# Heart Disease Prediction and Classification using Machine Learning

Foundations of Artificial Intelligence - Prof: Petia Georgieva (petia@ua.pt) & Eugénio Rocha (eugenio@ua.pt)

Academic Year 2021/22

André Reis Fernandes Number: 97977 Computacional Engineering Physics Department andre.fernandes16@ua.pt WorkRate: 50%

Abstract-In this document we use 6 Machine Learning algorithms implemented both in Python and in the Rapid Miner software to predict heart disease using a given data set as well

Filter Index Terms—machine learning, artificial intelligence, confuse matrix, performance metrics, label, parameters, hyperparameters tunning, ROC, AUC, Cost/Loss function.

as study which model is the best. After that we will conclude

this project by applying an Hidden Markov Model and Kalman

## I. INTRODUCTION

This project was proposed for the Foundations of Artificial Intelligence class by our teachers Petia Georgieva and Eugénio Rocha, an 3rd year class of the 1st cycle degree in Computational Engineering. The interest in learning and use Artificial Intelligence and Machine Learning to our day-to-day problems is growing day by day especially in the use to predict diseases, because manually determine the odds of getting, for example, an heart disease based on risk factors it's difficult. We decided to choose this theme because it reveals great importance to the society as well for us that learn more about AI and ML.

#### II. THE DATA SET

The dataset used in this article is the Cleveland Heart Disease dataset taken from the UCI repository. The dataset consists of 297 individuals data. There are 14 columns in the dataset, which are described below.

- 1. Age, in years
- 2. Sex, 1 = male; 0 = female
- 3. cp: chest pain type
  - Value 0: typical angina
  - Value 1: atypical angina
  - Value 2: non-anginal pain
  - Value 3: asymptomatic
- 4. trestbps: resting blood pressure (in mm Hg on admission to the hospital)
- 5. chol: serum cholestoral in mg/dl

Number: 98012 Computacional Engineering

Gonçalo Jorge Loureiro de Freitas

Physics Department goncaloifreitas@ua.pt WorkRate: 50%

- 6. fbs: (fasting blood sugar > 120 mg/dl) 1 = true; 0 =
- 7. restecg: resting electrocardiographic results
  - Value 0: normal
  - Value 1: having ST-T wave abnormality (T wave inversions and/or ST elevation or depression of > 0.05 mV
  - Value 2: showing probable or definite left ventricular hypertrophy by Estes' criteria
- 8. thalach: maximum heart rate achieved
- 9. exang: exercise induced angina, 1 = yes; 0 = no
- 10. oldpeak = ST depression induced by exercise relative to
- 11. slope: the slope of the peak exercise ST segment
  - Value 0: upsloping
  - Value 1: flat
  - Value 2: downsloping
- 12. ca: number of major vessels (0-3) colored by flourosopy
- 13. thal: 0 = normal; 1 = fixed defect; 2 = reversable defect
- 14. condition (target): 0 = no disease, 1 = disease

### III. THE APPROACH - PART 1

To study this data set we implemented 6 models, using both Python the Rapid Miner software. The code, rapid miner processes and the data can be found in our github repository

In this article we will be using the following classification models for classification:

- 1) Logistic Regression (Python)
- 2) Support Vector Machine (Python)
- 3) Gaussian Naive Bayes (Python)
- 4) Decision Tree (Python)
- 5) K-Nearest-Neighbor (Python)
- 6) Neural Networks (Rapid Miner)

It is commom to use a 60:20:20 ratio which the middle 20% is the validation set which is used to find the hyper-parameters, but in this article, for all models, we divide the data in an 80:20 ratio, that is, the train set is 80% and test set is 20% of the whole data. The train set will be used to train the model, i.e, finding the parameters that minimizes our error in the training set.

# A. Data Overview

Firstly we need to check if there is null values that can mislead us. The data that we use is already pre-processed, which means, there aren't any null values or unbalanced data, so we can jump right into applying the models. If there were null values we needed to drop/eliminate them to ensure an higher performance.

Let's take a look on how the data is arranged by comparing each feature with the frequency and condition, remembering that condition = 1 (orange) implies a disease and = 0 (green) implies that there isn't a disease

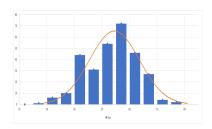


Fig. 1: Age distribution following a normal distribution.

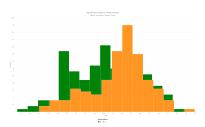


Fig. 2: Age Variation in relation to the Heart Condition.

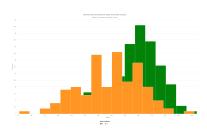


Fig. 3: Maximum heart rate achieved in relation to the Heart Condition.

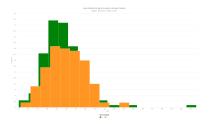


Fig. 4: Serum Cholesterol (in mg/dl) in relation to the Heart Condition.

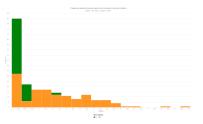


Fig. 5: ST depression (induced by exercise relative to rest) in relation to the Heart Condition.

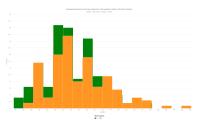


Fig. 6: Resting blood pressure (in mm Hg on admission to the hospital) in relation to the Heart Condition.

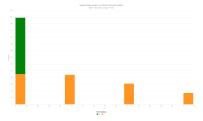


Fig. 7: Number of major vessels (0-3) in relation to the Heart Condition.

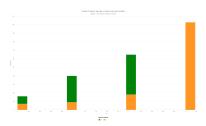


Fig. 8: Number of Chest pain type in relation to the Heart Condition.



Fig. 9: Exercise induced angina in relation to the Heart Condition.



Fig. 10: Fasting blood sugar ( > 120 mg/dl) in relation to the Heart Condition.



Fig. 11: Resting electrocardiography results in relation to the Heart Condition.



Fig. 12: Sex in relation to the Heart Condition.



Fig. 13: The slope of the peak exercise ST segment in relation to the Heart Condition.

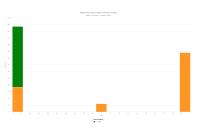


Fig. 14: Thallium stress result in relation to the Heart Condition.

