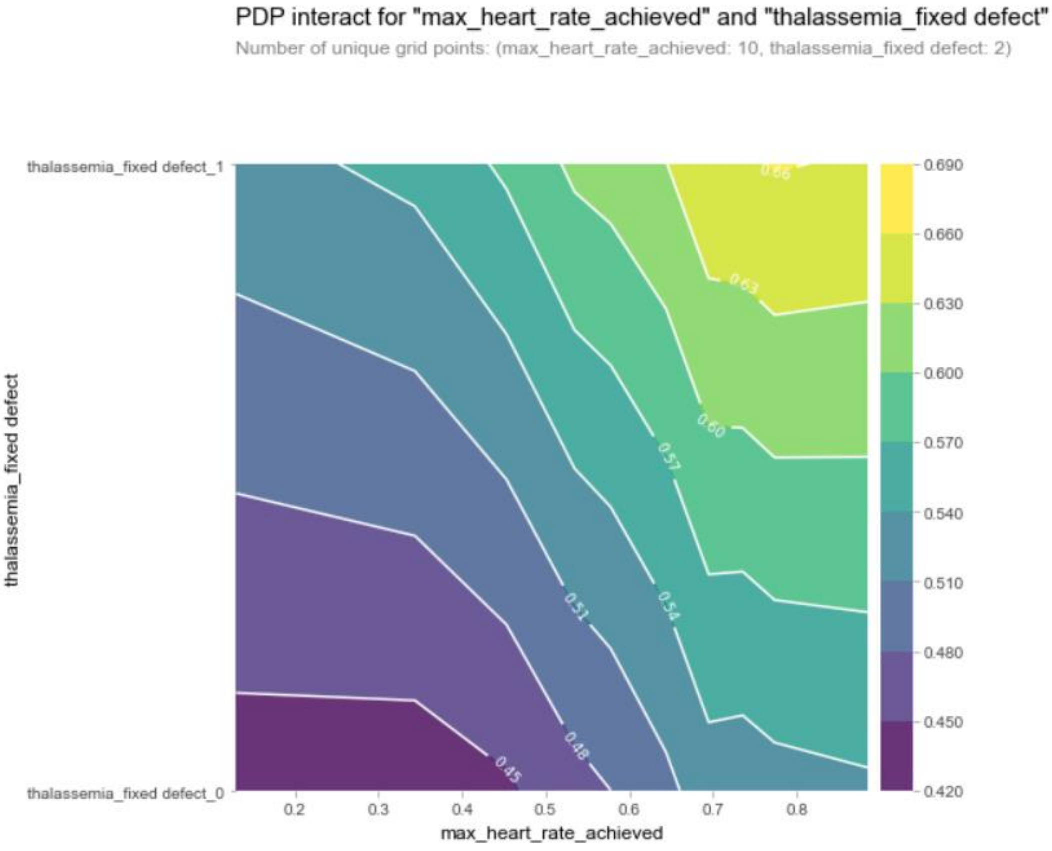
- **So, we can see when st_slope_downsloping increases, the probability of heart disease increases. That makes sense Upward or downward shifts can represent decreased blood flow to the heart from a variety of causes, including heart attack**



- **So, we can see when rest_ecg_ST-T wave abnormality increases, the probability of heart disease increases. That makes sense**

