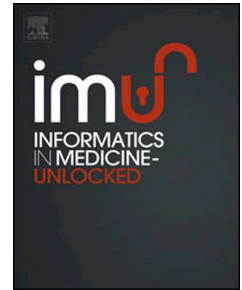


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Classification models for heart disease prediction using feature selection and PCA

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Abstract

The prediction of cardiac disease helps practitioners make more accurate decisions regarding patients' health. Therefore, the use of machine learning (ML) is a solution to reduce and understand the symptoms related to heart disease. The aim of this work is the proposal of a dimensionality reduction method and finding features of heart disease by applying a feature selection technique. The information used for this analysis was obtained from the UCI Machine Learning Repository called Heart Disease. The dataset contains 74 features and a label that we validated by six ML classifiers. Chi-square and principal component analysis (CHI-PCA) with random forests (RF) had the highest accuracy, with 98.7% for Cleveland, 99.0% for Hungarian, and 99.4% for Cleveland-Hungarian (CH) datasets. From the analysis, ChiSqSelector derived features of anatomical and physiological relevance, such as cholesterol, highest heart rate, chest pain, features related to ST depression, and heart vessels. The experimental results proved that the combination of chi-square with PCA obtains greater performance in most classifiers. The usage of PCA directly from the raw data computed lower results and would require greater dimensionality to improve the results.

Keywords: Machine Learning, Heart Disease, Apache Spark, PCA, Feature selection.

1 Introduction

The World Health Organization (WHO) [1] lists cardiovascular diseases as the leading cause of death globally with 17.9 million people dying every year. The risk of heart disease increases due to harmful behavior that leads to overweight and obesity, hypertension, hyperglycemia, and high cholesterol [1]. Furthermore, the American Heart Association [2] complements symptoms with weight gain (1-2 kg per day), sleep problems, leg swelling, chronic cough and high heart rate [3]. Diagnosis is a problem for practitioners due the symptoms' nature of being common to other conditions or confused with signs of aging.

The growth in medical data collection presents a new opportunity for physicians to improve patient diagnosis. In recent years, practitioners have increased their usage of computer technologies to improve decision-making support. In the health care industry, machine learning is becoming an important solution to aid the diagnosis of patients. Machine learning is an analytical tool used when a task is large and difficult to program, such as transforming medical record into knowledge, pandemic predictions, and genomic data analysis [4].

Recent studies have used machine learning techniques to diagnose different cardiac problems and make a prediction. Melillo et al. [5] contributed to an automatic classifier for patients with congestive heart failure (CHF) that separates patients with minimal risk from those at high risk. The classification and regression tree (CART) computed a sensitivity and specificity of 93.3% and 63.5%, respectively. Rahhal et al. [6] proposed a deep neural network (DNN) classification of electrocardiogram (ECG) signals to learn the best set of features and improved the performance. Guidi et al. [7] contributed to a clinical decision support system (CDSS) for the analysis of heart failure (HF). They compared the performance of different machine learning classifiers, such as neural network (NN), support vector machine (SVM), a system with fuzzy rules that uses CART, and random forests (RF). The CART model and RF obtained the best performance with an accuracy of 87.6%. Zhang et al. [8] found a NYHA

class for HF from unstructured clinical notes using natural language processing (NLP) and the rule-based method, calculating an accuracy of 93.37%. Parthiban et al. [9] scrutinized an SVM technique to diagnose heart disease in patients with diabetes, obtaining an accuracy of 94.60% and predicting features such as age, blood pressure, and blood sugar.

A major problem of machine learning is the high dimensionality of the dataset [10]. The analysis of many features requires a large amount of memory and leads to an overfitting, so the weighting features decrease redundant data and processing time, thus improving the performance of the algorithm [11-15]. Finding a small set of features characterizes different diseases of health management, genome expression, medical images, and IoT. Dimensionality reduction uses feature extraction to transform and simplify data, while feature selection reduces the dataset by removing useless features [16].

In the literature, the use of feature selection techniques improved the prediction of heart disease. Dun et al. [17] studied the presence of heart disease through deep learning techniques, random forests, logistic regression, and SVM with hyperparameter tuning and feature selection. NN had the best accuracy at 78.3%. Sewak et al. [18] reduced cardiovascular features using the Fisher ranking method, generalized discriminant analysis (GDA), and a binary classifier as extreme learning machine (ELM). They detected coronary heart disease with an accuracy improvement of 100%. Yaghoubi et al. [19] classified arrhythmias with heart rate variability (HRV). They achieved 100% accuracy using GDA for feature reduction and multilayer perceptron (MLP) neural network as a classifier. Mohammadzadeh et al. [20] classified 15 features from HRV signal. GDA reduced the features to five and computed 100% precision using SVM.

Principal component analysis (PCA) creates new components that store the most valuable information of the features by capturing a high variance [21]. Recently, several studies have used PCA as a feature extraction technique for classification in health care. Rajagopal et al. [22] compared an automatic classification of cardiac arrhythmia using five different linear and non-linear unsupervised dimensional reduction techniques with the neural network (PNN) classifier. With a minimum of 10 components, fastICA computed an F1 score of 99.83%. Zhang et al. [23] detected breast cancer using an AdaBoost algorithm based on PCA. Negi et al. [24] combined PCA with a feature reduction technique called uncorrelated linear discriminant analysis (ULDA) to obtain the best features that control upper limb motions. Avendaño-Valencia et al. [25] applied PCA to time frequency representations (TFR) to reduce heart sounds and improve performance. Kamencay et al. [26] presented a new method using PCA-KNN called the scale-invariant feature transform (SIFT) descriptor in different medical images, which resulted in an accuracy of 83.6% when training 200 images. Ratnasari et al. [27] reduced X-ray images using a threshold-based ROI and PCA. They obtained the best gray-level threshold of 150.

Earlier studies worked with a heart disease subset of 13 features (Subset-A). The aim of classification was to predict whether a patient had heart disease using, in most cases, the dataset of Cleveland [28]. Some remarkable results were presented: decision tree with an accuracy of 89.1% [29], random forests with an accuracy of 89.2% [30], artificial neural network with an accuracy of 92.7% [30], 89.0% [31], and 89.7% [32], and SVM with an accuracy of 88.0% [32]. GA+NN [33] computed the most notable hybrid model with 94.2% accuracy. PCA+regression and PCA1+NN [34] obtained the best PCA models with an accuracy of 92.0% and 95.2%, respectively.

The classification learning models combined with dimensionality reduction seek to achieve three primary objectives: (i) to learn the best feature representation of the dataset used; (ii) to validate the performance of PCA in conjunction with a feature selection technique; and (iii) to learn the classification model that computes the best performance. Six classifiers compute the 74 features: logistic regression, decision tree, random forest, gradient-boosted tree, multilayer perceptron, and Naïve Bayes.

We propose a model based on chi-square and PCA for the detection of heart disease. Experimental results have shown that PCA delivers a better prediction concerning the high dimensional classification problem by setting the features provided by chi-square, as seen when comparing PCA with raw data. Chi-square ranks the independent features most compatible with the label. We selected $k=13$ to perform a comparison with the subset of 13 features (Subset-A) used in the literature [28]. For PCA, we tried for the raw data a latent dimensional k greater than a variance of one. This implies $k=13$ for Cleveland, $k=14$ for Hungarian, and $k=11$ for CH (the datasets of Cleveland and Hungarian). Considering the results, the proposed approach improved most of the machine learning techniques.

