Binary Classification: Comparative Study of Machine Learning Algorithms in Pima Indians Dataset

Guilherme Michel Lima de Carvalho *, Jaqueline Lopes Dias^{+} and Marcos Jardel Henriques$^{@}$

Abstract— **This work proposes, through machine learning techniques, to analyze a diabetes database: Pima Indians. This database is composed of data that brings results from a group of Native American women who live in Arizona, where research was carried out on the main factors related to diabetes. Thus, in this article this data set was analyzed using the techniques: Naive Bayes, Logistic Regression, Support Vector Machine, K Nearest Neighbors, Decision Trees, Random Forest, Perceptron and Multilayer Perceptron. The missing data were treated using regression techniques. In addition, to deal with unbalanced data, the SMOTE technique was used. The results obtained by these techniques were compared using the following criteria AUC and Accuracy. Defining the selected models, the best models were KNN, with 3 closest neighbors and Minkonski's distance, (accuracy of 85%), random forest with number of estimators 600 and entropy method (determination of 90%) and MLP with 1000 hidden layers of 1000 neurons and with activation function (accuracy of 85%). Finally, combining the three best models using ensemble methods: voting classifier and stacking classifier (with a neural network with final estimator). The accuracy of the ensemble methods was 92% and 92%, respectively.**

Keywords: Diabetes, Classifiers, Pima Indian database, Machine learning

I. INTRODUCTION

Currently, Diabetes is among the ten diseases that kill the most in the world [1]. Diabetes is defined as a group of metabolic disorders exerting significant pressure on human health worldwide [2]. Responsible for triggering several other diseases, diabetes has been widely studied by researchers from all over the planet. Diabetes, also called Diabetes Mellitus, is a metabolic disease that increases blood sugar levels, for longer periods of time, when compared to a person without the disease [3]. There are several symptoms and among them are excesses: of giving in, of urine and of hunger. When left untreated it ends up triggering several complications in the individual. There are three main types of Diabetes: Diabetes Mellitus type I, type II and gestational [4]. As it is a silent disease, it is always necessary to pay attention mainly to cases in the family, as well as to foods consumed frequently.

Diabetes is in the group pf chronic diseases, the main characteristic of which is changes in the levels of insulin in the blood. Whether it is inappropriate production or use by the body. The disease is also a risk factor for others, such as kidney disease, blood vessel damage, blindness and heart disease development [5]. Diabetes is a global public health problem, often diagnosed in middle age to elderly people.

Research that contributes to early diagnosis, helped people to have a better quality of life. Supervised machine learning techniques can be applied as a way to improve the diagnosis. Patients who have a high probability of developing the disease can change habits that decrease the chance of developing the disease. How to adopt better nutrition, weight loss and exercise.

In this sense, Diabetes, like other diseases, needs attention ranging from special care to cutting-edge scientific research. In most studies like this, it is desired to know the relationship that one or more variables in a studied condition, more specifically, it is desirable to establish the chance of occurrence of such condition, given a specific image of the symptoms. In the presence of a disease in a person it is a binary event, and this random variable can be denoted by Y, whose assumed values are 0 for the absence of the disease and 1 for the presence. This brings us to classification models.

The binary classification proposes to classify elements of a given data set into two groups. That is, based on the characteristics of individuals, it tries to predict which group each one will belong to. One of the models, which comes to mind, when you want to work with binary classification, is the logistic model. This is because, one of the appropriate models to estimate the probability of an individual presenting the studied condition or the chance of acquiring it is the *Logistic Model* [6].

However, there are a variety of binary classification models for working with classification problems. Among them, we can mention: Naive Bayes, Logistic Regression, Support Vector Machine, K Nearest Neighbors, Decision Trees, Random Forest, Perceptron and Neural Networks. All of these classification techniques will be addressed in this work, which will be compared using the following criteria: accuracy, precision, recall and F1 score.

Therefore, this work proposes, through machine learning techniques, to analyze a Diabetes database: Pima Indians is a database that brings results from group of females Native Americans living in Arizona, where research was on the major factors related to diabetes [5].

The work is divided as follows: chapter 1 provides an introduction about the disease and the classifiers, as well as, which techniques will be used in this article. Chapter 2 presents the result of five articles that modeled the same database. Chapter 3 describes the data, presents a descriptive

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analysis and the methods used in this article. Chapter 4 presents the results and conclusions.

II. Related Works

When carrying out surveys of works that have already analyzed the database that this article proposes to analyze, a range of published works is found. Several of them use statistical techniques, as well as machine learning. Among the works listed by us, which analyzed the Pima Indians Diabetes database, the work of Kriještorac *et al.* [7], which obtained good results, as well as good specificities and sensitivities after transforming the data, draws attention. These authors used several algorithms and among them was: Random Forest, SVM, J48 and KNN.

Researchers Jhaldiyal and Mishra [8] also studied the Pima Indians Diabetes data set using two techniques: main components and SVM. When analyzing the data using the main component technique, to reduce the number of dimensions and, using the error pruning reduction tree to train the data, they obtained an accuracy close to 79%. When working with SVM, also using main components, with the same objective of the first situation, they reached an accuracy of approximately 97%.

Kordos *et al.* [9], using the nearest K-neighbor algorithm (K-NN), when working with this database, after good parameter adjustments, it obtained an accuracy of approximately 77%.

Purnami *et al.* [10], achieved an accuracy of 76.73% in an attempt to predict people who in the future would be diabetics. This result was obtained using soft support vector machines (SSVM).

Using a ratio of $70\% - 30\%$ to conduct training and testing, with the intention of detecting Diabetes, Jahangeer *et al.* [11], modeled and compared three machine learning techniques : nearest K-neighbor algorithm (K-NN), with k = 1 and k = 3; Decision Tree-CART and SVM. With that, they were able to see that the parameter adjustments are essential in the modeling. Through these different techniques, the following precision was reached: Decision Tree-CART = $76,60\%$; K-NN com K = 1: $64,60\%$; SVM = $74,21\%$ e K-NN com K = 3: $68,79\%$. In this same sense, Shirke *et al.* [12], working with the SVM and Decision Tree classifiers reached the precision are 79.39% and 76.10% respectively.

Christobel *et al.* [13], worked on this problem using cross-validation and the nearest K-neighbor algorithm (K-NN). Through data processing, normalization, dimensioning and imputation, they achieved an accuracy of 74.74% through the use of cross-validation twice. When they performed cross-validation ten times, they reached an accuracy of 71.84%. An accuracy of 73.59% was obtained using kNN.