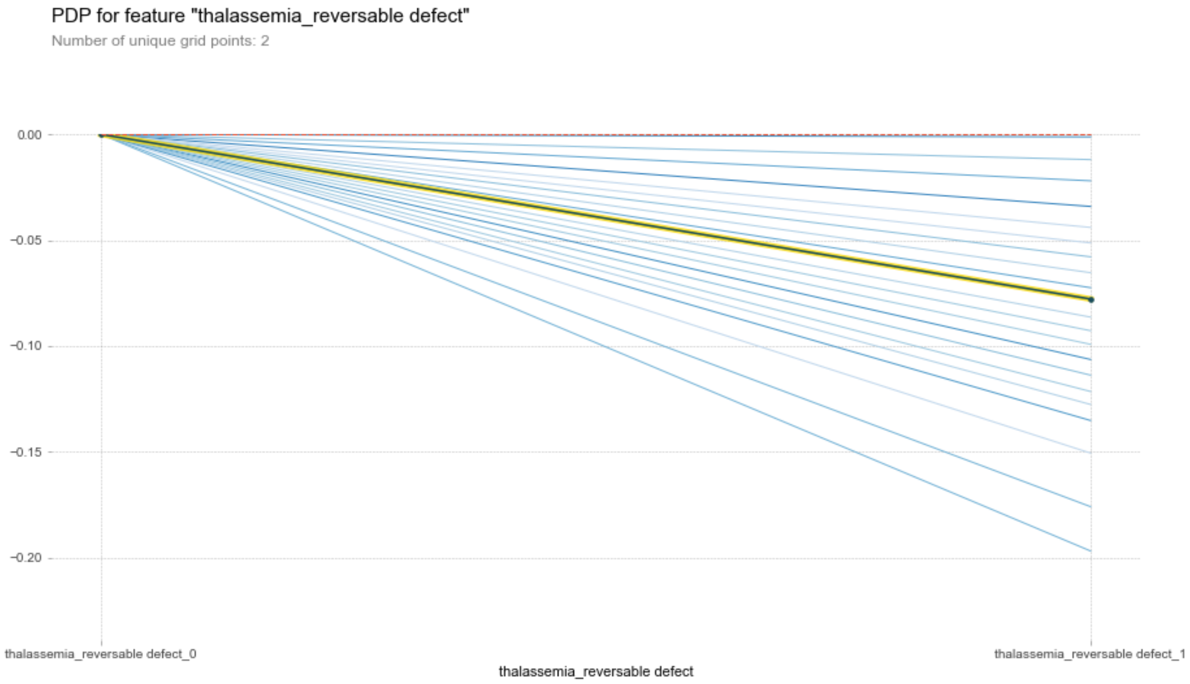
2D Partial Dependence Plots

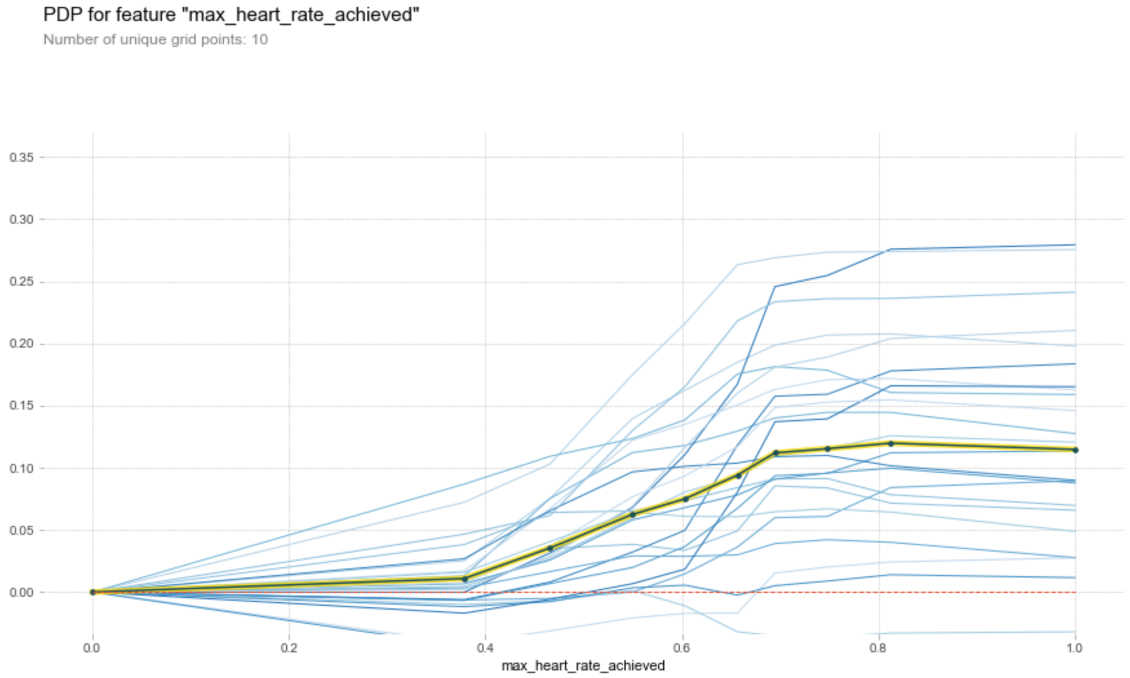
We can also visualize the partial dependence of two features at once using 2D Partial plots.



we can see when max_heart_rate_achieved & thalassemia_fixed defect increases, the probability of heart disease increases.