Table 1. Features of the Heart Disease Data set

Serial Number	Group	Feature Names	Features Descriptions
1		ID	Patient identification number
2		CCF	Social security number (replaces this with a dummy value of 0)
3	Patient record data	AGE	Age in years
4	Patient record data	SEX	1=male; 0=female
5	Patient record data	PAINLOC	Chest pain location (1=substernal; 0=otherwise)
6	Patient record data	PAINEXER	1=provoked by exertion; 0=otherwise
7	Patient record data	RELREST	1=relieved after rest; 0=otherwise
8	Patient record data	PNCADEN	Sum of 5, 6, and 7
9	Patient record data	CP	Chest pain type: 1=typical angina; 2=atypical angina; 3=non-angina pain; 4=asymptomatic
10	Patient record data	TRESTBPS	Systolic blood pressure at rest (in mm Hg on admission to the hospital)
11	Patient record data	HTN	History of hypertension
12	Patient record data	CHOL	Serum cholesterol in mg/dl
13	Patient record data	SMOKE	1=yes; 0=no (is or is not a smoker)
14	Patient record data	CIGS	Cigarettes per day
15	Patient record data	YEARS	Number of years as a smoker
16	Patient record data	FBS	Fasting blood sugar > 120 mg/dl (1=true; 0=false)
17	Patient record data	DM	1=history of diabetes; 0=no such history
18	Patient record data	FAMHIST	Family history of coronary artery disease (1=yes; 0=no)
19	Patient record data	RESTECG	Resting electrocardiographic results: 0=normal; 1=having ST-T wave abnormality (T wave inversions and/or ST elevation or depression of > 0.05 mV); 2=showing probable or definite left ventricular hypertrophy by Estes' criteria
20	Patient record data	EKGMO	Month of exercise ECG reading
21	Patient record data	EKGDAY	Day of exercise ECG reading
22	Patient record data	EKGYR	Year of exercise ECG reading
23	Medication during exercise test	DIG	Digitalis is used during exercise ECG (1=yes; 0=no)
24	Medication during exercise test	PROP	Beta blocker used during exercise ECG (1=yes; 0=no)
25	Medication during exercise test	NITR	Nitrates used during exercise ECG (1=yes; 0=no)
26	Medication during exercise test	PRO	Calcium channel blocker used during exercise ECG (1=yes; 0=no)
27	Medication during exercise test	DIURETIC	Diuretic used during exercise ECG (1=yes; 0=no)
28	Exercise test	PROTO	Exercise protocol: 1=Bruce; 2=Kottus; 3=McHenry; 4=Fast Balke; 5=Balke; 6=Noughton; 7=bike 150 kpa min/min; 8=bike 125 kpa min/min; 9=bike 100 kpa min/min; 10=bike 75 kpa min/min; 11=bike 50 kpa min/min; 12=arm ergometer
29	Exercise electrocardiogram	THALDUR	Duration of exercise test in minutes
30	Exercise electrocardiogram	THALTIME	Time when ST measure depression was noted
31	Exercise electrocardiogram	MET	Mets achieved
32	Exercise electrocardiogram	THALACH	Maximum heart rate achieved
33	Exercise electrocardiogram	THALREST	Resting heart rate
34	Exercise electrocardiogram	TPEAKBPS	Peak exercise systolic blood pressure (first of 2 parts)
35	Exercise electrocardiogram	TPEAKBPD	Peak exercise systolic blood pressure (second of 2 parts)
36	Exercise electrocardiogram	DUMMY	The same value as trestbps
37	Exercise electrocardiogram	TRESTBPD	Resting blood pressure
38	Exercise electrocardiogram	EXANG	Exercise-induced angina (1=yes; 0=no)

Table 1. Features of the Heart Disease Data set (continuation)

Serial Number	Group	Feature Names	Features Descriptions
39	Exercise electrocardiogram	XHYPO	Exercise-induced hypotension (1=yes; 0=no)
40	Exercise electrocardiogram	OLDPEAK	Exercise-induced ST depression relative to rest
41	Exercise electrocardiogram	SLOPE	The slope of the peak exercise ST segment: 1=upsloping; 2=flat; 3=downsloping
42	Exercise electrocardiogram	RLDV5	Height at rest
43	Exercise electrocardiogram	RLDV5E	Height at peak exercise
44	Cardiac fluoroscopy	CA	Number of major vessels (0-3) colored by fluoroscopy
45	Cardiac fluoroscopy	RESTCKM	Irrelevant
46	Cardiac fluoroscopy	EXERCKM	Irrelevant
47	Cardiac fluoroscopy	RESTEF	Rest radionuclide ejection fraction
48	Cardiac fluoroscopy	RESTWM	Rest wall motion abnormality: 0=none; 1=mild of moderate; 2= moderate or severe; 3=akinesis or dyskinesis
49	Cardiac fluoroscopy	EXEREF	Exercise-induce radionuclide ejection fraction
50	Cardiac fluoroscopy	EXERWM	Exercise-induce wall motion abnormalities
51	Exercise thallium scintigraphy	THAL	Exercise Thallium heart scan: 3=normal; 6= fixed defect; 7=reversible defect
52	Exercise thallium scintigraphy	THALSEV	Not used
53	Exercise thallium scintigraphy	THALPUL	Not used
54	Exercise thallium scintigraphy	EARLPUL	Not used
55	Coronary angiograms	CMO	Month of cardiac cath
56	Coronary angiograms	CDAY	Day of cardiac cath
57	Coronary angiograms	CYR	Year of cardiac cath
58	Coronary angiograms	NUM	Diagnosis of heart disease (angiographic disease status): -0= <50% diameter narrowing -1= >50% diameter narrowing (in any major epicardial vessel attributes 59 through 68 are vessels)
59	Blood Vessels	LMT	Left main truck
60	Blood Vessels	LADPROX	Proximal left anterior descending artery
61	Blood Vessels	LADDIST	Distal left anterior descending artery
62	Blood Vessels	DIAG	Diagonal branches
63	Blood Vessels	CXMAIN	Circumflex
64	Blood Vessels	RAMUS	Ramus intermedius
65	Blood Vessels	OM1	First obtuse marginal branch
66	Blood Vessels	OM2	Second obtuse marginal branch
67	Blood Vessels	RCAPROX	Proximal right coronary artery
68	Blood Vessels	RCADIST	Distal right coronary artery
69		LVX1	Not used
70		LVX2	Not used
71		LVX3	Not used
72		LVX4	Not used
73		LVF	Not used
74		CATHEF	Not used
75		JUNK	Not used

2 Materials and Methods

2.1 Description of the dataset

The dataset used in the research was the “Heart Disease Dataset” of the UCI Machine Learning Repository [28] as shown in Table 1. It had a label called coronary angiography (NUM) and 74 independent features. NUM specified whether a patient has the presence or absence of heart disease. The presence of heart disease combined the values 1, 2, 3, and 4 from the original datasets. For the examination, patients supplied historical data and were physically examined by practitioners [42]. Three non-invasive tests were part of the protocol: exercise electrocardiogram, exercise thallium scintigraphy, and coronary calcium fluoroscopy. The cardiologist interpreted the coronary angiogram results without knowing the non-invasive results. Previous research [43] has explained some features as well as the complete protocol.

In the literature, a subset of 13 features [28] was used to create an algorithm relevant to clinical situations. The clinical variables considered relevant were AGE, SEX, CP, and TRESTBPS; the routine test data CHOL, FBS, and RESTECG; the exercise electrocardiography test with the features THALACH, EXANG, SLOPE, and OLDPEAK; and the non-invasive test, THAL, and CA. In addition, the label was NUM. For comparison, we call this set of 13 features as “Subset-A”.