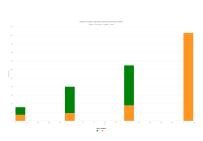


Fig. 15: Type of chest pain in relation to the Heart Condition.

	age	sex	ср	trestbps	chol	fbs	restecg	thalach
age	1							
sex	-0.0924	1						
ср	0.110471	0.008908	1					
trestbps	0.290476	-0.06634	-0.03698	1				
chol	0.202644	-0.19809	0.072088	0.131536	1			
fbs	0.132062	0.03885	-0.05766	0.18086	0.012708	1		
restecg	0.149917	0.033897	0.063905	0.149242	0.165046	0.068831	1	
thalach	-0.39456	-0.0605	-0.33931	-0.04911	-7.5E-05	-0.00784	-0.07229	1
exang	0.096489	0.143581	0.377525	0.066691	0.059339	-0.00089	0.081874	-0.38437
oldpeak	0.197123	0.106567	0.203244	0.191243	0.038596	0.008311	0.113726	-0.34764
slope	0.159405	0.033345	0.151079	0.121172	-0.00922	0.047819	0.135141	-0.38931
ca	0.36221	0.091925	0.235644	0.097954	0.115945	0.152086	0.129021	-0.26873
thal	0.120795	0.370556	0.266275	0.130612	0.023441	0.051038	0.013612	-0.25839

Fig. 16: Correlation Matrix

If we look now to Fig.2 we can see that as the age increases the number of persons with an heart diseases increases as well. From the Fig.3 we can see that the lower the thalach the higher probability the person with a disease. From Fig.4 and Fig.9 we conclude that there ins't a correlation between the chol and if the exercises induces angina or not with the condition. The Fig.5, Fig.6 and Fig.7 shows us that the higher the old peak, trestbps and the number of major vessels the more probability the person has to have an disease. Figures 8 and 10 shows that when the chest pain type is asymptomatic there is more cases of an condition while when studying the fasting blood sugar we see that if this is < 120 the cases raises as well. Fig.11 shows that there are more heart diseases when the resting electrocardiograph results shows probable or definite left ventricu- lar hypertrophy by Estes' criteria (Val 2). Fig.12 tell us that the males (1) are more prominent to an heart disease. From Fig.13 we see that the he flat exercise ST segment traduces in an higher probability of a condition. Finally, Fig.14 show us that the reversible defect thal leads to an higher number of conditions. With Fig.16 we can see how each feature correlates with one and another to the heart disease.

#### IV. MODELS

After a quick research we found that we can use the scikit-learn's GridSearchCV, which identifies the best parameters that you can included in the parameter grid based on predefined parameters by the users. This will be use to help us find the parameters that minimizes the error in the train set, by define the scoring parameter of GridSearchCV to 'neg\_mean\_absolute\_error'. This function is going to be used for the first 5 models. In the last model we use a different approach that will be explained in chapter IV-F.

#### A. Logistic Regression

This type of statistical analysis (also known as logit model) is often used for predictive analytics and modeling, and extends to applications in machine learning. It is used in statistical software to understand the relationship between the dependent variable and one or more independent variables by estimating probabilities using a logistic regression equation.

In order to map predicted values to probabilities, we use the sigmoid function. The function maps any real value into another value between 0 and 1

$$S(z) = \frac{1}{1 + \exp{-z}}$$

As this function returns a value between 0 and 1 we select a threshold value or tipping point above which we will classify values into class 1 and below which we classify values into class 0. This threshold is simply the value returned and if its  $\geq 0.5$  it will belong to the class 1, i.e, class positive (with disease), if lower than 0.5 the model would assume that there isn't an disease. [13]

There are many parameters for this model, for example the 'penalty' parameter; which has 4 possible parameters 'none',

# 

LOGISTIC REGRESSION

Fig. 17: Logistic Regression idea of model working

'12' (disperse the error terms in all the weights that leads to more accurate customized final models), '11' (gives output in binary weights from 0 to 1 for the model's features and is adopted for decreasing the number of features in a huge dimensional dataset) and 'elasticnet' (12 + 11 penalty); or the 'solver' parameter; with the options being 'newton-cg', 'lbfgs', 'liblinear', 'sag', 'saga'; and many more that can be found in the official documentation with the description of what each parameter does. Has we want the best accuracy we need to see which combination of these parameters gives us the lest error in the train set. Using the GridSearchCV function, where we compare every possible combination, between some predefined values of C, penalty and solver, it was found that the best parameters are C: 0.1, penalty: l2, solver:'newton-cq',with all the other parameters are set as default. The max\_iter parameter was also change to an higher value than the default value (100) to make sure that our model converges.

#### B. Support Vector Machine (SVM)

A Support Vector Machine is a supervised machine learning algorithm which can be used for both classification and regression problems. It follows a technique called the kernel trick to transform the data and based on these transformations, it finds an optimal boundary between the possible outputs.

The main idea is to identify the optimal separating hyperplane which maximizes the margin of the training data. Let us understand this objective term by term. A separating hyperplane it's a line (or other, depending on the dimension) that can separate the given data, which means, from one side we have all elements from one group and in the other side we have the elements of the another group. Maximizing the distance between the nearest points of each class and the hyper-plane would result in an optimal separating hyper-plane. This distance is called the margin.[1]

Using GridSearchCV, we found that the best possible parameters between kernel = ['rbf', 'poly', 'sigmoid'], C = [0.1, 1, 10, 100, 1000], gamma = [1, 0.1, 0.01, 0.001, 0.0001] the best are kernel = 'poly', C = 1 and gamma = 0.0001.

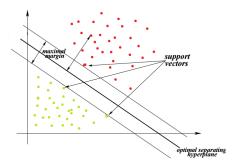


Fig. 18: Optional sparating hyper-plane

# C. Naive Bayes (Gaussian)

Naive Bayes is the easiest and rapidest classification method available, and it is well suited for dealing with enormous amounts of information. In several applications such as spam filtering, text classification, sentiment analysis the Naive Bayes classifier has shown to be effective. It makes predictions about unknown classes using the Bayes theory of probability.