ICE plots are similar to PD plots but offer a more detailed view about the behavior of near similar clusters around the PD plot average curve. ICE algorithm gives the user insight into the several variants of conditional relationships estimated by the black box.





Third Technique - SHAP Values

Understanding individual predictions

Finally, we will take a look at the Shapley values for different features. Shapley values are an idea that comes from game theory. For an input vector x , to compute the Shapley value of feature i , we consider all the possible subset of features that don't include i , and see how that model prediction would change if we included i . We then average of all such possible subsets. There are many theoretical properties of Shaply values which make them attractive. In particular, they are the only measure of feature importance which satisfy the following four properties simultaneously (we state these informally).

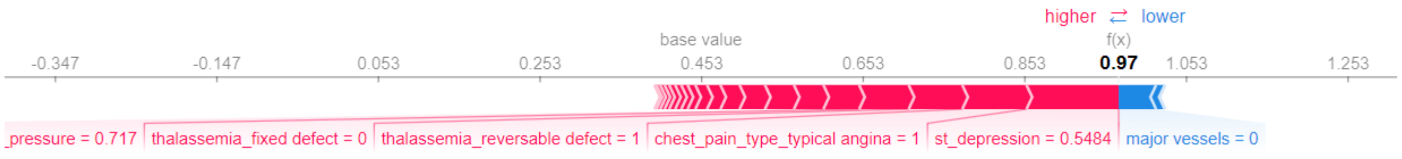
- Efficiency: The Shapley values of all features for a given prediction sum to the output of the model (i.e. the probability that target = 1).
- Symmetry: Any two features which have the same effect on the prediction are given the same Shapley value.
- Linearity: The Shapley value of a collection of features is the sum of the Shapley values of the features.
- Dummy: A feature which has no effect on the prediction has a Shapley value of 0.

We only compute the shap values for the random forest, and not logistic regression. There are a couple of reasons for this.

- TreeSHAP is a fast algorithm that comutes the exact Shapley values for the features and is unaffected by correlations in the data. For logistic regression we would have to use the KernelSHAP algorithm, which is much slower, is affected by correlations and only provides an approximation of the Shapley values.
- We will want to use Shapley values to plot dependency plots. Since logistic regression is a linear model, we already know that these plots will be linear.

Shap values show how much a given feature changed our prediction (compared to if we made that prediction at some baseline value of that feature).

- 20th record of test set :

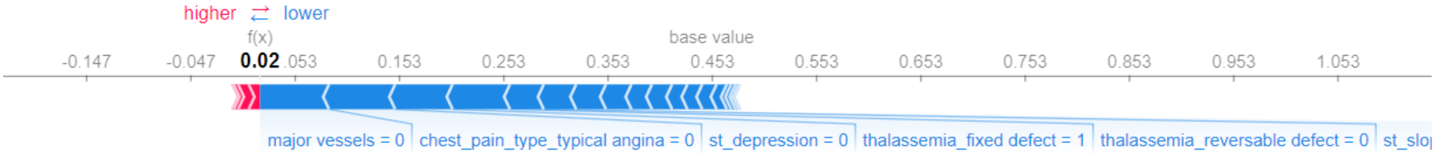


Interpretation

The above explanation shows features each contributing to pushing the model output from the base value (the average model output over the training dataset we passed) to the model output. Features pushing the prediction higher are shown in red, those pushing the prediction lower are in blue

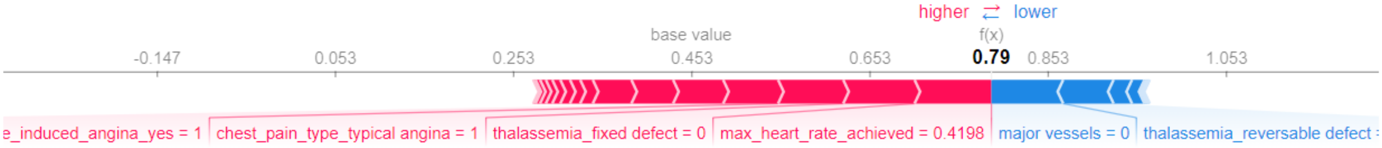
- The base_value here is 0.453 while our predicted value is 0.97.
- st_depression=0.5484 has the biggest impact on increasing the prediction, while
- major vessels=0 the feature has the biggest effect in decreasing the prediction.