Performing selection of variables Hashi *et al.* [14] and reduced them by 37.5% and 50%. And through KNN (with K = 10 and 11) the accuracy increased from 74.48% to 81.17%; through SVM the accuracy was increased from 77.17% to 87.01%.

Also working with KNN, Ster and Dobnikar [15], in the detection of Diabetes, they reached an accuracy of 71.90% testing cross-validations ten times. In addition, they realized that when the parameters were not adjusted, the neural network performed better.

Kandhasamy and Balamurali [16], worked with the classifiers KNN, SVM and Random Forest obtaining the accuracy of 73.17%, 73.74% and 71.74% respectively.

Shankaracharya et. al. [17], using the logistic regression technique and working with eight variables, obtained an accuracy of 79.17%. However, the accuracy increased slightly to 80.21% when the authors worked with only the four most important variables.

Choubey et. al. [18], working with this same data set, reached the accuracy: Naive Bayes (76%), Logistic Regression (78.69%) and KNN (76.47%).

Sisodia and Sisodia [19], working with this same data set, reached the following accuracy: Naive Bayes (76%), SVM (65.10%) and Decision Tree (73.8%)

III. Material and Methods

A. *Pima Indians Dataset*

This database is originally from the National Institute of Diabetes and Digestive and Kidney Diseases. The objective of the database is to diagnostically predict whether or not a patient has diabetes, based on certain diagnostic measurements included in the database. Several constraints were placed on the selection of these instances from a larger database. In particular, all patients here are females at least 21 years old of Pima Indian heritage, living in or near Arizona, USA, conducted in 1990. The database consists of several medical predictor variables and one target variable, Outcome. Predictor variables includes the number of pregnancies the patient has had, their BMI, insulin level, age, and so on.

Name	Description	Mean
NP	Numbers of times pregnant	3.8
GP	Plasma glucose concentration after 2 h	12.9
BP	Diastolic blood pressure (mmHg)	69.1
SKIN	Triceps skinfold thickness (mm)	20.5
INSULIN	Two-hour serum insulin	79.8
BMI	Body mass Index (weight (kg)/height m)	32
DPF	Diabetes pedigree function	0.5
AGE	Age of patient (years)	33.2

TABLE I: Predictor variables -Pima Indian diabetes database

Motivating the application of prediction techniques for this population is the slow and gradual onset of the disease [20]. Traditional diagnostic methods plasma glucose test can take up to 10 years to identify the disease [21]. The data set was chosen because it is widely used to test classification systems, making it easier to make comparisons between the results obtained with other models already proposed for the diagnosis of diabetes.

B. *Pre-processing and Exploratory Analysis*

Some observations have a value of zero, such as age and insulin, indicating that the database has some data reporting problems. Missing data are recorded as zero value in 376 of 768 observations in the Pima database. Due to the high proportion of values, the withdrawal of these observations would represent a great loss of data.

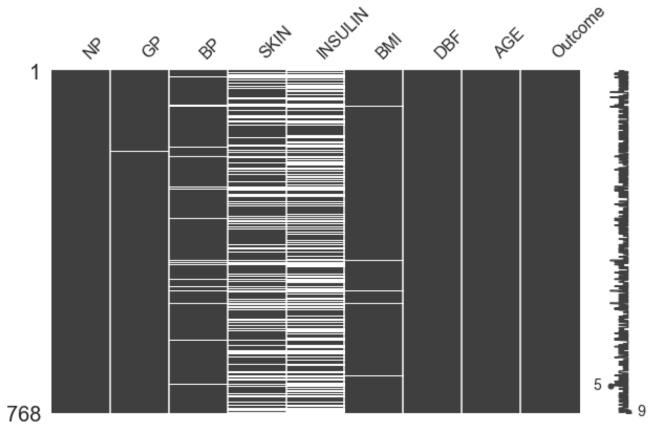


Fig. 1: Missing values for the variables

In the figure 1 , the missing data are represented with a white line.

The family history of diabetes increases the chances of developing the disease. Gestational diabetes is also positively associated with the risk of developing type II diabetes in the following years. With respect to age and weight, often people in middle age and overweight people, the disease develops more. The group is young, has an average age of 33 years, a minimum age of 21 years and a maximum age of 80 years.

As Figure 1, there is a lot of missing data in our database: Insulin (374), SkinThickness (227), BloodPressure (35), BMI (11) and Glucose (5). To deal with this, we have to use some technique. A common way is to replace the missing value with the average column value. In our work, we substitute these values for the average. As a result, there were major changes in the distribution format. These changes in distributions are shown clearly in the following figures:

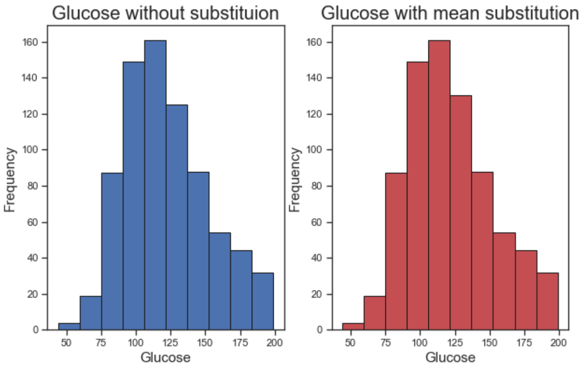


Fig. 2: Histogram of Glucose

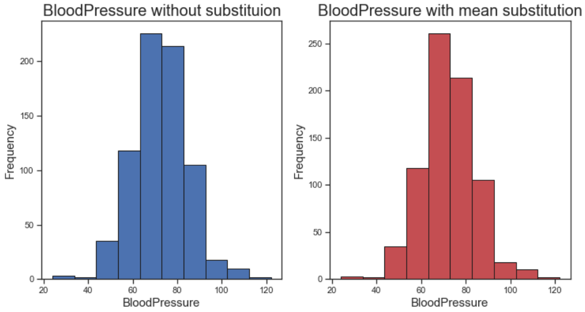


Fig. 3: Histogram of BloodPressure

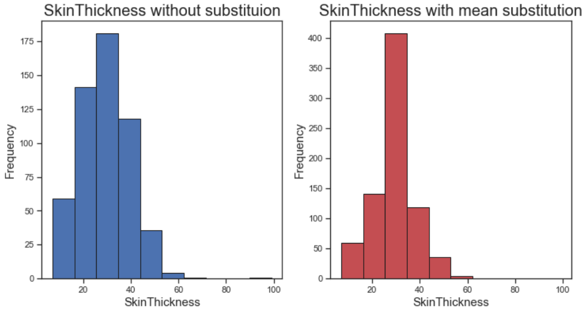


Fig. 4: Histogram of SkinThickness

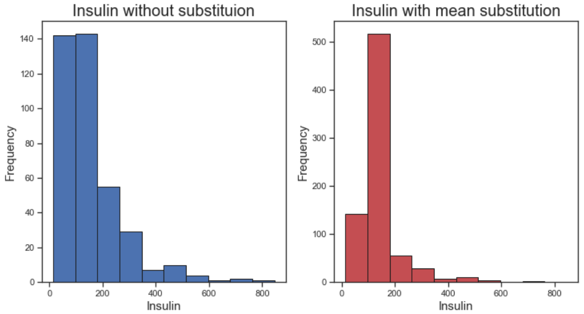


Fig. 5: Histogram of Insulin

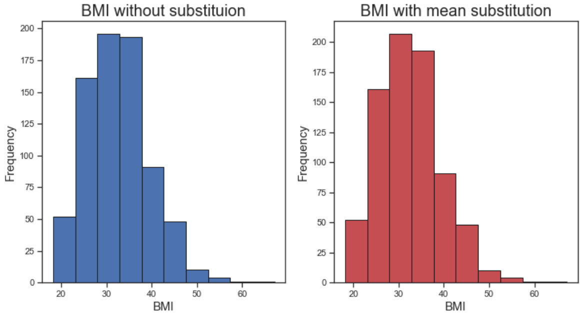


Fig. 6: Histogram of BMI

Another consideration in the exploratory analysis is that, the Pima Indian Database is unbalanced. We have more observations of the Class 0, that is, without diabetes. We show this in the following figure.

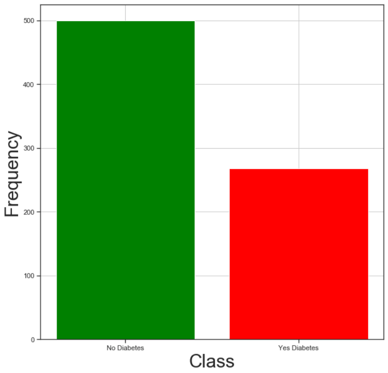


Fig. 7: Quantity of observations in each class

To overcome the problem of imbalance observed in the data set we use a technique called Synthetic Minority Over-sampling Technique(SMOTE),this approach is used to remove imbalance in the data by creating samples using the current data, see Ref. [22] for more details.

SMOTE selects the examples that are close in the resource space, separating a line between the data and generating a new sample at the limits of that line. For the k neighbors closest to the minority class observations, a neighbor is selected at random and a synthetic observation is created among the existing observations [23]. The method combines a random undersampling to identify minority observations, followed by SMOTE to increase the number of minority observations, balancing the sample. With this procedure it is possible to create as many synthetic examples of the minority class as needed. This combination has a better performance compared to simple sampling [22].

C. Feature Selection

We observed that the distribution of variables in the classes for some cases is very different. Thus, below are shown four graphs in figures 8, 9, 10 and 11. These graphs show the variables that have a great influence on the model.

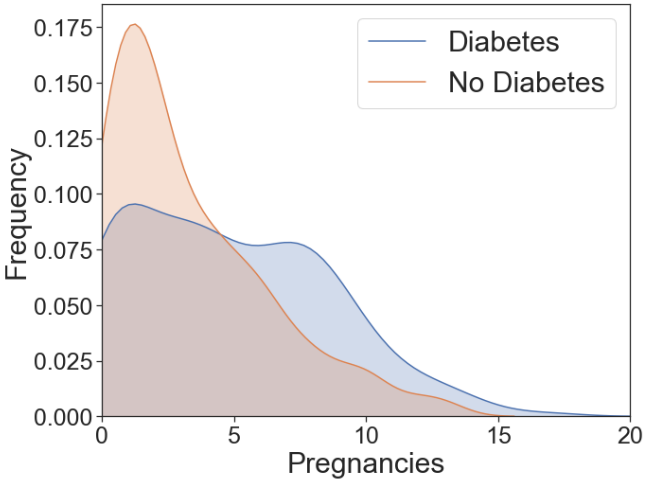


Fig. 8: Pregnancies distribution in the classes

In Figure 8, we can see the frequency distribution of the number of times that women became pregnant. At the first impression, it is noted that non-diabetic women had fewer children. In this case, fashion was around two children per woman. It is clearly seen that diabetic women had far more children than non-diabetic women. So far, visually, we can expect that the greater the number of children, the greater the chance of women having diabetes.

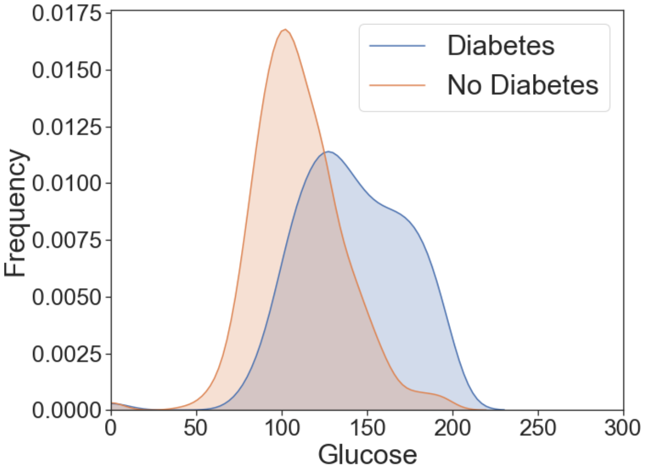


Fig. 9: Glucose distribution in the classes

Figure 9, on the other hand, shows the frequency distribution of the glycemic index among women. The fashion among non-diabetic women, that is, the vast majority of women who are not diabetic have a blood sugar around 100. Among diabetic women, most have a glycemic index of around 140, which according to OMS, is a typical index for a diabetic person. There is also a large percentage of women who have diabetes, a glycemic index above 150, exceeding 200.