There are 3 types of Naive Bayes Classification, the Gaussian, the Bernoulli and the Multinomial. In this article we just use the first one, which is employed when the predictor values are continuous and are expected to follow a Gaussian distribution, as ours does as we can see in Fig 1. It is worthy to note that this model is the easiest to program as it doesn't have any parameters to tunning.

1) Bayes Theorem: Bayes Theorem can be used to calculate conditional probability. Being a powerful tool in the study of probability, with the following formula.[2]

$$\mathcal{P}(A|B) = \frac{\mathcal{P}(B|A)(A)}{\mathcal{P}(B)}$$

Where  $\mathcal{P}(A|B)$  is the probability of event A occurring, given event B has occurred;  $\mathcal{P}(B|A)$  the probability of event B occurring, given event A has occurred; $\mathcal{P}(A)$  the probability of event A and  $\mathcal{P}(B)$  the probability of event B. Note that events A and B are independent events (i.e., the probability of the outcome of event A does not depend on the probability of the outcome of event B).

# D. Decision Tree

Decision Trees are powerful machine learning algorithms capable of performing regression and classification tasks. To understand a decision tree, let's look at an simple example which tries to predict if it is save to play golf, in Fig.19. We start at the root of the tree that contains our training data. At the root, we split our dataset into distinguished leaf nodes, following certain conditions like using an if/else loop. These splitting criteria are carefully calculated using a splitting technique.

With this tree we can easily decide if we can play golf in good conditions of it's better to stay home.

Outlook	Temp	Humidity	Windy	Golf?	
rainy	hot	high	false	no	
rainy	hot	high	true	no	Outlook
overcast	hot	high	false	yes	Outlook
sunny	mild	high	false	yes	
sunny	cool	normal	false	yes	sunny overcast rain
sunny	cool	normal	true	no	
overcast	cool	normal	true	yes	(Humidity)   yes   (Windy)
rainy	mild	high	false	no	
rainy	cool	normal	false	yes	/normal \ high / true \ false
sunny	mild	normal	false	yes	<del></del>
rainy	mild	normal	true	yes	yes no no yes
overcast	mild	high	true	yes	
overcast	hot	normal	false	yes	
sunny	mild	high	true	no	

Fig. 19: Example of a Decision Tree

So all-in-all, decision trees are a hierarchical series of binary decisions, and the antecedent nodes are simply the best split for the available training data at each level of our decision tree.

As we to minimize the error we also want the best splits, and these traduce in wanting the smallest tree and the most 'purest' (most homogeneous) nodes and for this we need to understand some fundamental splitting parameters that it uses to define those conditions, like *Gini Index*, *Entropy*, *Information Gain*, and *Classification error*.[14]

1) Gini Index: Every Machine Learning model has a loss function or a cost function, whose objective is to minimize the cost, i.e., the tentative distance between the predicted value and actual value. Gini Index is the cost/loss function that is used by decision trees to choose which feature will be used for splitting the data, and at what point the column should be split, and can be determined by:

$$GINI(node) = 1 - \sum_{Class_j} [\mathcal{P}(Class_j|node)]^2$$
 (1)

 $P(Class_j|node)$  being the probability of  $Class_j$  at a given node

An lower *Gini* score traduces in a lower cost which gives us the information that it was a good split.

2) Classification Error: Suppose that we cut off the growing process at various points over the growing process, and we evaluate the error of the tree at that point and time. This would lead to a graph of size vs. error (where error is the probability of making a mistake). There are two error rates to be considered; training/test error, i.e. fraction of mistakes made on the training/test set. These error curves are as follows:

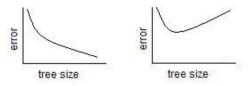


Fig. 20: Training (left) and Test error curves (right)

As the tree size increases, training error decreases. However, as the tree size increases, testing error decreases at first since we expect the test data to be similar to the training data, but

at a certain point, the training algorithm starts training to the noise in the data, becoming less accurate on the testing data. At this point we are no longer fitting the data but instead we are fitting the noise in the data. Therefore, the shape of the testing error curve will start to increase at a certain point at which the tree is too big and too complex to perform well on testing data (an application of Occam's razor). This is called overfitting to the data, in which the tree is fitted to spurious data. As the tree grows in size, it will fit the training data perfectly and not be of practical use for other data such as the testing set. We want to choose a tree at the minimum of the curve, but we are not aware of the test curve during training. We build the tree only using the training error curve, which appears to be decreasing with tree size. Again, we have two conflicting goals. There is a trade off between training error and tree size.

This error can be calculated using the follow equation:

$$Error(node) = 1 - \max_{Class_j}(\mathcal{P}(Class_j|node))$$
 (2)

3) Entropy: Entropy, H, measures the randomness or disorders in a system. In terms of data, we can define it as the randomness in the information we are processing. The higher the randomness, the higher the entropy. Hence, harder to conclude from that information, so we ideally want H=0. Mathematically, we calculate entropy as:

$$H(node) = -\sum_{Class_{j}} [\mathcal{P}(Class_{j}|node)log(\mathcal{P}(Class_{j}|node))]$$

4) Information Gain: Information gain,  $I_{gain}$ , measures the amount of information provided by a given feature or attribute about a particular target class, i.e. how much uncertainty was reduced after splitting on a given feature. While creating a decision tree, our goal is to find the attribute having the highest Information Gain, and conversely, the lowest entropy. Mathematically, it is calculated as the difference of the initial and final entropy.

$$I_{gain}(node) = \mathcal{H}_i - \mathcal{H}_f \tag{4}$$

- 5) Working with data: While training, our decision tree model evaluates all possible splits across all possible columns and picks the split with the lowest Gini Score. With the first split, all the data according to a specific condition falls towards either the left or the right of the root node. Now, for each side of training data under the root node, all possible splits are calculated again and the split with the lowest Gini Index is chosen. The process repeats for both left and right sides till we reach the terminating nodes representing a class in the target column.
- 6) Finding the best Parameters: Now that we have explained the importance of the splitting parameters we need to find the best ones for our dataset. As with first 2 models explained above we can use the GridSearchCV to obtain the parameters giving us the better possible accuracy.

We also need to pay attention than if we use Information Gain as a criterion, we assume that our attributes are categorical, and as per Gini index, we assume that our attributes are continuous. For our data set, we will work with Gini Index.