- 22th record of test set :

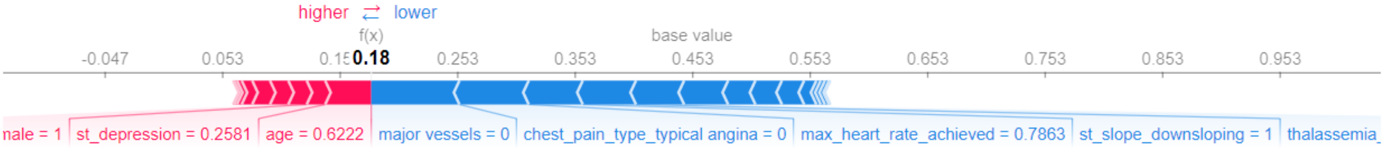


major vessels=0, chest_pain_type_typical angina=0 features has the biggest effect in decreasing the prediction.

- 23th record of test set :



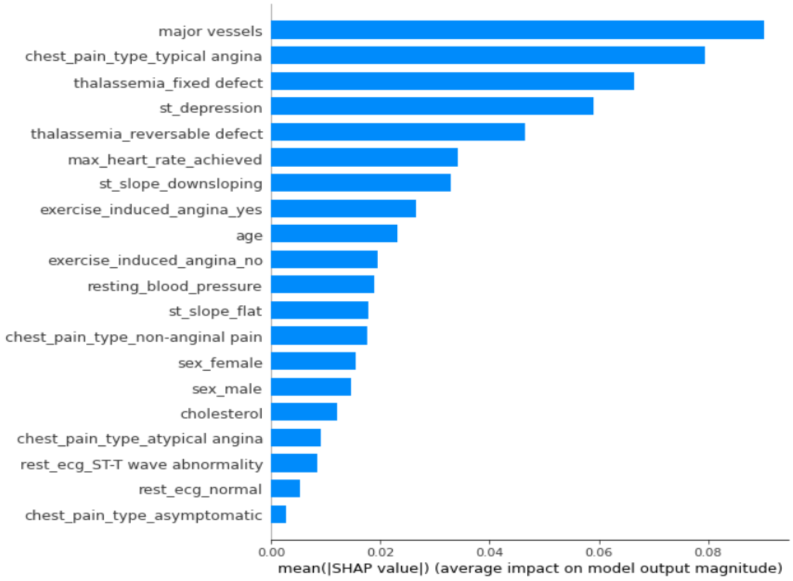
- 10th record of test set :



- **Feature values causing increased predictions are in pink, and their visual size shows the magnitude of the feature's effect.**
- **Feature values decreasing the prediction are in blue**

SHAP Feature Importance Plot

The global mean(|Tree SHAP|) method applied to the heart disease prediction model. The x-axis is essentially the average magnitude change in model output when a feature is "hidden" from the model (for this model the output has log-odds units).