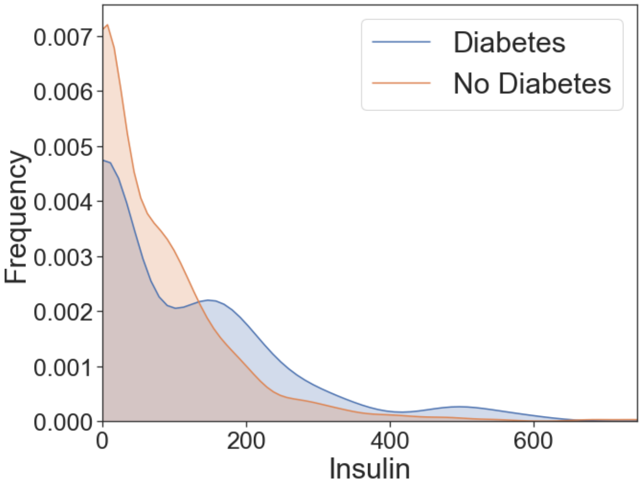


Fig. 10: Insulin distribution in the classes

Figure 10 shows the distribution of insulin in the blood of patients after the examination of insulin resistance. The insulin resistance test is performed as follows: first, blood glucose is measured with the fasting person. Then the patient ingests $75mg$ of glucose and after two hours the blood glucose level is adjusted again. In this graph there is a large amount of missing data, where the missing data is zero values (that is why the vast majority of people are around zero). Other than that, in this graph, it is noted that from the value 175 for the glycemic index, diabetic people appear more frequently.

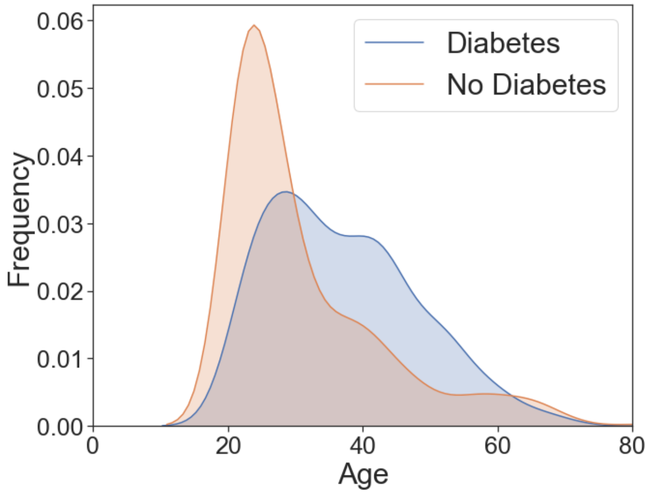
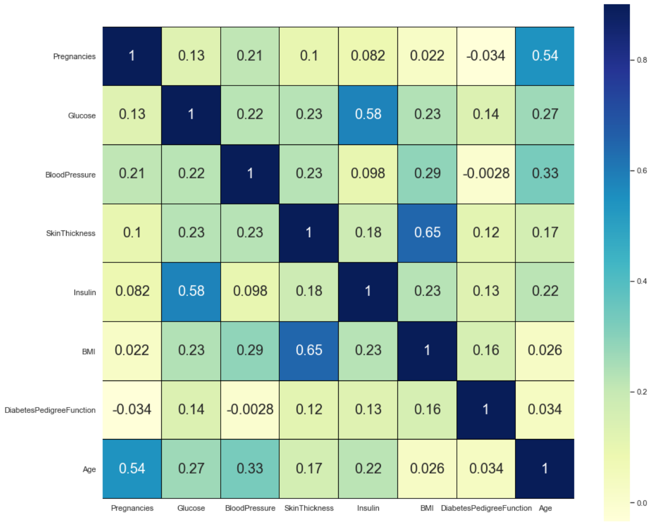


Fig. 11: Age distribution in the classes

Figure 11 shows the frequency distribution of ages, between diabetic and non-diabetic individuals. It can be noted that among non-diabetics are the youngest, where the average age is close to 20 (perhaps a little more). The average age of diabetic people, on the other hand, approaches 40 years. Among diabetics the dispersion of ages is greater; the younger is the opposite, that is, the dispersion of ages among the younger is less.

Now we show the correlation matrix of the covariables.



	Pregnancies	Glucose	BloodPressure	SkinThickness	Insulin	BMI	DiabetesPedigreeFunction	Age
Pregnancies	1	0.13	0.21	0.1	0.082	0.022	-0.034	0.54
Glucose	0.13	1	0.22	0.23	0.58	0.23	0.14	0.27
BloodPressure	0.21	0.22	1	0.23	0.098	0.29	-0.0028	0.33
SkinThickness	0.1	0.23	0.23	1	0.18	0.65	0.12	0.17
Insulin	0.082	0.58	0.098	0.18	1	0.23	0.13	0.22
BMI	0.022	0.23	0.29	0.65	0.23	1	0.16	0.026
DiabetesPedigreeFunction	-0.034	0.14	-0.0028	0.12	0.13	0.16	1	0.034
Age	0.54	0.27	0.33	0.17	0.22	0.026	0.034	1

Fig. 12: Correlation Matrix

The most correlated variables are SkinThickness and BMI, with 0.65 pearson correlation. So in this database do not have to much correlation between the features and the feature space have a low dimension, therefore we use all the variables in the modelling.

D. Classification Models

1) Naive Bayes: Consider we have a sample of independent observations in a training set, lets say: $(\mathbf{x_1}, Y_1), (\mathbf{x_2}, Y_2), \cdots, (\mathbf{x_n}, Y_n) \sim (\mathbf{X}, Y)$. Where, $\mathbf{x_1}, \cdots, \mathbf{x_n}$ are the d dimensional vectors of features, and $Y_1, \cdots, Y_n$ are the target, in this case, Y_i are binary variables. Our goal is to build a function to predict new observations, based on this sample.