The datasets used for the analysis were Cleveland, Hungarian, and a combination of both called CH (Cleveland-Hungarian). Table 2 displays the data distribution. Cleveland had a more uniform distribution than Hungarian and CH for both healthy individuals and patients with heart disease.

2.2 Proposed approach for the dimensionality reduction and classification

The proposed approach was applied to the three datasets referred in Section 2.1. We pre-processed and cleaned the datasets from Cleveland, Hungarian, and CH, as mentioned in Section 2.3. In addition, some of the features were

Table 2. Datasets distribution

Dataset	Total # of instances	Presence HF	Absence HF
Cleveland	283	157 (55%)	126 (45%)
Hungarian	294	188 (64.9%)	106 (35.1%)
CH	577	345 (59.8%)	232 (40.2%)

not considered for the analysis, as stated in Table 3. Further, we performed four type of experiments for analysis. We assessed the raw data first with all six classifiers. In the second experiment, we applied the feature selection technique of chi-square to obtain a unique and reduced set of ranking-based features with the diagnosis of the heart disease (NUM) and validate them with the classifiers. The third test used the reduced datasets obtained by chi-square and then applied PCA. The final experiment was the use of PCA directly from raw data. The validation and analysis module used the performance metrics mentioned in Section 2.6, such as accuracy, precision, recall, F1 score, Matthews correlation coefficient (MCC), and Cohen’s Kappa coefficient (κ). The representation of this approach is illustrated in Figure 1.

Table 3. Features not included

Category	Features not included in the model
Irrelevant	ID (patient identification number), social security number (CCF), PNCADEN (sum of PAINLOC, PAINEXER and RELREST), EKGMO (month of exercise ECG reading), EKGDAY (day of exercise ECG reading), EKGYR (year of exercise ECG reading), CMO (month of cardiac cath), CDAY (day of cardiac cath), CYR (year of cardiac cath)
Repeated	DUMMY (same as TRESTBPS)
Unexplained	RESTCKM, EXERCKM, THALSEV, THALPUL, EARLOBE, LVX1, LVX2, LVX3, LVX4, LVF, CATHEF, JUNK, NAME
Null data	RESTCKM, EXERCKM, RESTEF (rest radionuclide ejection fraction), RESTWM (rest wall motion abnormality), EXEREF (exercise radionuclide ejection fraction), EXERWM (exercise-induce wall motion abnormalities), THALSEV, THALPUL, EARLOBE

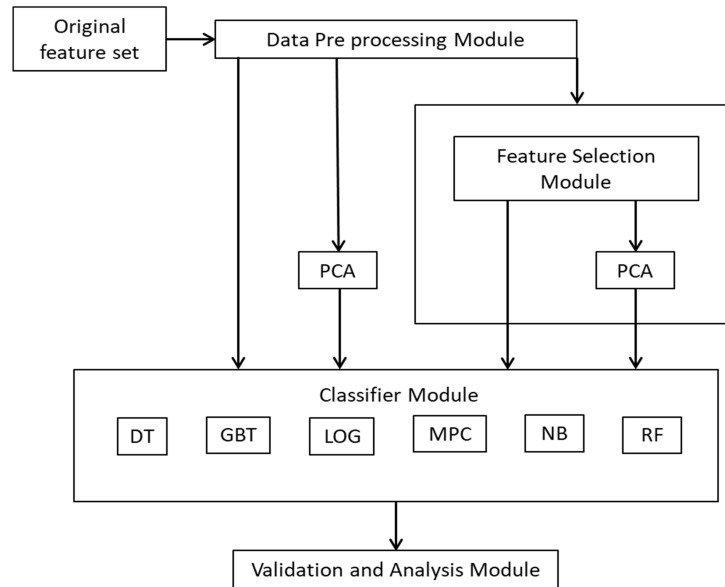


Figure 1. Schematic Diagram of Proposed Approach

2.3 Preprocessing information and cleansing considerations

The datasets had irrelevant, unexplained, null, or repeated features. Table 3 shows the features not included in the analysis. For this investigation, Cleveland contained 41 features, Hungarian contained 45 features, and CH contained 38 features. The most important considerations for cleansing were to assign a single category for missing values called 'null value' and to create rules that consider data consistency. An example of this is that a patient cannot have cholesterol or age equal to zero. If this occurs, the value will be changed to the 'null value' category.

The complete considerations of the cleaning process were: (1) classes 1, 2, 3, and 4 were converted to the same class (patient with heart disease); (2) null values were replaced by a unique label; (3) zero was unacceptable in continuous results, therefore it was changed as null; (4) if SMOKE was unanswered but CIGS or YEARS were, SMOKE was changed from null to number 1 (patient is a smoker). If CIGS and YEARS had a value of 0, SMOKE was converted to 0; (5) if THALTIME had a value greater than THALDUR, the response was removed; (6) THALACH could not be lower than THALREST; (7) if OLDPEAK had a value of 0, THALTIME was changed to 0; and (8) DUMMY was the same feature as TRESTBPS, so it was eliminated.

2.4 Dimensionality reduction

Dimensionality reduction [10] is the process of reducing the number of variables considered. It can be used to extract latent features from raw datasets or to reduce the data while maintaining the structure. This research proposed two different dimensionality reduction methods, for feature selection was selected the chi-square test of independence and for feature extraction, the principal component analysis (PCA).

2.4.1 Chi-square

Chi-square test (CHI) sorts features based on the class and filters out the top features on which depends the class label. ChiSqSelector (CHI) of Apache Spark MLlib is used for feature selection in the model construction. CHI filters the features and sorts them, through repeated iterations, for selection. For this study, we selected the top 13 features using CHI to make a comparison with the literature. Table 4 contemplates the amount of complete data and the correlation between the features and the label. Of the first 13, Cleveland and Hungarian selected 4 vessel features, while CH selected 5; the vessels were LADDIST, RCAPROX, OM1, CXMAIN, and LADPROX. Cleveland used the non-invasive test features, THAL, and CA, while Hungarian selected EXANG. Chest pain values included CP, RELREST, and PAINEXER. The patient records incorporated only CHOL. Exercise

electrocardiogram features indicated THALACH, THALDUR, and ST segment values such as THALTIME, OLDPEAK, and SLOPE. The uncorrelated features involved medications during exercise test, PAINLOC, HTN, SMOKE, FBS, DM, FAMHIST, RESTECG, RAMUS, and OM2. Overall, the common features across the three datasets should be considered as risk factors for heart disease, including CHOL, THALACH, LADDIST, OLDPEAK, THALTIME, RCAPROX, CP, and CXMAIN.