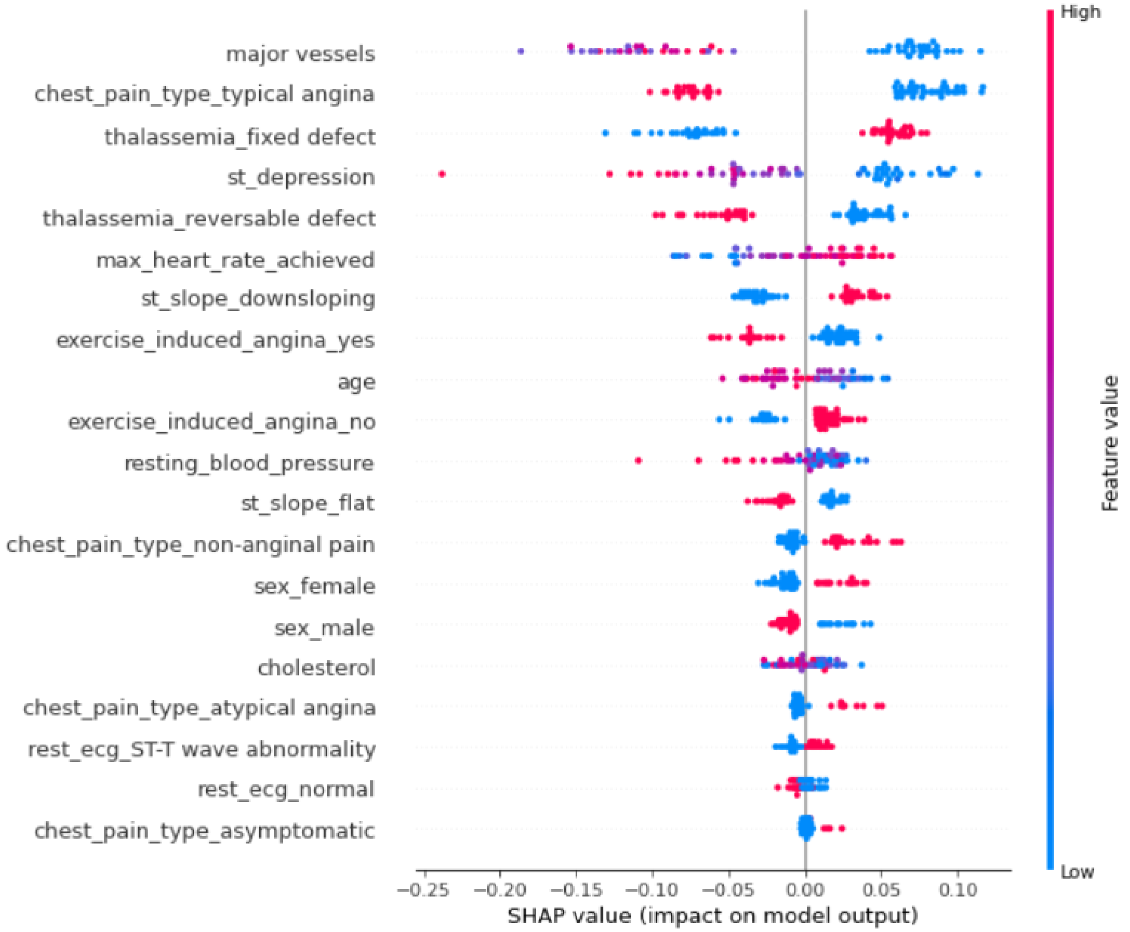


SHAP Summary Plot

To get an overview of which features are most important for a model we can plot the SHAP values of every feature for every sample. The summary plot tells which features are most important, and also their range of effects over the dataset.

For every dot:

- Vertical location shows what features it is depicting.
- The color shows whether that feature was high or low for that row of the dataset.
- Horizontal location shows whether the effect of that value caused a higher or lower prediction.