We can use the following Risk function to train the model:

$$R(g) = P(Y \neq g(X)) \tag{1}$$

So, we have to maximize:

$$g(x) = \underset{c \in \{0,1\}}{argmax} P(Y = c|\mathbf{x}) \tag{2}$$

Now, we have to estimate $P(Y = c|\mathbf{x})$, for this let's consider the Bayes theorem:

$$P(Y = c|\mathbf{x}) = \frac{f(\mathbf{x}|Y = c)P(Y = c)}{\sum_{s \in \{0,1\}} f(\mathbf{x}|Y = s)P(Y = s)} \tag{3}$$

To get the estimate for $P(Y = c|\mathbf{x})$ we have to estimate everything in the right side of the (4) equation. The estimates for $P(Y = c)$ for $c \in \{0, 1\}$ are easily to get, using the proportion of this classes in the sample. The Naive-Bayes method assume that, for every $c \in \{0, 1\}$, $f(\mathbf{x}|Y = c)$ can be factored:

$$f((\mathbf{x_1}, \mathbf{x_2}, \cdots, \mathbf{x_d})|Y = c) = \prod_{j=1}^{d} f(\mathbf{x_j}|Y = c) \tag{4}$$

By assuming that distributions are independent. So, we can estimate every $f(\mathbf{x_j}|Y = c)$ by assuming for example:

$$X_j|Y = c \sim N(\mu_{j,c}, \sigma^2_{j,c}) \tag{5}$$

And the estimates for $\mu_{j,c}$ and $\sigma^2_{j,c}$ are given by maximum likelihood. Therefore, we have:

$$\hat{P}(Y = c|\mathbf{x}) = \frac{\hat{f}(\mathbf{x}|Y = c)\hat{P}(Y = c)}{\sum_{c \in \{0,1\}} \hat{f}(\mathbf{x}|Y = s)\hat{P}(Y = s)} \tag{6}$$

Finally we have:

$$g(x) = \underset{c \in \{0,1\}}{argmax} \hat{P}(Y = c|\mathbf{x}) \tag{7}$$

And the decision rule can be: $g(x) = 0$ if $\hat{P}(Y = 0|\mathbf{x}) \geq \hat{P}(Y = 1|\mathbf{x})$ and $g(x) = 1$ otherwise.

2) Logistic Regression: In the logistic model, we use the values of a series of independent variables to predict the occurrence of the dependent variable (disease or condition). Thus, all variables considered in the model are controlled among themselves. As we use a series of independent variables, it is a multivariable problem. The regression model Multiple logistics is used for the case of regression with more than one explanatory variable.

According to Agresti (2007) [24]; Hosmer and Lemeshow (2013) [25] the general model for logistic regression with multiple Explanatory variables are defined as follows. Denote k predictors for an answer binary Y by $x_1, x_2, \ldots, x_k$. The model for the *odds log* is given by

$$\begin{aligned}\text{logit}(\text{P}(\text{Y}=1)) = \ln\left[\frac{\pi(x)}{1-\pi(x)}\right] \\ = \alpha + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k,\end{aligned}$$

The parameter β_i refers to the effect of x_i in the *odds log* when $Y = 1$, controlling the others $x's$. In addition, perhaps the most important interpretation of the logistics model is in the calculation of the **odds** ($Odds$ - O) and the **odds ratio** ($OddsRatio$ - OR), which allows to quantify the magnitude of association between the explanatory variables and the response variable. $Odds$ are given by

$$\frac{\pi(\boldsymbol{x})}{1-\pi(\boldsymbol{x})} = \exp\left(\alpha + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k\right).$$

This exponential relationship provides an interpretation for $\beta's$: The product by $\exp(\beta_i)$ for each unit plus x_i. See that when $\beta_i = 0$, $\exp(\beta_i) = 1$, therefore, the odds does not change when x_i changes [24].

3) Support Vector Machine: Developed in the 1990s, support vector machines - SVM, initially designed only for binary problems, ended up becoming a good classifier for a range of situations. With that, it became a reference when it comes to statistical machine learning. SVM is based on hyperplane concepts, which requires good knowledge of algebra [26].

Mathematically speaking, a definition of a hyperplane is not very complex and can be represented as:

$$\beta_0 + \beta_1 x_1 + \beta_2 x_2 = 0$$

What can be generalized to:

$$\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p = 0$$

Thus, all points of the vector $\mathbf{x} = x_1, x_2, \cdots, x_p$, which satisfy the equation, will belong to the hyperplane.

Otherwise,

$$\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p < 0$$

$$\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p > 0$$

With that, we just need to calculate the sign of the equation, to know where the point under analysis is.

A classic example of how to increase the dimensionality of data is by transforming a two-dimensional space into a three-dimensional one

$$f(x_1, x_2) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$

When the limit of separation of the vectors is, even if approximately, linear, the SVM will present good results. When linearity is bad, just increase the dimensions to solve this problem.

The following are some ways to increase these dimensions:

- Linear kernel

  $$K(\mathbf{X}, \mathbf{X}') = \mathbf{X} * \mathbf{X}'$$

  When using a linear kernel, we will have results equal to the results obtained by SVM.
- Polynomial kernel

  $$K(\mathbf{X}, \mathbf{X}') = (\mathbf{X} * \mathbf{X}' + c)^d$$

  For $d = 1$ and $c = 0$, we will have results equal to SVM and the linear kernel. However, when $d > 1$ the linearity will be increased, proportionally to its growth.
- Gaussian Kernel (RBF)

  $$K(\mathbf{X}, \mathbf{X}') = exp(\gamma||\mathbf{X} - \mathbf{X}'||^2)$$

  The value of $\ gamma$ controls the value of the kernel. The higher the value of $\ gamma$, the greater the flexibility of the model.

These are four of many other ways to increase dimensionality to solve the linearity problem. Each with its advantages and disadvantages, where, its hyperparameters can be found through cross-validation. Deciding which kernel to use will depend a lot on the situation you have to resolve. However, the Gaussian Kernel (RBF) is the most suitable for having only two hyperparameters to be optimized, and it is very flexible as to the classifier complexity.

4) K-Nearest Neighbours: The K-nearest neighbors (KNN) technique is a method of imputing and classifying data through the nearest neighbor. This method was proposed by Fukunaga and Narendra [27]. The method selects K objects with profiles similar to a missing observation Y_i through a distance measurement, such as Euclidean distance. After calculate all distances, one of the K observations closest to $_i$ what value occurs most often (for categorical data), or the average weighted of these values (for quantitative data), to fill in the missing value Y_i. This process does not change the variance or the average of the data set.

Two things must be defined to work with the KNN method: the metric of the distance calculation to be used and the size of K.

The metrics are chosen according to the problem, and the most used in calculating the distance between two points are:

- Euclidean Distance

$$D_E(p,q) = \sqrt{\sum_{i=1}^{n}(p_i - q_i)^2}$$

- Minkowski distance

$$D_M(p,q) = \left(\sum_{i=1}^{n}|p_i - q_i|^r\right)^{1/r}$$

- Chebyshev Distance

$$D_C(p,q) = \max_i(|p_i - q_i|)$$

In any case, $p = (p_1, \ldots, p_n)$ e $q = (q_1, \ldots, q_n)$ are two n-dimensional points and in the equation $D_M(p,q)$, r will be a chosen chosen constant.