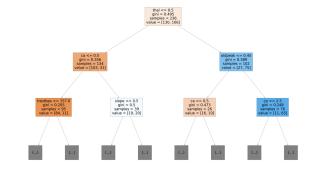


Fig. 21: Decision Tree for our data with  $max_{depth} = 2$ 

You can create the tree to whatsoever depth using the  $max_{depth}$  parameter, only two layers of the output are shown above. Let's break the blocks in the above visualization:

- 1)  $thal \le 0.5$  Is the condition on which the data is being split. (where that is the column name).
- 2) Gini: Is the Gini Index. Although the root node has a Gini index of 0.495, which is not so great, we can imagine what the other Gini scores would have looked like.
- 3) Samples: The number of data rows before the split.
- 4) Values=[x,y]: Provides the split rows of training data into the following leaf nodes. Since we are doing binary classification, there are only two values.

Now all we have to do is find the hyper-parameters. For this model we will we use the GridSearchCV which give us back that the best values which are max\_depth=5, max\_features='log2', max\_leaf\_nodes=30, min\_samples\_leaf=8, min\_weight\_fraction\_leaf=0.3. It's possible to get other parameters and results due to the randomness of this model, i.e, for example, a different first split would change everything. So this aren't the ultimate best parameters but the best parameters between some tests we made.

#### E. K-Nearest-Neighbor (KNN)

The KNN algorithm assumes that similar things exist in close proximity. In other words, similar things are near to each other. This is a very used algorithm due to being simple, easy to implement and very versatile as it can be used for classification, regression, and search problems. However it got one big disadvantaged, the algorithm gets significantly slower as the number of examples and/or predictors/independent variables increase. [7]

This algorithm can be explained in few steps as following:

- 1) Select the number of the neighbors, K
- 2) Calculate the Euclidean (5) distance of K number of neighbors

- 3) Take the K nearest neighbors as per the calculated Euclidean distance
- 4) Among these K neighbors, count the number of the data points in each category
- 5) Assign the new data points to that category for which the number of the neighbor is maximum
- 6) The model is ready

With the Euclidean Distance of  $A(X_1,Y_1)$  and  $B(X_2,Y_2)$  being:

$$ED_{\langle A,B\rangle} = \sqrt{(X_1 - X_2)^2 + (Y_1 - Y_2)^2}$$
 (5)

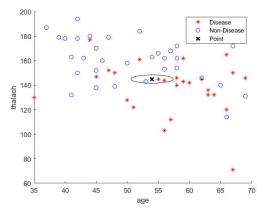


Fig. 22: Example of K = 3 for our train set of thalach-age

As we can see in the figure above, after selecting K=3 and the model choosing an random point, X the model identifies the 3 nearest points, based on the euclidean distance. The class label of the new record is the label of the majority of the nearest neighbors, in this case the blue circle, o, would be change for the red star, \*.

Using GridSearchCV we found that the best parameters from leaf\_size = [1,2,...,49]; n\_neighbors = [1,2,...,29] and p = [1,2] are [leaf\_size=1, n\_neighbors=23, p=1] with all the others parameters set to default and being n\_neighbors the value of our K.

# F. Neural Network (NN)

Neural networks, also known as artificial neural networks (ANNs) or simulated neural networks (SNNs), are a subset of machine learning and is at the heart of deep learning algorithms however, we have used it as a non-deep classifier. Their name and structure are inspired by the human brain, mimicking the way that biological neurons signal to one another [8]. Neural networks are ideally suited to help people solve complex problems in real-life situations. They can learn and model the relationships between inputs and outputs that are nonlinear and complex, make generalizations, reveal hidden relationships, patterns and predictions, and model highly volatile data and variances needed to predict rare events [19]. Neural networks are composed of a certain number of layers, an input and output layer and then, it could have one or more hidden layers. Each layer is composed of set of nodes, the

artificial neurons. Each neuron has the ability to let through or not data, depending if his value is above the threshold, letting through the data to the next layer of neurons.

Each node has its own weight assigned and when data meets it, as an input, it gets multiplied by the weight and then summed. If that output exceeds the given threshold the activation function is "fired" and the data is passed to the next layer i.e. the input of a neuron becomes the output of the next node [8].

To play this model the software used was RapidMiner Studio. The first step, shown in the figure 23, is to apply a numerical to polynomial operator that changes the type of selected numeric attributes to a polynomial type and maps all values of these attributes to corresponding polynomial values. In other words, each numerical value is simply used as nominal value of the new attribute, the condition. As numerical attributes can have a huge number of different values even in a small range, converting such a numerical attribute to polynomial form will generate a huge number of possible values for the new attribute.

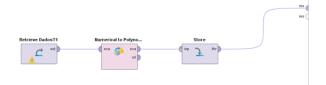


Fig. 23: Neuronal Net.

The next step is represented in figure 24. Firstly is applied a split data operator where we have created a ratio of 80% / 20%, to use it, already mentioned before, 80% of data to train and 20% to test. Neural Net operator is applied and getting the 80% as input. This operator, as well mention above, can have hidden layers yet, since the focus of this course is non-deep strand, we've used only one hidden layer. Each layer has a certain size associated. The number of layers and the number of nodes in each hidden layer are known as hyperparameters and they must be specified. The most reliable way to configure these hyperparameters is via systematic experimentation [6]. Regarding the choice of the number of neurons there are many rule-of-thumb methods for determining the correct number of neurons to use in the hidden layers [12]. In this work, to calculate the number of neurons in the hidden layer, we have used two thirds of the number of neurons in the input layer plus number of neurons in the output layer [12].

Other parameter in the NN operator is the training cycles. This parameter specifies the number of training cycles used for the neural network training. Its default number is two-hundred, but after some testing we figured that four-hundred was the ideal number.

Learning rate, the amount of change to the model during each step [5]. This hyperparameter controls the rate or speed at which the model learns. Typical values for a neural network

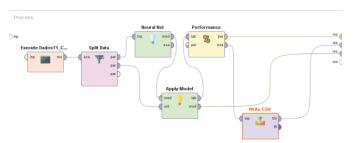


Fig. 24: Neuronal Net.

learning rate are less than 1 and greater than  $10^{-6}$  [5]. On the other hand, a traditional default value for the learning rate is 0.1 or 0.01. After some attempts of different learning rates, the best one was 0.001.