Table 4. Features selected by CHI from raw data

#SF	LF	%DC	Corr	LF	%DC	Corr	LF	%DC	Corr
	Cleveland Dataset			Hungarian Dataset			CH Dataset		
1	CHOL	100.0	0.12	CHOL	93.2	0.20	CHOL	96.5	0.17
2	THALACH	100.0	-0.40	SLOPE	35.4	0.54	OLDPEAK	100.0	0.48
3	RLDVSE	100.0	0.07	THALTIME	35.4	0.49	CP	100.0	0.46
4	LADDIST	100.0	0.57	CXMAIN	100.0	0.59	CXMAIN	100.0	0.54
5	OLDPEAK	100.0	0.42	LADPROX	100.0	0.56	THALTIME	55.0	0.38
6	THALDUR	100.0	-0.25	EXANG	99.7	0.41	LADDIST	100.0	0.53
7	THALTIME	75.5	0.24	OLDPEAK	100.0	0.55	RCAPROX	100.0	0.52
8	THAL	99.3	0.44	THALACH	99.7	-0.30	LADPROX	100.0	0.52
9	RCAPROX	100.0	0.51	CP	100.0	0.51	EXANG	99.8	0.41
10	CP	100.0	0.40	PAINEXER	100.0	0.54	THALACH	99.8	-0.32
11	OM1	100.0	0.49	RCAPROX	100.0	0.52	SLOPE	67.0	0.35
12	CA	99.3	0.34	LADDIST	100.0	0.34	RLDVSE	100.0	0.11
13	CXMAIN	100.0	0.48	RELREST	100.0	0.45	OM1	100.0	0.44

#SF= # of selected features; LF=List of Features; %DC=# of data complete; Corr= correlation

2.4.2 Principal components

To determine the number of meaningful components to be retained, we select the eigenvalue-one criterion for the analysis. With this, we kept all the components with an eigenvalue greater than 1.00. As individual variables, each component counts for one unit of variance. Therefore, components with an eigenvalue greater than 1.00 stood for a higher variance than their contribution as individual variables. In contrast, components with eigenvalues less than 1.00 contributed less than their individual value and were removed from analysis.

The first 13 components of Cleveland had a variance greater than 1.00 and an accumulated proportion of 0.678. The first two components had a cumulative proportion of 0.246; the amount of variance in component 1 was 5.445 and 4.396 in component 2. The principal components of Hungarian were represented in the first 14 components and had a variance greater than 1.00 and an accumulated proportion of 0.694. The amount of variance in component 1 was 6.340 and in component 2 was 4.451, with a cumulative of 0.240. The first 11 components of CH contained a variance of more than 1.00 and a cumulative proportion of 0.729 of the information. The first two components had an accumulated proportion of 0.399; the amount of variance in component 1 was 14.614 and in component 2 was 4.547. Hence, selecting components with an eigenvalue greater than 1.00 was the best choice, so we selected 13 components for Cleveland, 14 components for Hungarian, and 11 components for CH.

2.5 Classifiers proposed

For this research, ML Spark libraries were selected for feature validation. The version of Apache Spark used was 2.2.0 in Java language. MLlib has tools for preprocessing, basic statistics, dimensionality reduction, classification, regression, clustering, and association rules. This work used the CHI for feature selection and PCA for feature extraction. The most important parameter was the "Selection method", which chose the main features according to CHI as shown in Table 5. The other settings were the default ones.

The classification models use the default value for most of the hyperparameters. The models were: (1) decision tree (DT); (2) gradient-boosted tree (GBT); (3) logistic regression (LOG); (4) multilayer perceptron (MPC); (5)

Naïve Bayes (NB); and (6) random forests (RF). Table 6 describes the parameter settings for each classifier. The GBT and RF trees used several DT parameters as default values, except for Gini impurity. DT hyperparameters are the maximum depth of a tree equal to 5, and the maximum number of bins used when the discretization of continuous features was 32. In addition, LOG had an elasticity of 0.8 and a binomial family parameter. The parameters of MPC were set at a maximum iteration of 100. MPC had two hidden layers, the first with 5 neurons and the second with 4 neurons. The model type selected for NB was multinomial.

The 6 classifiers were run 10 times, the best result was added for this research, and the performance of the label evaluated, in compliance with the percentage of the correct classification. For the experiment, the Heart Disease datasets were divided into two datasets: (1) training dataset with the 70% of the information (80% for training and 20% for validation); and (2) testing dataset with 30% of the information.

Table 5. Parameter for feature selection techniques

Feature selection technique	Basic Hyperparameters
ChiSqSelector	Selection method=numTopFeatures; Top features= default set to 50

Table 6. Parameters tuning for classifier in Apache Spark

Classifier	Basic Parameters
DT	algo="Classification"; numClasses=2; maxDepth=5; minInstancesPerNode="auto"; minInfoGain="auto"; maxBins=32; maxMemoryInMB= 256 MB; subsamplingRate= "auto"; impurity "gini"
GBT	Loss="Log Loss"; numIterations="auto"; learningRate="auto"; algo="Classification"
LOG	numClasses=2; MaxIter=10; RegParam=0.3; ElasticNetParam=0.8; Family="binomial"
MPC	Layers="number of features, 2"; BlockSize=128; Seed=1234L; MaxIter=100; two hidden layers, the first with 5 neurons and the second with 4 neurons.
NB	Lambda="false"; ModelType="false"
RF	numClasses=2; numTrees="auto"; featureSubsetStrategy="false"; subsamplingRate="auto"; impurity="gini"; seed="false"

2.6 Evaluation process

The confusion matrix helps practitioners to form a clear idea of whether the results have a high performance. The confusion matrix elements were: (1) true positive (TP), which were patients who had heart disease and were correctly diagnosed; (2) true negative (TN), which were patients who did not have heart disease and were correctly diagnosed; (3) false negative (FN), which were patients who had heart disease and were misdiagnosed; and (4) false positive (FP), which were patients who did not have heart disease and were misdiagnosed. In the medical field, false negatives are the most dangerous predictions.

The different performance metrics were calculated using a confusion matrix. Accuracy (Acc) measured the properly classified instances [1]. The formula for calculating accuracy was given by

$$Accuracy = \frac{TP+TN}{TP+FN+FP+TN} \quad (1)$$

Precision was the positive predictive value defined by

$$Precision = \frac{TP}{TP+FP} \quad (2)$$

Recall identified the proportion of patients with heart disease given by

$$Recall = \frac{TP}{TP+FN} \quad (3)$$

The F1 score considered a harmonic average between precision in Eq. (2) and recall in Eq. (3) defined by

$$F1\ score = 2 \left(\frac{Precision \times Recall}{Precision + Recall} \right) \quad (4)$$

Matthews correlation coefficient (MCC) was introduced by Brian W. Matthews to predict the performance of protein secondary structure [52]. The results of MCC are in percentage. Therefore, MCC becomes a widely used performance metric in medical research for imbalanced data expressed by

$$MCC = \frac{TP \times TN - FP \times FN}{\sqrt{(TP+FP)(TP+FN)(TN+FP)(TN+FN)}} \quad (5)$$

Cohen's Kappa coefficient (κ) was introduced by J. Cohen [53] in 1960 to correlate the measurement of inter-rater reliability. Kappa measures the percentage of agreement between two raters. The formula to calculate Kappa is represented by

$$\kappa = \frac{p_0 - p_c}{1 - p_c} \quad (6)$$

where p_0 is the percent of agreement among raters, as in Eq. (1), and p_c is the chance agreement.



Figure 2. Comparison of ML classifiers for Cleveland using accuracy and F1 score

3 Results

Significant observations revealed that the use of the selected features of CHI with PCA had the best results with the classifiers across all three datasets in most cases. All performance metrics are in percentage.