The KNN method is often used to work with classification problems. Let's exemplify through the Euclidean distance, calculating the distance between two vectors.

$$e = \sqrt{\sum_{j=0}^{n}(X_{i,j} - X_{i+n,j})^2}$$

Given a point in space, KNN seeks to find the closest neighbors through the set of vectors:

$$\underset{X_{i,j} \subset X}{\arg\min} \sum_{i=0}^{K} \sqrt{\sum_{j=0}^{N}(X_{i,j} - t_i)^2}$$

Where: X, K and N are the neighbors and number of elements of the vector, and $X_{i,j}$ are the lines of the matrix.

What the vector will return $K_n = \{x_1, x_2, \cdots, x_n\}$ such that the sum of their distances is as short as possible, before the instance t.

5) Decision Trees: Decision tree is a supervised machine learning algorithm used in problems of classification and regression. Transforming a complex problem into multiple simpler problems, the algorithm is a strategy of dividing to win. For classifier a new item obtained from the tree is explained using set of rule taken on attribute values of training data. Through a simple algorithm to classify a new item, through of root nodes the instances with different features. The algorithm follows between questions and answers until reaches a leaf, that will be used as class for this case. The solutions to minor problems are combined into one tree, solving a more complex problem[28].

A decision tree can be easily and effectively converted into a set of rules, mapping from the root node to the leaf nodes step by step. Based on the concept of entropy and information gain [18]. We need to calculate two types of entropy using frequency tables as follows:

Entropy of of the target:

$$Entropy(T) = \sum_{i=1}^{c} -P_i log_2 P_i$$

and entropy using the frequency table of two features:

$$Entropy(T,X) = \sum_{c \in X} P(c)E(c)$$

The gain in information measures the reduction in entropy for each division:

$$Gain(T,X) = Entropy(T) - Entropy(T,X)$$

The objective is to maximize the gain.

Other classification criteria common is Gini

$$Gini(T) = \sum_i P_i(1 - P_i)$$

6) Random Forest: Random forest algorithm uses multiple learning algorithms seeking the best predictive performance. "The Random forest classifier creates multiple decision tree from randomly selected subset of training database. Aggregates the votes from different decision trees to decide the final class of test objects"[29]. It has two parts: Tree bagging and from tree bagging to random forest. Let n be the number of cases in sample at random of training set with replacement. The sample will be the training set of tree. We select the node that best split the node. There is no pruning, each tree is grown to the largest extent possible [16].

7) Perceptron: Rosenblatt's Perceptron is a simple Neural Network that can be composed by one single neuron, or several neurons arranged in a single layer. Is an algorithm for supervised learning of binary classifiers. The perceptron was invented in 1957 by Frank Rosenblatt [30]. The idea behind the Perceptron is to compose one or more output neurons, each of which is connected to several inputs units by means of connections that are characterized by weights [31]. One illustration of this model is presented bellow:

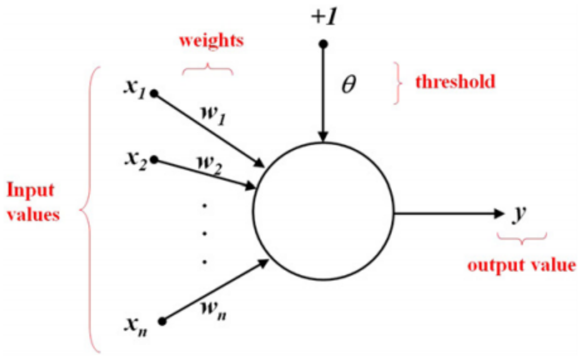


Fig. 13: Single Neural Perceptron, adapted from [31]

The output value is calculated as follows:

$$y = f(\sum_{i=1}^{n} w_i x_i + \theta) \tag{8}$$

The function f is called activation function and is given by:

$$f(x) = \begin{cases} 1, & \text{if } x > 0 \\ -1, & \text{otherwise} \end{cases} \tag{9}$$

In the Perceptron model we can use different penalty functions in regularization. Here we explore three: L1 norm, L2 norm and Elasticnet. For more details of regularization in Perceptron see Ref. [32].

8) Multilayer Perceptron: An Multilayer Perceptron(MLP) is an extension of Perceptron. In fact, MLP consists at least three layers of nodes. The following figure, adapted from [33] is showed an example of MLP.

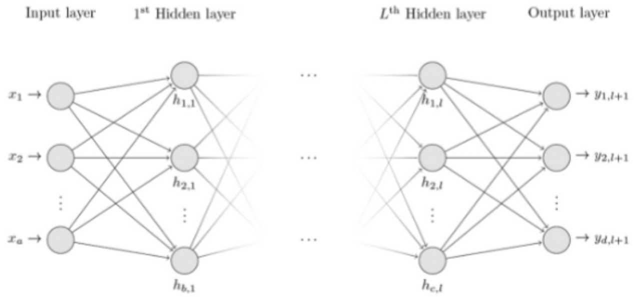


Fig. 14: MLP example, adapted from [33]

The learning processes occurs in MLP by changing connection weights, using backpropagation. For more details see Ref. [31]. In the case of MLP we can use several activation functions. Here we use logistic, identity, tanh and relu. This functions are:

Logistic:

$$f(x) = \frac{1}{1 + e^{(-x)}} \tag{10}$$

Identity:

$$f(x) = x \tag{11}$$

Tanh:

$$f(x) = tanh(x) \tag{12}$$

Relu:

$$f(x) = max(0, x) \tag{13}$$

9) Ensemble methods: Ensemble methods use several classifiers to obtain better predictive performance than each classifier alone. In this work we use two ensemble method: Voting Classifier/Majority Rule and the Stacking Classifier. The Voting classifier is very simple to understand, suppose for a certain classification problem we have three different classifications, the voting classifiers is a way to combine this three rules in one classifier. A common way to combine is to use the mode. The stacking classifier is similar, but the rule to get the final prediction is not only simple the mode, but every classification rule is passed to a new classifier and this meta classifier is used to get the final prediction.