For the momentum, that simply adds a fraction of the previous weight update to the current one leading to an increasing in the size of the steps taken towards the minimum of the gradient, we leave it on zero.

Then, the apply model was applied and ,as the name says, applies the model. It got as input the 20% data and of the splitting data operator and trained model of NN operator. Lastly, we integrate the performance operator. This operator has the function to evaluate the NN model's performance and the performance criteria are automatically determined in order to fit the NN model.

# V. RESULTS

#### A. Confusion Matrix and Performance Metrics

For each model it is possible to evaluate its performance. Every model has a confusion matrix, being the generic form represented in table I.

TABLE I: Confusion Matrix

	True 0	True 1
Pred 0	TP	FN
Pred 1	FP	TN

A confusion matrix is a summary of prediction results on a classification problem [17]. It shows the ways in which our classification model is confused when it makes predictions giving insights, not only into the errors being made, but more importantly the types of errors that are being made. Analysing the matrix we can extract the True Positive (TP), True Negative (TN), False Positive (FP) and the False Negative (FN) values.

For the Logistic Regression model the confusion matrix obtained is represented in table II. For this model we were able to get TP we got 27, for TN we got 26, for FP we got 5 and for FN we got 2.

TABLE II: Confusion Matrix - Logistic Regression

	True 0	True 1
Pred 0	27	2
Pred 1	5	26

For the Support Vector Machine (SVM) model the confusion matrix obtained is represented in table III. For this model we were able to get TP we got 24, for TN we got 24, for FP we got 7 and for FN we got 5.

TABLE III: Confusion Matrix - SVM

	True 0	True 1
Pred 0	24	5
Pred 1	7	24

For the Naive Bayes (Gaussian) model the confusion matrix obtained is represented in table IV. For this model we were able to get TP we got 25, for TN we got 26, for FP we got 5 and for FN we got 4.

TABLE IV: Confusion Matrix - Naive Bayes

	True 0	True 1
Pred 0	25	4
Pred 1	5	26

For the Decision Tree model the confusion matrix obtained is represented in table V. For this model we were able to get TP we got 23, for TN we got 25, for FP we got 6 and for FN we got 6.

TABLE V: Confusion Matrix - Decision Tree

	True 0	True 1
Pred 0	23	6
Pred 1	6	25

For the K-Nearest Neighbour (KNN) model the confusion matrix obtained is represented in table VII. For this model we were able to get TP we got 28, for TN we got 21, for FP we got 4 and for FN we got 6.

TABLE VI: Confusion Matrix - KNN

	True 0	True 1
Pred 0	22	11
Pred 1	8	19

For the Neural Network (NN) model the confusion matrix obtained is represented in table VII. For this model we were able to get TP we got 29, for TN we got 21, for FP we got 3 and for FN we got 6.

TABLE VII: Confusion Matrix - Neural Net

	True 0	True 1
Pred 0	29	6
Pred 1	3	21

With the confusion matrix it is possible to get the accuracy and precision of the model used. For the accuracy, the formula used was:

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

To obtain the precision, the formula is:

$$Precision = \frac{TP}{TP + FP}$$

It is also possible to get the F1 Score, a metric that is primarily used to compare the performance of two classifiers, with the confusion matrix. Its formula is:

$$F1 = 2*\frac{Recall*Precision}{Recall+Precision}$$

where Recall is the TPR.

It is also possible to get the True Positive Rate (TPR), also known as recall or sensitivity, which represents all positive examples the fraction of correctly classified, True Negative Rate (TNR), also known as specificity representing all negative examples the fraction of correctly classified, and False Positive Rate (FPR) that represents how often an actual negative instance will be classified as positive, a fals alarm.

$$TPR = \frac{TP}{TP + FN}$$

$$TNR = \frac{TN}{TN + FP}$$

$$FPR = \frac{FP}{FP + TN}$$

Finally, we can get, by using the confusion matrix, the balanced accuracy, often used when the two classes are imbalanced – that is, one class appears much more than the other. It is represented by the bellow formula:

$$Balanced_{Accuracy} = \frac{Recall + Specificity}{2}$$

Where Specificity is the TNR.

The table VIII show us all of these performance metrics by model.

TABLE VIII: Perfomace Metrics

(%)	Acc	Prec	F1	TPR	TNR	FPR	Bal Acc
LogReg	88.3	84.4	88.5	93.1	83.9	16.1	88.5
SVM	80.0	77.4	79.9	82.8	77.4	22.6	80.0
NB	85.0	83.3	84.7	86.2	83.8	16.1	85.0
DT	80.0	75.9	78.6	81.5	78.8	21.2	80.0
KNN	68.3	73.3	69.8	66.7	70.4	29.6	68.5
NN	84.75	90.63	83.71	77.78	87.50	12.50	82.64

# B. Comparing with other articles

We search other articles/works similar to ours to our data set and we notice that when using our data set various authors apply this same models, but using the default parameters. So for that, we applied all this models again but this time using the default parameters, and we obtained the following performance table:

TABLE IX: Perfomace Metrics - Default Parameters

(%)	Acc	Prec	F1	TPR	TNR	FPR	Bal Acc
LogReg	86.7	83.9	86.7	89.7	83.9	16.1	86.8
SVM	61.7	57.1	67.6	82.8	42.0	58.1	62.3
DT	68.3	72.4	68.9	65.6	71.4	28.6	68.5
KNN	66.7	71.0	68.8	66.7	66.7	33.3	66.7
NN	74.6	71.9	75.4	79.3	70.0	30.0	74.7

It's important to notice that all values are lower, as expected, as this aren't the best parameters for our data. Also, as Gaussian Naive Bayes doesn't have any parameters so the results are the same.