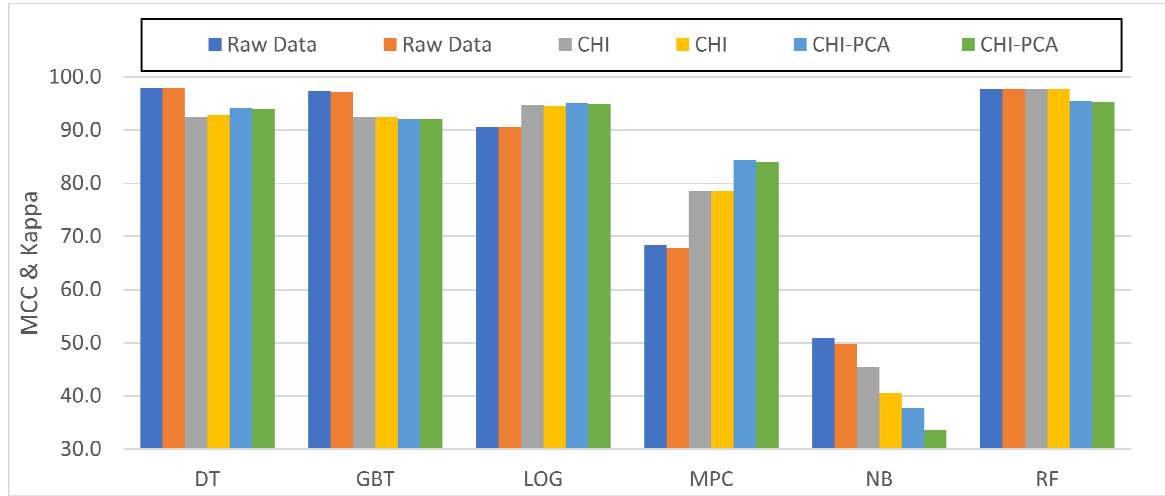


Figure 3. Comparison of ML classifiers for Cleveland using MCC and Kappa

3.1 Results comparing raw data with CHI-PCA

In this section, we will compare the best results of the raw data with CHI and PCA. For CHI, we selected 13 features, as shown in Table 4. PCA created the principal components using the same CHI features. Overall, Cleveland dataset obtained the best results using CHI-PCA (Figure 2 and Figure 3). Nevertheless, DT and GBT presented better results using raw data. Compared to the raw data, CHI and CHI-PCA improved in the computations of LOG, MPC, NB. However, the performance decreased with DT, and GBT. The greatest improvement was in MPC using the features of CHI-PCA. MPC had an 8.1% accuracy increase, and an F1 score of 9.1%, respectively. RF behavior was the same with raw data and CHI, computing a recall of 100%, an accuracy of 98.9%, an F1 score of 98.8%, an MCC of 97.7%, and a Kappa of 97.7%. CHI-PCA-NB presented the worst value, with an accuracy of 68.4%, an F1 score of 75.7%, an MCC of 37.7%, and a Kappa of 33.7%. GBT presented a pattern when applied with CHI and PCA as shown in Figure 2. The values of MCC and Kappa are consistent among them.

Figure 4 and Figure 5 present the best computations in the Hungarian dataset. The greatest result was CHI-PCA-RF with 99.0% accuracy, 100.0% precision, 96.8% recall, 98.4% F1 score, 97.7% MCC, and 97.6% Kappa. Therefore, CHI-PCA presented the most remarkable performance. GBT, LOG, and RF obtained equivalent results when using CHI-PCA. Even with a lower accuracy, CHI-PCA-GBT computed a perfect recall of 100% and an F1 score of 98.5%, only RF exceeds the result by obtaining a better MCC and Kappa. The computations of DT and NB decreased compared to the raw data. CHI computed the highest values using MPC and DT. Likewise, GBT, LOG, and RF calculated greater results than raw data with CHI features.

Figure 6 and Figure 7 show the performance of the CH dataset. GBT with raw data, CHI-DT, CHI-PCA-LOG, and CHI-PCA-RF computed the highest accuracy of 99.4%. The F1 score was similar in all cases, with a variation of 0.2%. Most models performed better with CHI and CHI-PCA, except for GBT and NB. The greatest improvements between raw data and CHI-PCA were LOG with accuracy increase of 4.5%, F1 score of 4.8%, MCC of 7.5%, and Kappa of 7.5%, respectively. In addition, the values of MCC and Kappa using CHI and CHI-PCA are similar in some cases.