TABLE II Confusion Matrix

		True diagnosis		
		Positive	Negative	Total
Predicted	Positive	TP	FP	$TP + FP$
	Negative	FN	TN	$FN + TN$
	Total	$TP + FN$	$FP + TN$	N

10) Performance Metrics: For evaluate our models we choose four different metrics: Accuracy, Recall, Precision and F1-Score. The choice of the evaluation metrics influences the firm that measures the performance of machine learning algorithms, different performance metrics were adopted to evaluate the algorithms. First we have to define the confusion matrix, it a kind of contingency table with two dimensions. Based on the confusion matrix, the relationship between true and false positives and negatives. Where we seek to minimize false negative and positive results.

- Accuracy: number of correct predictions made by the model. That is, the proportion of the true positives and negatives in relation to all the predictions of the confusion matrix. Applied to classes with proportions of data are nearly balanced.
- Recall: proportion of true positives in relation to those who actually tested positive. To minimize false negatives, the measure will approach
- Precision: discover the proportion of true positives in relation to those that are true and false positives.
- pandas: used for data analysis and manipulation tool.
- f1-score: a unique score to represent precision and recall, based on the harmonic average between the two metrics.

In terms of Confusion Matrix these metrics are defined by:

Accuracy

$$ACC = \frac{TP + TN}{TP + TN + FP + FN} \tag{14}$$

Recall

$$Recall = \frac{TP}{TP + FN} \tag{15}$$

Precision

$$Precision = \frac{TP}{TP + FP} \tag{16}$$

F1-Score

$$F1 = \frac{2TP}{2TP + FP + FN} \tag{17}$$

To evaluate our models we alse use the ROC curve. The ROC curve is created by plotting the true positive rate (TPR) against the false positive rate (FPR) at various threshold settings. The true-positive rate is also known as recall. The FPR is defined by $\frac{TN}{TN+FP}$.

E. Implementation:

We use python to implement all of this methods. The following libraries are required:

- NumPy: used for linear algebra and other operations.

- seaborn: used for statistical data visualization.
- matplotlib: used for plot and data visualization.
- pandas: used for data analysis and manipulation tool.
- scikit-learn: used for all the classification methods and preprocessing methods.
- Impyute: used for deal with missing data imputation.
- imblearn: used for deal with imbalanced data.

IV. Experiments

A. Description of experiments and performance of classifiers

For each model we describe in the Section of material and methods we try a few experiments. Each measure for performances of the models is an average of 10-fold cross validation. The database we use in each experiment is the database with replacement of the miss values with the mean and we balanced the data using SMOTE technique, which is implemented in the package imblearn.

1) Naive-Bayes: First we use the simple model Naive-Bayes, defined before.

2) Logistic Regression: We also use a simple logistic regression, defined before.

3) Support Vector Machine: We use SVM Classifier with differents kernels. We use polynomial kernel of degree 2 and degree 3. In our work we also use the linear kernel and the Radial basis.

4) K-Nearest-Neighbors: We use different configurations of KNN, with 3 or 5 Nearest Neighbors and the Minkowski distance with different values for p.

5) Decision Trees: We choose two decision tree, one with gini criterion and the other with entropy.The maximum number of features to consider when looking the best split was the total number of features in the database.

6) Random Forest: For the random forest classifier we test two criterion, gini and entropy. In addition, we choose the number of estimators as 100 and 600.

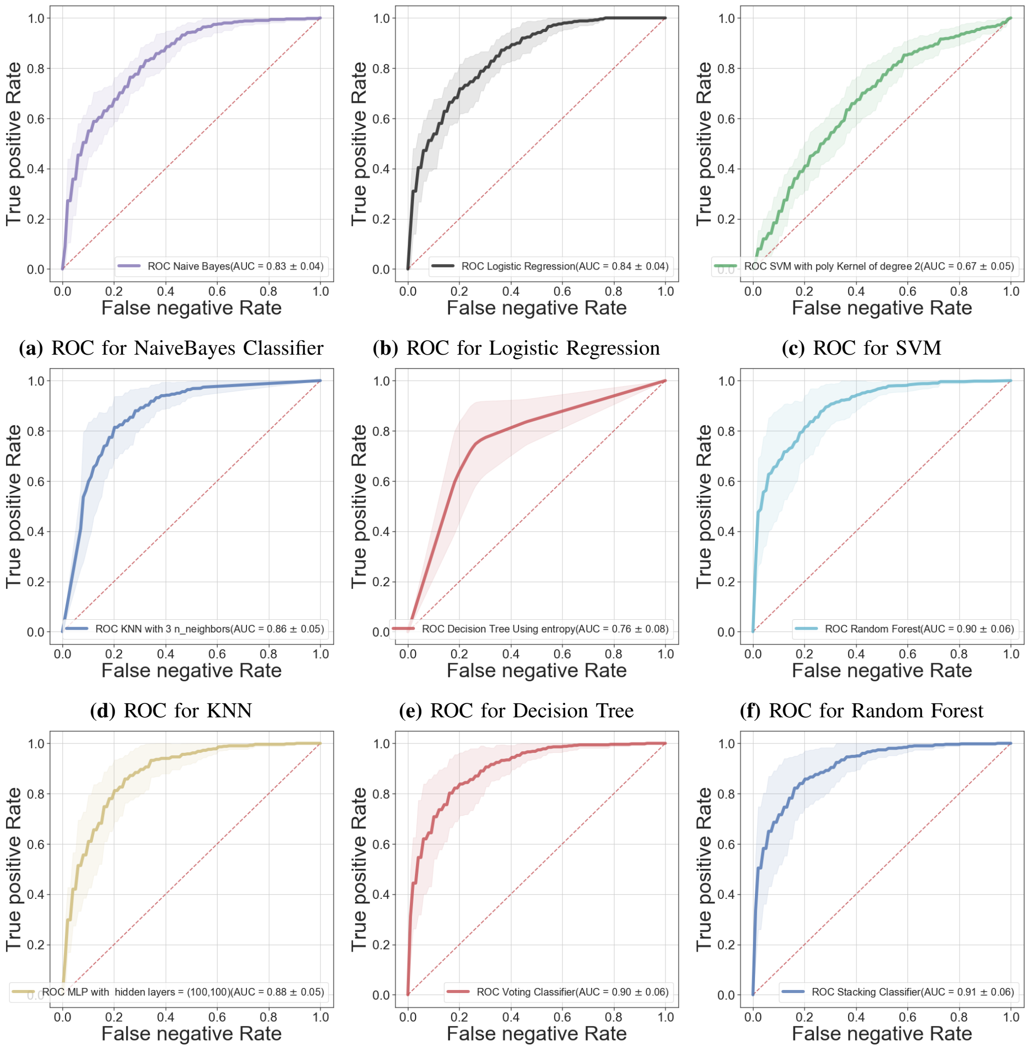
7) Multilayer Perceptron: We use 1000 hidden layers with 1000 neurons for MLP Classifier and differents activation functions. We test the following activations functions: Logistic, identity, relu and Tanh.