#### C. ROC and AUC curves

The Receiver Operator Characteristic (ROC) curve is an evaluation metric for binary classification problems. It is a probability curve that plots the TPR against FPR at various threshold values and essentially separates the 'signal' from the 'noise'. The Area Under the Curve (AUC) is the measure of the ability of a classifier to distinguish between classes and is used as a summary of the ROC curve. The higher the AUC, the better the performance of the model at distinguishing between the positive and negative classes. [5]

When AUC = 1, then the classifier is able to perfectly distinguish between all the Positive and the Negative class points correctly. If, however, the AUC had been 0, then the classifier would be predicting all Negatives as Positives, and all Positives as Negatives. When 0.5<AUC<1, there is a high chance that the classifier will be able to distinguish the positive class values from the negative class values. This is so because the classifier is able to detect more numbers of True positives and True negatives than False negatives and False positives. When AUC=0.5, then the classifier is not able to distinguish between Positive and Negative class points. Meaning either the classifier is predicting random class or constant class for all the data points. [17]

So, the higher the AUC value for a classifier, the better its ability to distinguish between positive and negative classes.

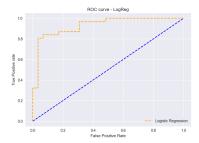


Fig. 25: ROC - Logistic Regression

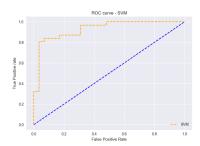


Fig. 26: ROC - SVM

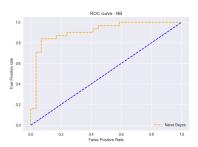


Fig. 27: ROC - Naive Bayes

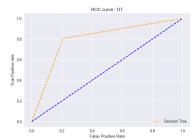


Fig. 28: ROC - Decision Tree

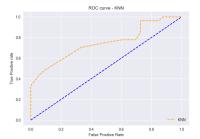


Fig. 29: ROC - K-nearest Neighbor



Fig. 30: ROC - Neural Network

The models from figures 25, 26, 27, 28 and 29 got an AUC of 0.93,0.93,0.91, 0.80 and 0.75. As the AUC of the first 3 models is very close to 1 we can conclude that the model can perfectly distinguish between all the Positive and the Negative class correctly, where as for the Decision Tree and K-nearest Neighbor, although its not perfect, there is a high chance than it can distinguish them correctly.

The ROC graph represented in 30 was made on RapidMiner software and the AUC obtained was 0.89. As it can be seen, it has two lines where the red represents the ROC function and the blue the threshold ROC function. Both line share the same x-axis however their y-axes are different, TPR for ROC and a threshold value for Threshold ROC. The ROC curve is built by decreasing the thresholds, from 1 to 0 and, at each value a confusion matrix is calculated giving a point in the graph (FPR versus TPR) i.e. the ROC graph. Well, the blue curve was built by using the thresholds that were used to build the ROC.

#### D. Error Functions

To study this functions we just used 2 features, age as X and thalach as Y, this 2 were chosen randomly and we could have selected any of the other features.

1) Loss Function: Loss function is also known as cost function. This function basically means how much far away our predicted line is from the generic data [18]. This function measure the difference between the estimator (the dataset) and the estimated value (the prediction, data after model) [15]. The function used to calculate the cost function was:

$$\mathcal{J}(\theta) = \frac{1}{m} \sum_{i=1}^{m} (h_{\theta}(x^i) - y^i)^2$$

Where m represents the length of the variable in Y axis and  $h_{\theta}$  represents the hypothesis. When we applying it, it should be applied for different values of  $\theta$  so we can see the minimum of the function [15].

2) Gradient Descent: Gradient descent is an optimization algorithm that's used when training a machine learning model. It's based on a convex function and tweaks its parameters iterative to minimize a given function to its local minimum. [10]

Gradient descent algorithm does not work for all functions. There are two specific requirements. A function has to be differentiable and convex. The function used to obtain the gradient for all the models descent is:

$$\frac{\partial \mathcal{J}(\theta)}{\partial \theta} = \frac{1}{m} \sum_{i=1}^{m} (h_{\theta}(x^{i}) - y^{i}) x_{j}^{i}$$

We also need to see if we are using a good value for the learning rate, in Fig.31 we see the format we want our curve to take and with this we can try different values for the learning rate and see which one applies better.

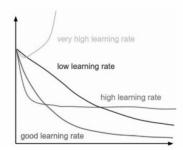


Fig. 31: Good and Bad Learning Rates

After all this requirements we implement the gradient function to our data with an learning rate of 0.01 and we got the following curve.

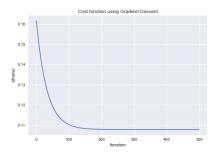


Fig. 32: Gradient Descent, learning rate = 0.01

As we can see just a bit after the 100 iterations our model converges. It is worth noting that to compute the gradient descent it is necessary to choose two attributes. In this case we have 13 of them, so we've chose the attribute age and thalach.

# VI. CONCLUSION - PART 1

Heart Disease is one of the major concerns for society today. It is difficult to manually determine the odds of getting heart disease based on risk factors. However, machine learning techniques are useful to predict the output from existing data. For that, it's important to get the best prediction, and this only happen when working with the best parameters for the data set in study and with comparing models to see which one gives us a best result.

As seen in chapter V the best model for classification of this data set is the Logistic Regression followed by the Naive Bayes (Gaussian) due to being the models with best accuracy of the test set.

#### VII. HIDDEN MARKOV-MODEL

Hidden Markov models (HMMs) are sequence models. That is, given a sequence of inputs, such as words, an HMM will compute a sequence of outputs of the same length. An HMM model is a graph where nodes are probability distributions over labels and edges give the probability of transitioning from one node to the other. Together, these can be used to compute the probability of a label sequence given the input sequence.

HMM is a statistical Markov model in which the system being modeled is assumed to be a Markov process with unobserved (hidden) states. In our case, the hidden states are the condition, disease and non disease. HMM also has another layer, another states, which are called observations, i.e, something you can observe so, in our case the observations will be a sequence composed by the 13 features studied in this data set, II.