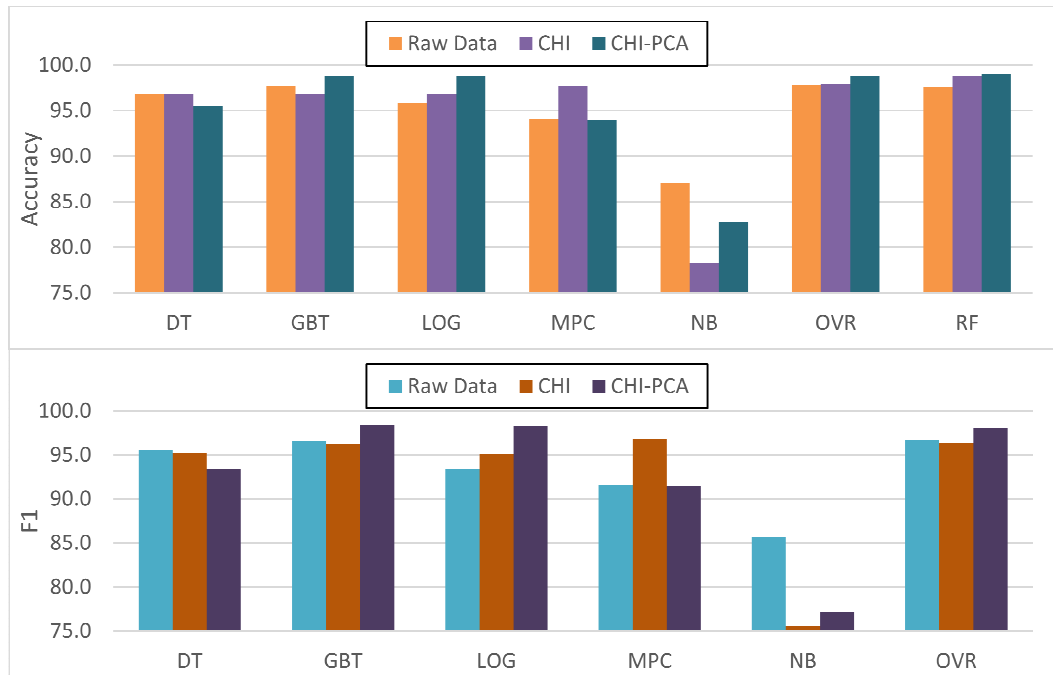


Figure 4. Comparison of ML classifiers for Hungarian using accuracy and F1 score

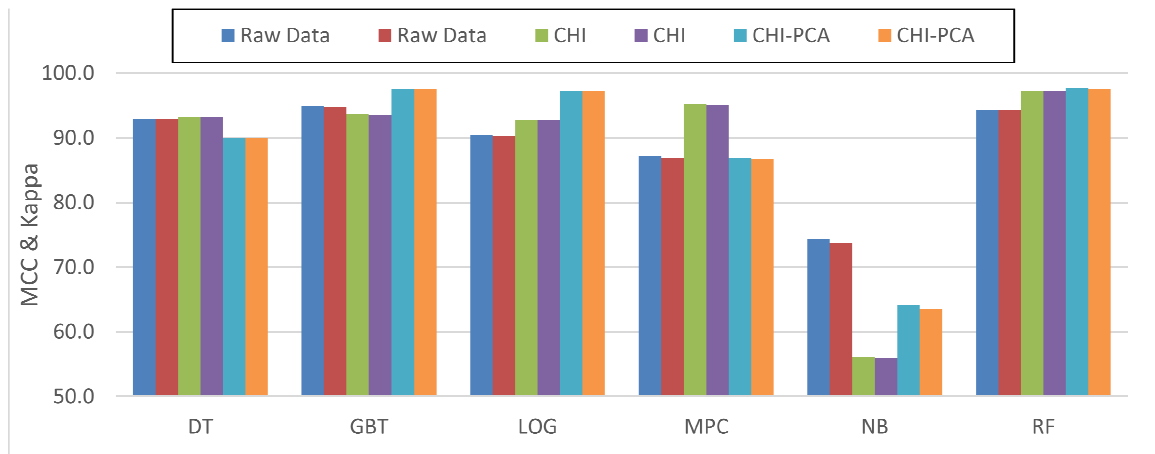


Figure 5. Comparison of ML classifiers for Hungarian using MCC and Kappa

3.2 Results of the comparison of PCA using raw data and CHI

Table 7 displays a comparison between PCA performance using the features of CHI and the raw data. The use of PCA in raw data had poor results in Cleveland and CH. The performance of the classifiers was reduced to around 30% except for NB and MPC. NB was 3.4% higher in Cleveland and 2.7% higher in Hungarian; MPC computed an accuracy 1.5% greater in Hungarian. Although Hungarian computed lower results in raw data, they were closer to CHI-PCA. Except for MPC, the classifiers were between 4% and 9% lower in accuracy and 6% and 15% inferior in F1 score. As can be seen, PCA retained enough information from the raw data when k was adequate and became less competitive when k was too low or too high. For a large number of features and instances, PCA performance was superior when using CHI features.

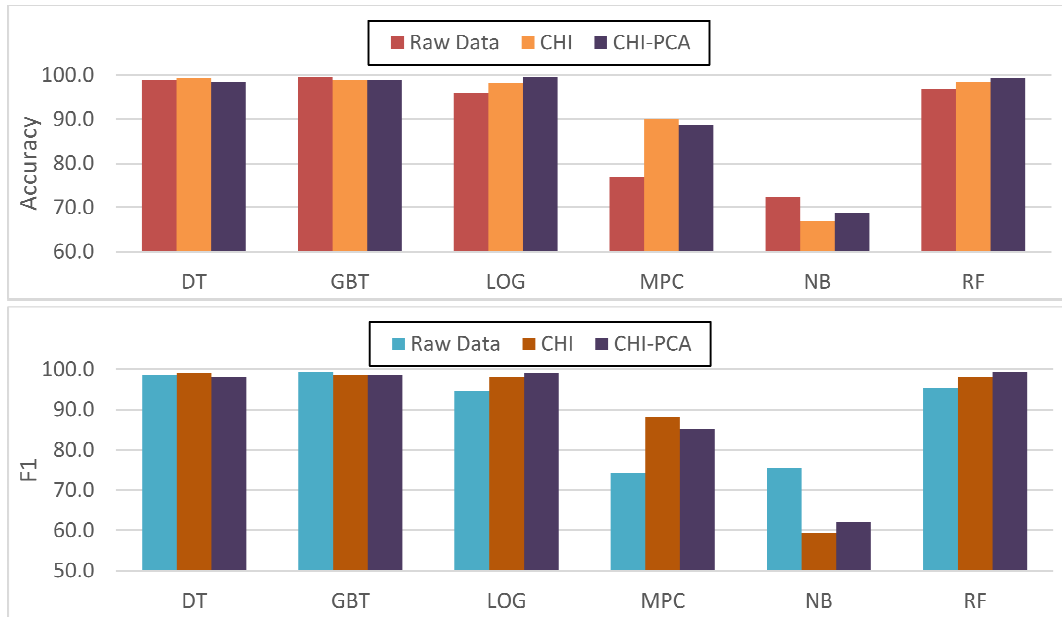


Figure 6. Comparison of ML classifiers for CH using accuracy and F1 score

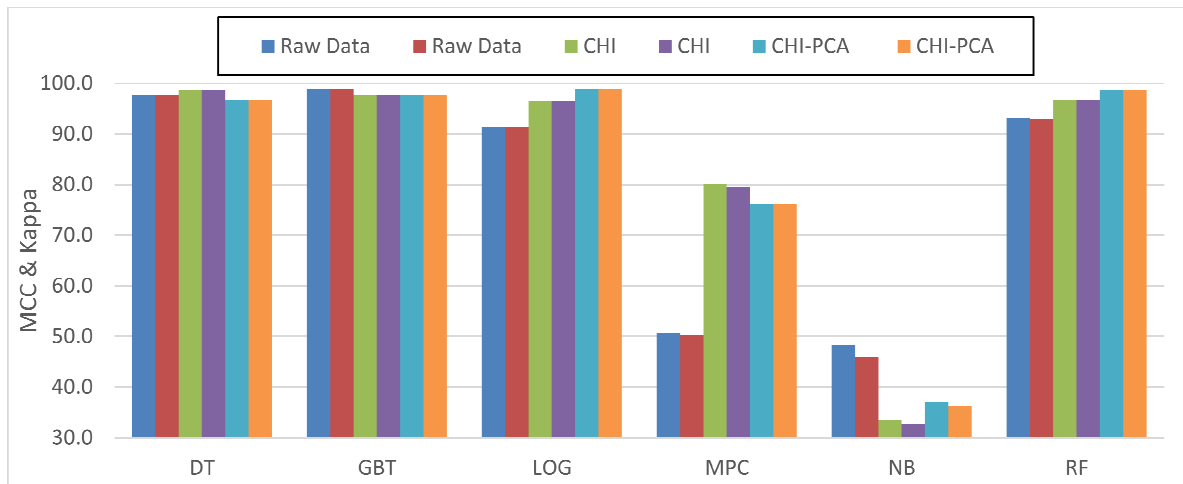


Figure 7. Comparison of ML classifiers for CH using MCC and Kappa

3.3 Results of the classifiers comparing non-invasive test features

We tested the results obtained by the non-invasive test in Table 8. The features involved were the thallium heart scan (THAL), the number of major vessels colored by fluoroscopy (CA), and whether exercise-induced angina (EXANG). In the case of Cleveland, these features had high data quality. If the results are compared to the Subset-A of Cleveland, some classifiers computed greater values than logistic regression, NB, and SVM. For Hungarian, CA did not exist, and THAL had a weak representation with only 9.5% completed. As a result, a deficient performance is reasonable considering the lack of information. In the case of CH, the representation of THAL was 53.5%. Some classifiers, such as DT, GBT, and NB, achieved competitive results.

Table 7. Performance of the raw data and CHI-PCA

	Performance	DT	GBT	LOG	MPC	NB	RF
Cleveland							
CHI-PCA	Accuracy (%)	97.3	96.1	97.6	92.1	68.4	98.7
	Precision (%)	100.0	97.1	100.0	95.2	65.0	100.0
	Recall (%)	92.3	94.3	94.1	88.9	90.7	97.1
	F1 (%)	96.0	95.7	97.0	92.0	75.7	98.6
Raw Data-PCA	Accuracy (%)	62.8	74.7	73.3	74.0	70.7	67.9
	Precision (%)	57.1	59.5	60.0	74.2	67.9	77.1
	Recall (%)	66.7	73.3	77.8	65.7	55.9	58.7
	F1 (%)	61.5	65.7	67.7	69.7	61.3	66.7
Hungarian							
CHI-PCA	Accuracy (%)	95.5	98.8	98.8	94.0	82.8	99.0
	Precision (%)	90.3	97.0	100.0	88.9	84.4	100.0
	Recall (%)	96.6	100.0	96.6	94.1	71.1	96.8
	F1 (%)	93.3	98.5	98.2	91.4	77.1	98.4
Raw Data-PCA	Accuracy (%)	88.8	89.7	94.9	95.5	78.0	93.2
	Precision (%)	88.0	87.0	91.4	92.6	63.6	93.1
	Recall (%)	78.6	80.0	94.1	92.6	72.4	87.1
	F1 (%)	83.0	83.3	92.8	92.6	67.7	90.0
CH							
CHI-PCA	Accuracy (%)	98.4	98.9	99.4	88.6	68.8	99.4
	Precision (%)	100.0	97.3	100.0	87.1	70.8	100.0
	Recall (%)	96.3	100.0	98.6	83.6	55.3	98.6
	F1 (%)	98.1	98.6	99.3	85.3	62.1	99.3
Raw Data-PCA	Accuracy (%)	73.7	74.3	78.6	80.5	71.5	75.1
	Precision (%)	70.8	63.6	71.4	74.6	62.7	66.2
	Recall (%)	52.3	60.3	70.4	72.3	88.1	70.8
	F1 (%)	60.2	61.9	70.9	73.4	73.2	68.5