8) Ensemble Methods: We use meta-classifiers including Voting Classifier and Stacking Classifier. For do this we choose the best three models defined before by the AUC criterion and perform the ensemble classifier. The models are: MLP with 1000 hidden layers and 1000 neurons each layer and $tanh$ activation, Random Forest with 600 number of estimators and Gini criterion and KNN with 3 nearest neighbors and Minkoski distance with $p = 1$. For the Stacking Classifier we use a MLP with the final estimator with 1000 hidden layers and 1000 neurons.

All algorithms were tested considering all variables and applying 10-fold cross-validation, due to their efficiency in small data sets. Previous studies [7] that explored different combinations of variables in the same data set, achieved better results using all variables. From the results obtained it can be concluded that the ensemble methods (Stacking Classifier and Random Forest) and neural networks (MLP), present a better performance. Considering different weaker algorithms proved to be more powerful in both accuracy and precision for the classification of diabetes for the Pima database. Ensemble Methods Stacking Classifier, get the highest accuracy to be 92% and Random Forest with 600 estimators and considering entropy decision criteria (accuracy 90%).

The SVM classification model using the RBF kernel function obtained a better accuracy performance (82%) when compared with its linear application (77%) and polynomial of degree 3 (73%), a similar result found by other experiments [5]. Obtaining better results than Decision Tree with gini criterion, Logistic Regression and Naive Bayes algorithms, as in previous experiments [11]. However, the results were lower than the KNN considering the three closest neighbors (85%). One interesting thing to observe is that, the KNN classifier give to us a very high recall measure, which means, this method don't give any false negative in three configurations tested. Decision Tree model uses Gini criterion and entropy criterion, the first being the one with the highest accuracy (82%) and precision (84%). Obtaining a low performance, surpassing only Naive Bayes (75%) and logistic regression (78%).

The figure 15i shows the ROC (Receiver Operating Characteristic) curves used to evaluate the classifier's performance. The area under the curve (AUC) is calculated, we can obtain a metric to compare different classifiers. The ROC curve shows the rate of the really positive in relation to the rate of the false positives, the closer to a better and below 0.5 we have a bad model [34]. The models with the best performance according to this criterion are Stacking Classifier (AUC = 0.91), Voting Classifier (AUC = 0.90), Random Forest (AUC = 0.90), MLP (AUC = 0.88), KNN with 3nn (AUC = 0.86) , Logistic Regression (AUC = 0.84), Naive Bayes (AUC = 0.83), Decision Tree (AUC = 0.76) and SVM with poly Kernel of degree 2 (AUC = 0.67). The Ensemble Stacking Classifier method performed better according to its AUC.



(a) ROC for NaiveBayes Classifier

(b) ROC for Logistic Regression

(c) ROC for SVM

(d) ROC for KNN

(e) ROC for Decision Tree

(f) ROC for Random Forest

(g) ROC for MLP

(h) ROC for Voting Classifier

(i) ROC for Stacking Classifier

Fig. 15: Roc Curves

TABLE III Comparison of results (accuracy)

Methods	Our	[9]	[10]	[11]	[12]	[13]	[14]	[15]	[16]	[17]	[18]	[19]
Naive Bayes	0.75										0.76	0.76
Logistic Regression	0.78									0.8021	0.7869	
SVM with poly Kernel of degree 2	0.59		0.7673*	0.7421	0.7939		0.8701		0.7374			0.6510
SVM with poly Kernel of degree 3	0.73											
SVM linear	0.77											
SVM with rbf Kernel	0.82											
KNN with 3nn, distance metric with p=1	0.85	0.77		0.6879		0.7474	0.8117	0.7190	0.7317		0.7347	
KNN with 3nn, distance metric with p=2	0.82											
KNN with 5nn, distance metric with p=1	0.80											
KNN with 5nn, distance metric with p=2	0.83											
Decision Tree with gini criterion	0.82			0.7660**	0.7610							0.738
Decision Tree with entropy criterion	0.86											
Random Forest, nestimators=100, Gini	0.90								0.7174			
Random Forest, nestimators=100, Entropy	0.92											
Random Forest, nestimators=600, Gini	0.89											
Random Forest, nestimators=600, Entropy	0.90											
MLP with (1000,1000)(Activation logistic)	0.78											
MLP with (1000,1000)(Activation identity)	0.78											
MLP with (1000,1000)(Activation tanh)	0.85											
MLP with (1000,1000)(Activation relu)	0.85											
Ensemble Methods: Voting Classifier	0.92											
Ensemble Methods: Stacking Classifier	0.92											

*Soft Support Vectormachines (SSVM)

**Decision Tree-CART

Table III contains all the results of the accuracy obtained in this work, through the nine classification methods used. In addition, this same table also contains the values of the highest accuracy obtained by the works that were cited in this article. The ten articles referenced in this work, basically used the classification techniques Logistic Regression, SVM, KNN, Decision Tree and Random Forest. Considering all the references that worked with Decision Tree, KNN and Random Forest, our article showed superior accuracy. In relation to the six works that used KNN, only one, [8], obtained a greater accuracy than those presented in this article.

V. Conclusions

In this article we review the main current techniques that can be used for binary classification using the Pima Indian Database. We use techniques to deal with the missing values and imbalanced classes. To deal with missing data we use a regression technique to replace them. Besides that, to deal with imbalanced data we use the SMOTE technique [22]. We compared several classifiers, Naive-Bayes, Logistic Regression, SVM, KNN, Decision Tree,Random Forest and Multilayer Perceptron using different hyperparameters. Considering the models separately the best models are KNN, with 3 nearest neighbors and Minkonski distance,(85% accuracy), Random forest with 600 number of estimators and Gini criterion(89% accuracy) and MLP with 1000 hidden layers of 1000 neurons and $tanh$ in activation function(85% accuracy). Finally we combined this three best models using the AUC criterion and perform ensemble methods, voting classifier and stacking classifier(with a neural network in final estimator), the accuracy of the ensemble methods was 92% and 92%, respectively.

VI. Source Code

All the code used in this paper can be access in the following link: `https://github.com/gmichelcarvalho/Binary-Classication`.

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