Instead of using all the 13 features we will only use 3. As the Logistic Regression model was the one with best results we decided to use this model to calculate the feature importance, [4], which gave us the features with most importance, with the 3 with a higher value being sex, ca and thal. We also try to choose features where the correlation wasn't high so we don't influence the results. Remembering that sex could be 0 (female) or 1 (male), ca could be 0,1,2 or 3 based on the number of major vessels colored by flourosopy and thal could be 0 (normal), 1 (fixed defect) or 2 (reversable deffect). With this we have  $2 \times 4 \times 3 = 24$  sequence possibilities ([000],[001],[002], etc.), we would assume that the order of the sequences are sex, ca and thal, i.e., for the example 001 this means sex = 0, ca = 0 and thal = 1. As described above our Markov Chain hidden states would be the condition, 0 (no disease) and 1 (disease), with this first we have to calculate the following probabilities, also known as Transition probabilities:

- 1. P(condition = 1)
- 2. P(condition = 0)
- 3.  $P(condition_i = 0 \text{ and } condition_{i+1} = 0)$
- 4.  $P(condition_i = 1 \text{ and } condition_{i+1} = 0)$
- 5.  $P(condition_i = 0 \text{ and } condition_{i+1} = 1)$
- 6.  $P(condition_i = 1 \text{ and } condition_{i+1} = 1).$

Our observations will be that 24 sequences made from the 3 most important features. We now need to calculate the Emission, which are the probabilities of an sequence given having an disease or not, per example, P(001|condition=1) With all the Emission and Transition probabilities calculated we get following Markov Chain, represented in Fig.33.

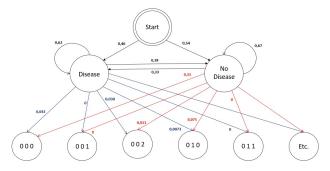


Fig. 33: Markov Chain of our model

With this probabilities we can see what a person with or without an heart disease is more likely to have between these 3 parameters. In the table X, we have the 3 most commons sequences that leads to a person with disease and without an disease, remembering that the order is sex,ca,thal.

TABLE X: Sequences with higher probability

(sex,ca,thal)	Disease	Non Disease
1st	112 and 102	000
2nd	122	100
3rd	110	102

With this we can conclude that a person with an heart disease is more likely to be a man with 1 or 0 major vessel colored by flourosopy and reversable deffect thal, whilst a person without an heart disease is more likely to be a women with 0 major vessel colored by flourosop and an normal thal. Studying the other probabilities, we notice something interesting, we see that if sex is 1 (male) all possibles sequences of the other features have events when the condition is 1 (disease), i.e, every possible sequence for a man can result in a disease what doesn't happen when sex is 0 (female), with this we can conclude that men are more prone to an heart disease than women.

A women that starts with ca=0 and thal=0 and then her ca is changed to 2 and her thal is alternate with 1 or 2, our module assumes that condition is always equal to 0 (no disease), this means that, based in our HMM, if a women starts with 0 major vessels colored by flourosopy and a normal thal when her number of vessels is changed to 2 and her thal varies between normal, fixed and reversable deffect this alterations are not enough to provoke an heart disease to the a woman. This still happens when she return to the initial state, i.e, sex=ca=thal=0. The sequence to study this problem is the following:

$$000 \rightarrow 020 \rightarrow 021 \rightarrow 022 \rightarrow 021 \rightarrow 020 \rightarrow 000$$

Now, let's begin in the same initial state as the example before, but now, the thal of this woman is changed to reversable deffect (2), and her major vessels change between the 4 possibilities. The exact same thing happens, this alterations doesn't change the condition of the woman. The sequence now is:

$$000 \rightarrow 002 \rightarrow 012 \rightarrow 022 \rightarrow 032 \rightarrow 022 \rightarrow 012 \rightarrow 002 \rightarrow 000$$

But woman are not super humans, and there are some alterations that we study that can change the condition of a woman. Let's go back to the last sequence. Let's pick up the last sequence when the woman goes to 012 for the second time. If we stopped where or take the sequence above, she wouldn't be diagnosed with a disease but, if, for some reason, she instead of returning to 0 major vessels, instead her thal is changed to normal, keeping the 1 major vessels, this alteration is enough for the woman to be diagnosed with an heart disease. The sequence assumed here is the following:

$$000 \rightarrow 002 \rightarrow 012 \rightarrow 022 \rightarrow 032 \rightarrow 022 \rightarrow 012 \rightarrow 010$$

We can study more possible sequences, but the most interesting behaviours are when a woman starts or her ca and thal are changed 1 major vessel and normal, our model, always assume that this change provokes a change in the condition, diagnosing her with a disease, with the other interesting behaviour being that when a women starts or her ca and thal are changed 1 major vessel and reversable deffect the model assumes that this change is only significant when the previous/next state is 020 or, due to behaviour above described, 010.

Now, looking to what happens when sex is 1 (male). Starting with a man with 1 major vessel and normal thal (and condition = 0) if we alternate the thal (by any order), this alteration doesn't change his condition. The same happens when the thal is fixed to normal and we change the number of major vessels but, after we have 3 major vessels and the thal is changed, we only see an alteration in the diagnostic when the thal is changed to fixed deffect. The sequences are shown bellow:

$$110 \rightarrow 120 \rightarrow 130 \rightarrow 131 \rightarrow Disease$$
 
$$110 \rightarrow 120 \rightarrow 130 \rightarrow 132 \rightarrow NoDisease$$

For the final example, let's say we have this sequence:

$$101 \rightarrow 111 \rightarrow 112 \rightarrow 122 \rightarrow 121 \rightarrow 120 \rightarrow 110 \rightarrow 100$$

Our model assumes that the only change that changes the condition is the last step (110 to 100). There's also a interesting behavior when studying the case for men, when he starts or change to 1 major vessel and fixed deffect thal its always assume that the diagnostic is a disease. Other interesting fact is that a man that changes to 0 major vessels and a reversable deffect thal always is diagnosed with a disease, if the previous/following states aren't 132, 122, 130 or 101.

For the study of this problem, when a patient has diagnosed with a disease we stopped the sequence because we assume that a person with a heart disease can't cure from the disease, we also assume that a person can change to the opposite gender, to make the examples being the more accurate to real

medical cases has possible. We can study other changes of 3 features studied and, with this, we can try to predict what changes can and cannot provoke a change of the diagnostic, which is very help-full to a medic staff when analysing a patient.

# VIII. BAYESIAN NETWORK

Bayesian networks are a widely-used class of probabilistic graphical models. They consist of two parts: a structure and parameters. The structure is a directed acyclic graph (DAG) that expresses conditional independencies and dependencies among random variables associated with nodes. The parameters consist of conditional probability distributions associated with each node. A Bayesian network is a compact, flexible and interpretable representation of a joint probability distribution. It is also an useful tool in knowledge discovery as directed acyclic graphs allow representing causal relations between variables and at providing a convenient and coherent way to represent uncertainty in uncertain models and are increasingly used for representing uncertain knowledge. Typically, a Bayesian network is learned from data.