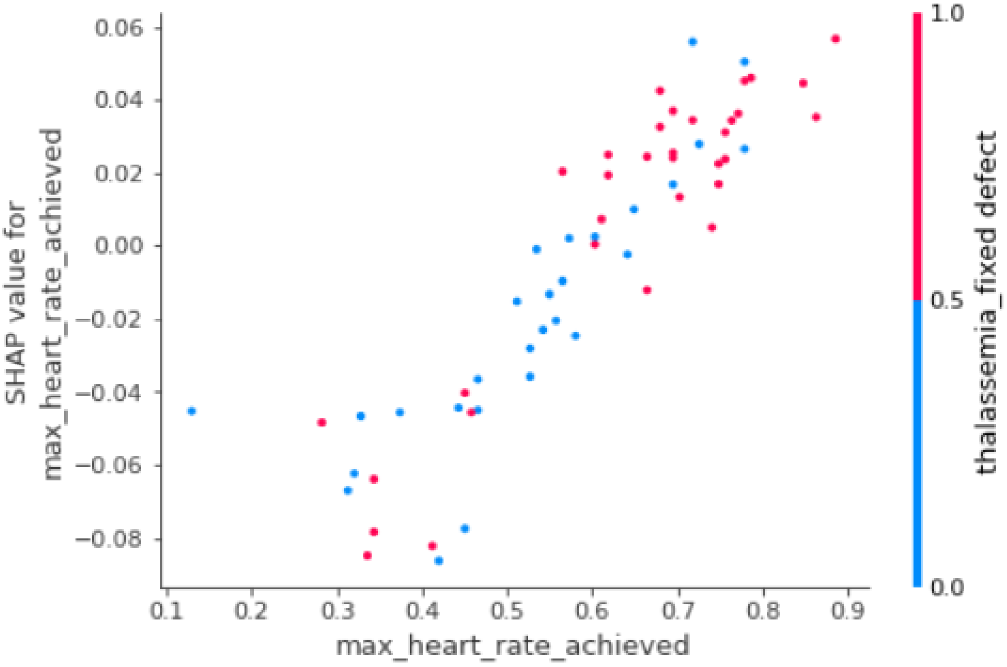


The higher the SHAP value of a feature, the higher is the log odds of heart disease in this heart disease prediction model. Every patient in the dataset is run through the model and a dot is created for each feature attribution value, so one patient gets one dot on each feature’s line. Dot’s are colored by the feature’s value for that patient and pile up vertically to show density.

- **The number of major vessels division is pretty clear, and it's saying that low values are bad (blue on the right), the probability of heart disease increases.**
- **The number of chest_pain_type_typical angina division is pretty clear, and it's saying that low values are bad (blue on the right).**
- **Higher values of thalasemia_fixed_defect increases the risk of heart disease whereas its lower values decreases the chances of heart disease.**
- **The thalassemia 'reversable defect' division is very clear (yes = red = good, no = blue = bad).**
- **The thalassemia 'thalassemia_fixed defect' division is very clear (yes = red = bad, no = blue = good).**
- **The thalassemia 'st_slope_upsloping' division is very clear (yes = red = bad, no = blue = good).**

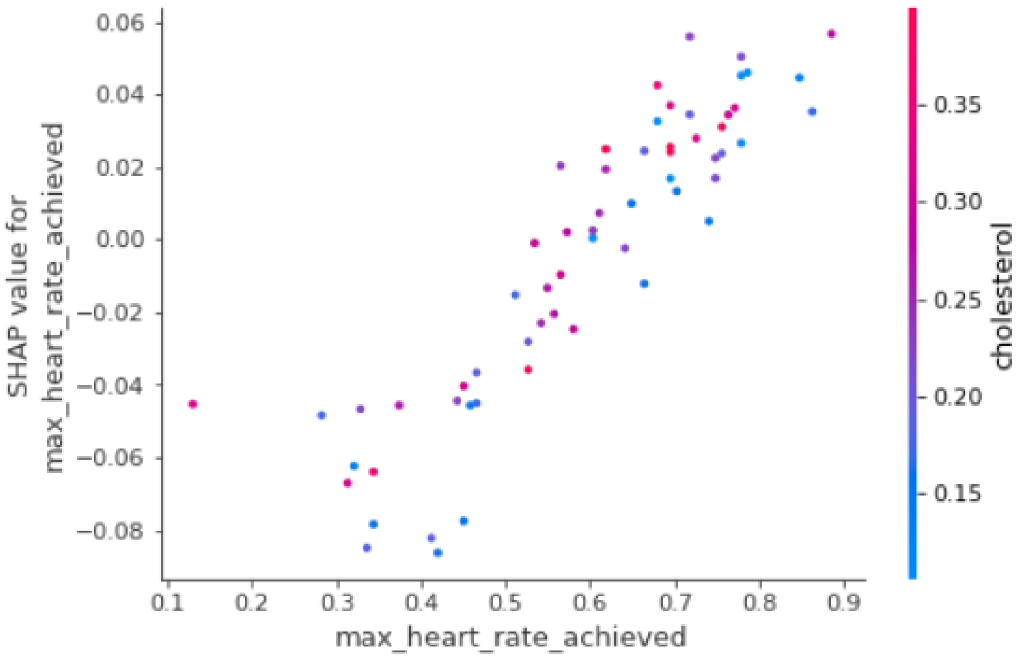
SHAP Dependence Contribution Plots

While a SHAP summary plot gives a general overview of each feature, a SHAP dependence plot shows how the model output varies by a feature value. SHAP dependence contribution plots provide a similar insight to PDPs, but they add a lot more detail.



Start by focusing on the shape, and we'll come back to color in a minute. Each dot represents a row of the data. The horizontal location is the actual value from the dataset, and the vertical location shows what having that value did to the prediction.

- **we can see when max_heart_rate_achieved & thalassemia_fixed defect increases, the probability of heart disease increases.**



Fourth (Extra) technique - LIME(Local Interpretable Model-agnostic Explanations)

Local surrogate models are interpretable models that are used to explain individual predictions of black box machine learning models. Surrogate models are trained to approximate the predictions of the underlying black box model. Instead of training a global surrogate model, LIME focuses on training local surrogate models to explain individual predictions.

The recipe for training local surrogate models:

1.Select your instance of interest for which you want to have an explanation of its black box prediction.

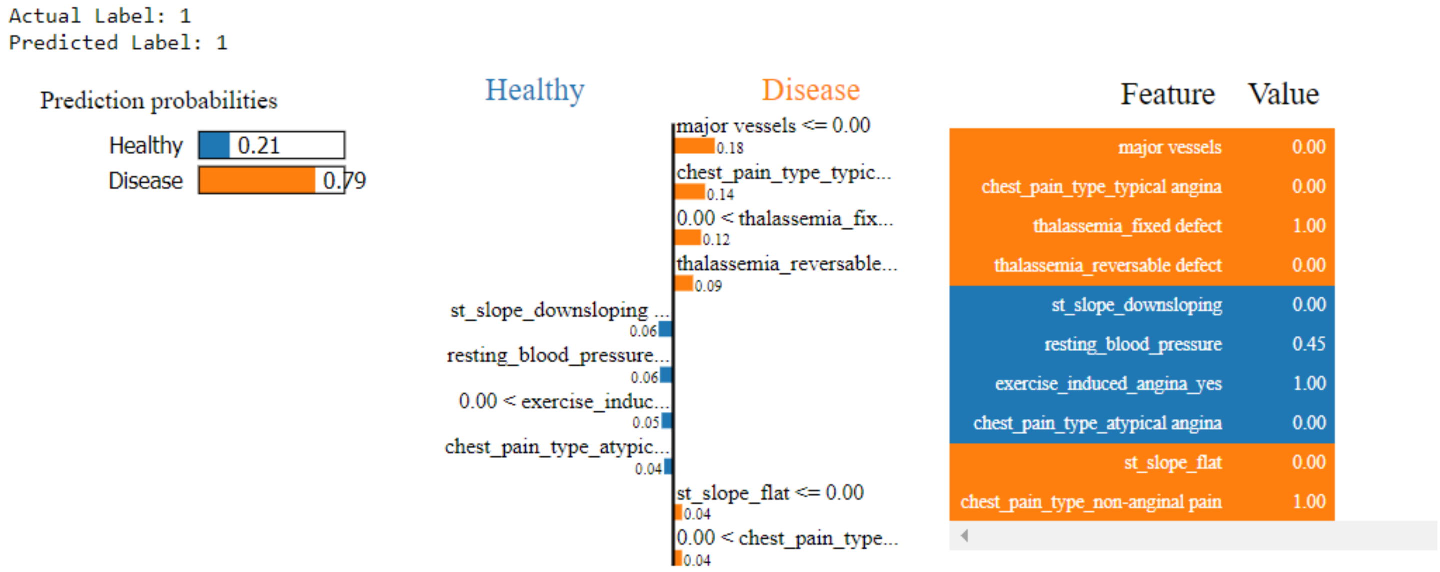
2.Perturb your dataset and get the black box predictions for these new points.

3.Weight the new samples according to their proximity to the instance of interest.

4.Train a weighted, interpretable model on the dataset with the variations.

5.Explain the prediction by interpreting the local model.

Interpretable Machine Learning book : https://christophm.github.io/interpretable-ml-book/lime.html



```
Actual Label: 1
Predicted Label: 1
```

Feature	Value
major vessels	0.00
chest_pain_type_typical angina	0.00
thalassemia_fixed defect	1.00
thalassemia_reversable defect	0.00
st_slope_downsloping	0.00
resting_blood_pressure	0.45
exercise_induced_angina_yes	1.00
chest_pain_type_atypical angina	0.00
st_slope_flat	0.00
chest_pain_type_non-anginal pain	1.00

Interpretability Conclusion

Machine Learning doesn’t have to be a black box anymore. What use is a good model if we cannot explain the results to others? Interpretability is as important as creating a model. To achieve wider acceptance among the population, it is crucial that Machine learning systems are able to provide satisfactory explanations for their decisions. As Albert Einstein said,” If you can’t explain it simply, you don’t understand it well enough”.