4 Discussion

4.1 Discussion comparing raw data with CHI-PCA

Promising results were obtained with the use of CHI and PCA. In the first part of Section 3, only DT and GBT lacked improvement in some of the tests. This suggests that tree performance improves when using a large number of features due to supplying more options for the trees. NB dropped the worst results in all the tests. The classifiers LOG had remarkable results when using CHI-PCA. The MPC classifier obtained better results with CHI than CHI-PCA, however the performance was below the rest of the classifiers in most tests due to a network overfit on the training dataset. When we increased the layers or neurons, the performance of the metrics decreased, suggesting that for a small input, such as the datasets in this study, MPC is more stable when using a smaller number of layers. Despite Cleveland, RF made an improvement using CHI-PCA. CHI obtained a remarkable result, and the 13 features selected were prominent for heart disease detection. Significant observations revealed that PCA works best using LOG and CHI using MPC. Overall, LOG, and RF were the classifiers with the best performance and improvement with a smaller number of features.

In most models, the precision value exceeded the recall. Thus, the classifiers computed models that were more sensible to false negatives than false positives. As false positives are examined by practitioners, it is more dangerous to have false negatives. Even so, the value of precision should not be diminished, so it is important to use the F1 score to obtain the optimal balance between precision and recall.

Table 8. Performance of non-invasive test values

Dataset	Performance	DT	GBT	LOG	MPC	NB	RF
Cleveland	Acc (%)	86.6	87.7	88.0	86.8	76.1	86.2
	Precision (%)	88.9	85.0	90.6	92.7	68.0	87.8
	Recall (%)	82.1	85.0	82.9	80.9	85.0	81.8
	F1 (%)	85.3	85.0	86.6	86.4	75.6	84.7
	MCC (%)	73.8	78.5	79.0	73.4	52.0	79.9
	Kappa (%)	72.7	77.9	78.7	71.4	80.8	78.8
Hungarian	Acc (%)	82.9	82.3	81.9	81.5	78.7	81.3
	Precision (%)	81.5	75.0	75.0	68.0	68.8	80.0
	Recall (%)	71.0	72.3	67.7	73.9	71.0	68.6
	F1 (%)	75.9	73.8	71.2	70.8	69.8	73.8
	MCC (%)	63.1	60.5	58.2	57.3	55.3	59.9
	Kappa (%)	62.8	60.5	58.1	57.1	55.2	59.4
CH	Acc (%)	87.3	85.6	80.2	80.5	74.9	86.4
	Precision (%)	84.9	90.0	81.4	80.9	100.0	86.5
	Recall (%)	78.9	76.1	66.7	63.3	40.5	81.0
	F1 (%)	81.8	82.0	73.3	71.0	57.7	84.0
	MCC (%)	68.6	71.1	57.4	57.6	44.0	72.2
	Kappa (%)	68.6	70.4	56.8	56.7	32.5	72.1

Contrary to accuracy and F1 score, MCC and Kappa show the susceptibility of imbalanced data. In addition, the results were similar between MCC and Kappa in each classifier. LOG computed the best results using CHI-PCA. The Hungarian and CH datasets presented an imbalanced classification problem in which the rate of healthy patients was higher. The raw data in the imbalanced datasets had a greater difference in performance between accuracy and F1 score than the dimensionality reduction results (Table 9). The performance between accuracy and F1 score decreased in the datasets. The difference in Cleveland was not noted in the raw data due to the balance between the two classes. The greatest difference on average was when CHI was used. Even so, each result was lower than the overall average of 0.9%. Hungarian had the biggest difference between accuracy and F1 score due to an imbalance. The CHI and CHI-PCA averages decreased by 0.5% compared to the raw data. CH computed a 1.2% difference in raw data, which was higher than the average. The CHI and CHI-PCA values were 0.5% and 0.7%, respectively. MPC performed better on a balanced dataset such as Cleveland with an average of 0.4%, while Hungarian and CH had the worst performances with 2.0% and 2.7%, respectively. The models with the smallest differences between accuracy and F1 score were GBT, MPC, and RF. NB obtained the poorest results and was excluded from the average results.

Table 9. Comparison of the difference in performance between accuracy and F1 score

Dataset	Method	DT	GBT	LOG	MPC	RF	Average
Cleveland	Raw data %	0.3	0.0	1.2	1.1	0.1	0.54
	CHI %	0.5	2.1	1.0	0.1	0.1	0.76
	CHI-PCA %	1.3	0.4	0.6	0.1	0.5	0.58
Hungarian	Raw data %	1.3	1.1	2.5	2.5	1.6	1.8
	CHI %	1.6	0.6	1.7	1.0	0.8	1.14
	CHI-PCA %	2.2	0.3	0.6	2.6	0.6	1.26
CH	Raw data %	0.3	0.0	1.4	2.7	1.3	1.14
	CHI %	0.1	0.1	0.3	2.0	0.4	0.58
	CHI-PCA %	0.3	0.3	0.1	3.3	0.1	0.82
Average		0.87	0.54	1.04	1.71	0.61	0.96

4.2 Discussion of the features selected by chi-square and the PCA results

As in other studies [21, 44-46], the use of PCA after a reduction technique improved the results. The raw dataset produced poorer results in most of the cases (Table 7). The experiment in Section 3.2 compared the performance of raw data with our method. Like the other results, RF improved the computation when using raw data, while MPC

was completely superior using CHI. CHI-PCA outperformed most experiments, especially with LOG as seen in Section 3.1, Section 3.3, and Section 3.4. NB did not present a competitive performance for any of the tests given.

The top 13 features selected by CHI had a great validation for the compilers. The datasets had five vessels. Of these, four of the vessels were part of the left main coronary artery (LAD), considered the most important because it supplies more than half of the blood to the heart. The vessels were the proximal left anterior descending artery (LADPROX), the distal left anterior descending artery (LADDIST), the first obtuse marginal branch (OM1), and the circumflex (CXMAIN). Remaining was the proximal right coronary artery (RCAPROX), which is part of the right coronary artery (RCA). For the non-invasive, the selector considered THAL and CA with a high ranking. Features related to risk factors were not highly ranked by the selector, except for cholesterol. Physicians obtained other features that are part of the exercise test and correlated with heart disease and ST segment values. Taken together, the information obtained by the different tests aided in the diagnosis of heart disease and must be considered for model prediction.

The risk factors that performed best in this study and that are cited by the WHO and the American Heart Association were high blood cholesterol, chest discomfort, inadequate physical activity (seen in the exercise electrocardiogram features). Other features, such as history of hypertension, smoking and the fasting blood sugar, were not complete and were difficult to compare with WHO and American Heart Association standards.