One of the most given examples of application is the fact that a Bayesian network could represent the probabilistic relationships between diseases and symptoms, which is the case of our study.

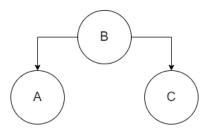
So, we can conclude that a Bayesian network is a graphical model that contains information about probabilities of relationships between variables that are normally used to make decisions.

# A. Example

We can make Bayesian Networks concrete with a small example. [3]

Consider a problem with three random variables: A, B, and C. A is dependent upon B,e.g. P(A|B), and C is dependent upon B, e.g. P(C|B). P(A|B) and P(C|B) are the conditional dependencies. As for the conditional independencies, this are the flowing, A is conditionally independent from C, e.g. P(A|B,C), and C is conditionally independent from A, e.g. P(C|B,A).

As A and C are dependent upon B, in the graph we have edges like (B,A) and (B,C), i.e., an arrow from B to A and an arrow from B to C. The graph is has follow:



Bayesian networks satisfy the local Markov property, which states that a node is conditionally independent of its non-descendants given its parents. In this example, P(A|B,C) =

P(A|B), since A is conditionally independent of its non-descendant, C, given B.

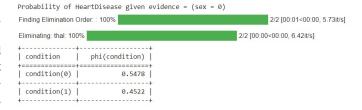
This property allows us to reduce the amount of required computation, since most nodes will have few parents relative to the overall size of the network.

# B. Implementation

For this problem, we did 2 simple implementations. In the first one we only use the 3 features from feature importance, i.e. sex, ca and thal. This features, plus the condition, will be the nodes. As for the edges we defined them as [('sex', 'condition'), ('ca', 'condition'), ('thal', 'condition')].

In the first implementation, we've used 'MaximumLikelihoodEstimator' as a model fit estimator. Maximum likelihood estimation is a method that determines values for the parameters of a model. The parameter values are found such that they maximise the likelihood that the process described by the model produced the data that were actually observed. In general, given a data set and a statistical model (Bayesian Network), the maximum likelihood method estimates the values of the different parameters of the statistical model in order to maximize the probability of the observed data.

It was also applied inferencing. Machine learning inference is the process of running data points into a machine learning model to calculate an output. This process is also referred to as "operationalizing a machine learning model" or "putting a machine learning model into production". In the developed code, a query was applied that allows changing the evidence parameter to the feature and its values that are pretended to be studied. For this example, studying the sex = 0, we get:



This means that the thal feature is going to be the deleted branch. Eliminating features is the same as eliminating edges because we are eliminating every edge that was correlated with the feature thal. After a delectation it is possible to assume that every condition probability with thal child's is a fixed value. This method gives exact results of the network.

In this implementation we have also gotten the performance metrics, from the test set on a 80:20 (training:test) split, shown in the following matrix:

TABLE XI: Perfomace Metrics - Bayesian Networks

(%)	Acc	Prec	F1	TPR	TNR	FPR	Bal Acc
BN	33.9	33.9	50.6	100.0	0.0	100.0	0.5

As for the second implementation we've used all the features except ca, slope, thal and oldpeak. After some research, we defined the edges as ('age', 'trestbps'), ('age', 'fbs'),

('trestbps', 'condition'), ('fbs', 'condition'), ('sex', 'trestbps'), ('exang', 'trestbps'), ('condition', 'restecg'), ('condition', 'thalach'), ('condition', 'chol').

For example, for age = 29, in the data set used, the result we've got is:



With the exang being eliminated.

As for the second part of this implementation we have developed a Bayesian Network that accepts input values by the user in the features age, sex, exang and fbs. With this we can see if a person with the values, inserted by the user, is more prone to a disease or not and, as normal, see what branch is being deleted. For example, setting the input values as age = 29, sex = 1, exang = 0 and fbs = 1, we get the following:



In this example, the branch deleted is the trestbps.

#### IX. KALMAN FILTER

Kalman filtering is an algorithm that provides estimates of some unknown variables given the measurements observed over time. Kalman filters have been demonstrating its usefulness in various applications.[11]

The Kalman filter process has two steps: the prediction step, where the next state of the system is predicted given the previous measurements, and the update step, where the current state of the system is estimated given the measurement at that time step.

This were not implemented in this project, but the idea of the application of this model is that based on an initial start sequence of the features values, like sex, ca and thal, we predict the next sequence and predict if the new sequence provokes a change on the diagnostic of the person.

#### X. COMPARING WITH OTHER ARTICLES

Although it wasn't possible to find other articles with this exact data-set about the 2 models applied we were able to find other articles in the same area, like, [16] and [9]. In this, and many other similar articles, the authors consider other features but, the idea is the same as our project, based on a features-set predict if a person as an heart disease or not. This allows us to conclude that using machine learning models/algorithms to

studying this type of day-to-day problems is beginning to be something more and more common and it's very helpful to the study of this problems

# XI. CONCLUSION - PART 2

In the Hidden Markov Model we can see that, when studying the sequences, there are a lot more no disease results than diseases, this is due to the low number of features considered, i.e. has we use a sub-set from the original data-set, we consider that the condition depends only on sex, ca and thal, what it's false. Due to this, the results will not be so accurate as if we considered all the features, because the condition returned is the condition with the highest probability based on just the sequence of 3 features selected. In the end, we can conclude that, for more accurate/real results, more features should be considered.

A Hidden Markov Model applied to our data set can be very help-full to the medical staff. By keeping tracks of the sex, ca, thal of a patient we can use this model to tried to predict if any changes in this features happens they are able to provoke a change in the condition of the patient, what you can't do directly with the other models presented in this project.

As for the Bayesian Network, the results were not great, so we can conclude that this model is not the best model, presented in this project, to predict an heart disease based on some features.

# XII. FUTURE WORK

The future work of this project would see the Kalman Filter applied on this data set as well as other models like Fuzzy Logic or a more deep application of the Bayesian Networks.

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