4.3 Discussion of the invasive and non-invasive test

The vessels' models were enough to achieve a great result. The invasive test's limitation was its exclusive use in patients with a previous heart attack, severe chest pain, abnormal electrocardiogram or stress test. The non-invasive features performed poorly, so they must be completed with more information. In the literature, other studies worked with the non-invasive testing. This study [51] compared psychological and physiological factors to predict angina on an exercise treadmill test (ETT), concluding that these factors are important in the prediction of exercise angina. Another study [59] concluded that there are sex differences in the experience of chest pain (pain features) and the prediction of exercise-induced angina, while [60] included some painful and non-painful sensations in the relationship with exercise-induced ischemia in women but not in men. [61] concluded that patients are more prone to have long-term survival from preoperative thallium scanning and coronary revascularization before major vascular surgery. Further studies should be conducted with the non-invasive variables.

4.4 Discussion of the results with the literature

We compared our results with earlier studies in Table 10 using Cleveland dataset. Our approach achieved greater results with raw data and the use of CHI with PCA. The accuracy, precision, and recall are used for the comparison. Hung et al. [48] classified the data using linear support vector machine (SVM), Naïve Bayes, and logistic regression. The best result was SVM obtaining 89.98% accuracy for raw data. Compared to our results, the values are lower than our classifiers, except for NB and MPC.

Table 10. Comparison with other studies using the Cleveland dataset

Author	Method	Accuracy	Precision	Recall	Features
Our study	ChiSqSelector+PCA and RF	98.7%	100.0%	97.1%	13
Shamosollahi, et al., 2019 [47]	C&RT	92.6%	92.6%	90.4%	20
Shamosollahi, et al., 2019 [47]	ANN	90.4%	97.1%	80.8%	20
Mounika Naiudu, et al., 2012 [49]	K-mean based MAFIA with ID3	85.0%	80.0%	85.0%	NA
Miao, et al., 2016 [50]	Adaptative Boosting	80.14%	81.5%	71.0%	29

Table 11. Comparison with other studies using CH dataset

Author	Method	Accuracy	Precision	Recall	Features
Our study	Gradient-boosted Tree (GBT)	99.4%	100.0%	98.7%	Raw data
Our study	ChiSqSelector+PCA and Logistic Regression	99.4%	97.6%	100.0%	13
Hung, et al., 2018 [48]	Linear SVM	89.9%	NA	87.0%	Raw data
Hung, et al., 2018 [48]	Infinite Latent Feature Selection (ILFS)	90.7%	NA	91.0%	39

Each of the classifiers that used CHI-PCA outperformed the literature. Using a dimensionality reduction technique, CHI with PCA and RF classifier computed the best result using 13 features. Shamosollahi, et al. [47] used clustering to determine the k number. After, they performed decision tree and artificial neural network (a hidden layer with 3 nodes). The best result was the C&RT decision tree with an accuracy of 92.6%, and neural networks computing 90.4% accuracy. Mounika Naidu et al. [49] proposed the use of K-mean based on Maximal Frequent Itemset Algorithm (MAFIA) with ID3. The data was clustered using K-means algorithm with k value as 2, then MAFIA used the relevant cluster of 13 features and the ID3. The result of the experimentation was 85.0% accuracy. Miai, et al. [50] used an adaptative Boosting algorithm with an accuracy of 80.14% on Cleveland dataset. In addition, the authors computed on the Hungarian dataset an accuracy of 89.12%, which is below our models, except NB. The results of Cleveland were superior in all the metrics in the literature.

Table 11 shows the comparative performance of CH with the literature. Hung et al. [48] performed the feature selection techniques of Infinite Latent Feature Selection (ILFS), Sort features according to pairwise correlations (CFS), Feature Selection and Kernel Learning for Local Learning-Based Clustering (LLCFS), and PCA. ILFS performed the best computation with 90.65% accuracy and was the classifier that used the least number of features. CFS, LLCFS, and PCA computed 89.93% accuracy, but they need at least 55 features to achieve that result. They used the datasets of Cleveland, Hungarian, and Switzerland. Our method outperformed the literature with a smaller number of features, such as in the case of Cleveland and Hungarian datasets.

Table 12. Best models accuracy with other studies using the Subset-A of Cleveland

Author	Method	Accuracy	Tool	Features	Dataset
Khanna, et al., 2015 [54]	Logistic Regression	84.80%	-	13	50% training, 50% testing
Khan, et al., 2016 [55]	Decision Tree C4.5	89.10%	WEKA	13	70% training, 30% testing
Khan, et al., 2016 [55]	Random Forest	89.25%	WEKA	13	70% training, 30% testing
Khanna, et al., 2015 [54]	SVM (linear)	87.60%	-	13	50% training, 50% testing
Kodati, et al., 2018 [56]	Naive Bayes	83.70%	WEKA	13	-
Uyar, et. al., 2017 [57]	GA based on RFNN	96.63%	-	13	85% training, 15% testing
Santhanam, et al., 2013 [58]	PCA1 +FFNN	95.20%	-	8 ±1	-
Alotaibi, 2019 [62]	SVM	92.30%	-	13	10-fold cross-validation
Latha & Jeeva, 2019 [63]	Majority vote with NB, BN, RF and MP	85.48%	-	9	-
Gupta et al., 2019 [64]	MIFH (Factor analysis of mixed data + RF)	93.44%	-	28	-

Table 12 contains the best models from the literature considering different methods using the features of Subset-A. Some studies had high accuracy [57, 58, 62, 64], but we must consider that most of them only used accuracy, and important metrics such as precision, recall, and F1 score were not considered for evaluation. Furthermore, the dataset division was not mentioned in the articles [56, 58, 63, 64], or the testing dataset was small, as in [57], with only 45 test instances, which can lead to an error in the results. The non-hybrid models computed promising results for the trees [55], but SVM [62] was the only one with more than 90% accuracy. There is a gap in the SVM results between [54] and [62] of 4.7% with the only difference in the dataset, this must be address and verify in the future. According to the hybrid models comparison, when the dimensionality reduction was used, a better prediction of heart disease was obtained. Similar to our model, some of the hybrid models in the literature outperformed the others with the use of RF. Our CHI-PCA logistic regression model had the second greatest improvement when compared with raw data, this can be observed in [54] where the performance was the worst among the non-hybrid models.

Based on these results, our model outperformed those in the literature. It is important when practitioners can only work with three or four times less than the given number of features and achieve competitive results compared to full features. Our method helps to reduce unnecessary patients' attributes and reduce the amount of data.

5 Conclusion

In this paper, we proposed the use of a chi-square (CHI) with PCA to improve the prediction of machine learning models. The goal for the classifier was to predict whether a patient has heart disease. Use of complete features is not feasible when the system resources need to be considered. In this study, we successfully applied dimensionality reduction techniques to improve the raw data results. For the 74 features given, we selected three groups of features and achieved the best performance. It was found that among the classifiers, **CHI-PCA with RF had the maximum performance**, with **98.7% accuracy for Cleveland, 99.0% accuracy for Hungarian, and 99.4% accuracy for CH**. Our aim is to find the best dimensionality reduction method for the prediction of heart disease in terms of performance, for this reason, CHI-PCA was the most consistent and preferable method.

From the analysis, chi-square derived features of anatomical and physiological relevance, such as cholesterol, maximum heart rate, chest pain, features related to ST depression, and heart vessels. Our method can be employed in many real-life applications or in other medical diagnoses to analyze great amounts of data and identify the risk factors involved in different diseases. Our main limitation is the difficulty to extend these findings on heart disease due to the small sample size. For future developments, we plan to apply our method to a larger dataset and perform the analysis of some other disease with different feature selection techniques.

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Declaration of interests

☒ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

☐ The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: