

Optimizing explainability of Breast Cancer Recurrence using FuzzyGenetic

Fabio Cardoso¹, Thiago Medeiros¹, Marley Vellasco¹, Karla Figueiredo²

¹ Pontifical Catholic University of Rio de Janeiro slynrick@gmail.com,
thiago.medeiros.carvalho@gmail.com, marley@ele.puc-rio.br

² Rio de Janeiro State University karlafigueiredo@ime.uerj.br

Abstract. Breast cancer is the most common cancer diagnosed in the world, being the cause of death of 685,000 people worldwide in 2020. Due to the aggressiveness of the disease, early-stage identification, treatment, and remission detection are important to ensure longevity to those who may have cancer. In this paper, we propose a fuzzy-genetic approach for breast cancer recurrence classification. To this end, we use a Genetic Algorithm to design automatically the fuzzy inference system with the objective of balancing between accuracy and explainability. The proposed system achieved an accuracy of 91.30%, finding eleven rules with a maximum of three antecedents per rule, which provided a competitive result compared to other Machine Learning approaches.

Keywords: Fuzzy System · Genetic Algorithm · Classification · Breast Cancer.

1 Introduction

Cancer is recognized as a significant public concern worldwide due to its lethality and apparition in different organs [21]. One of the main problems related to this disease is the difficulty in detecting it in the early stages, in which the chances of treatment are considerably higher. Therefore, recent efforts have been made to create cancer treatment and a mechanism for the early identification of such pathology

Breast cancer is the most commonly detected disease among all types of cancer in the world [12]. This occurrence is considerably higher in women, being one of the leading causes of death [2]. This problem led the World Health Organization to launch a global initiative to raise awareness regarding the breast cancer problem [1].

In medical applications, Machine Learning (ML) approaches are especially useful to assist doctors in diagnostics and treatments. Depending on the task, different approaches can be suitable for automatic diagnosing the disease. Gravina *et al.* [9], for example, presented an ML strategy to classify prostate cancer using biopsy data of the patients. To detect breast cancer in its early stages, different authors proposed computer vision approaches to identify this disease, using digital mammography and even infrared images [16, 8].

As such approaches are used in a critical application, it is desirable that the results provided by ML methods should be reliable and understandable. To this end, explainable techniques are often employed to enhance the explainability of black-box models, which is the case for most ML methods. In medical application cases, techniques like Shapley [15] are used to explain the results provided to black-box models [25]. However, as those explainability approaches are considered post-hoc methods, they may lead to unreliable or even hard-to-understand explanations [22].

Interpretable models play an important role in Artificial Intelligence methods that can be easily understood by humans. One approach is the Fuzzy Inference System (FIS), which uses fuzzy logic, linguistic terms, and fuzzy rules to model the problem. The FIS is known to incorporate human reasoning and linguistic rules by construction, which verse in favor of a more reliable model in terms of understandability. Therefore, this approach can be suitable for medical applications. Boadh *et al.* [3] proposed a FIS with the objective of identifying the percentage of prostate cancer risk, using as input data the patient’s age, the prostate volume, and the result of the prostate antigen test (PSA).

In this work, we propose an automatic design of FIS for breast cancer remission classification. The contributions are three-fold:

- We develop a fuzzy-genetic approach to automatically discover the rules and the parameter of the membership functions of the fuzzy sets.
- We model the design of automatic FIS to create a more interpretable model, by adjusting the objective function to reduce the number of antecedents and rules generated.
- We evaluate the proposed approach in the breast cancer remission classification, comparing it with traditional ML approaches. Also, we assess the interpretability of our approach in both qualitative and quantitative terms.

The paper is organized as follows: Section 2 presents the literature review of ML and explainability techniques in medical applications. Section 3 presents the proposed approach for the automatic design of the FIS system. Then, in Section 4 we present the experimental details of the problem, with results and discussions presented in Section 5. In section 6, we summarize our findings and present the future directions of this work.

2 Related works

In the literature, there is a great deal of interest in the development of ML for classification in areas of high medical importance, such as the case of cancer identification that brings death to many every year [12]. Ravele *et al.* [20] developed an automated detection system using machine learning techniques. The best approach was using Neighbor Component Analysis (NCA) with K-nearest neighbor to classify breast cancer, achieving an accuracy of approximately 98.50%.

Gupta *et al.* [10] presented a solution using Multi-layer Perceptron (MLP) for prostate tumor classification between malignant and benign. Data balancing

tests using techniques were performed and the best result found, using all input variables, was 97.00% accuracy using a hybrid balancing technique by under-sampling and oversampling.

Erdem *et al.* [6] also presented a solution for prostate cancer diagnosis comparing the machine learning models Naive Bayes (NB), Logistic Regression, k-Nearest Neighbor (k-NN), Support Vector Machines (SVM), Linear Regression, Random Forest (RF), Linear Discrimination Analysis (LDA), Multi-Layer Perceptron (MLP) and Deep Neural Network (DNN). The best result was with the MLP model, which achieved an accuracy of 97.00%. In this work, no variable selection techniques were used, therefore, the result used all eight variables available in the database.

To have greater interpretability of the results, Janssen *et al.* [13] presented an eX-treme Gradient Boosting (XGB) model to identify the chance of survival of prostate cancer patients using the Shapley Additive Explanations (SHAP) technique to inform the contribution of each model input to the result. This is an interesting proposal as many models that are "black boxes" hiding the reasons why the model achieved its results [5].

Kit-Sang *et al.* [24] presented a proposal to search for a minimum set of rules and membership functions of a SIF, using an implementation of a Genetic Algorithm that they called hierarchical. In this work, it was possible to achieve a result with performance compatible with techniques such as adaptive control and the conventional fuzzy approach with Genetic Algorithm and has the potential to become a low-cost system.

Gupta *et al.* [11] develop a fuzzy system for breast cancer classification. This work used a decision tree to derive the rules to be used in the fuzzy system with a total of 27 rules and achieved an accuracy of 97.00% with the system with those rules.

Despite the profusion of research in cancer classification for medical applications, the analysis of cancer recurrence remains relatively unexplored in the literature. Our work aims to fill this gap by introducing an approach that combines ML model design, explainability, and Auto ML. We propose a fuzzy-genetic approach that considers the accuracy metrics, but also focuses on generating interpretable fuzzy rules for human understanding. This approach not only enhances the accuracy of cancer recurrence analysis but also provides valuable insights into the underlying patterns and factors contributing to recurrence

3 Automatic Fuzzy System Design

In medical applications, an interpretable result is one of the most desirable characteristics in automatic diagnosis problems, given that doctors can directly audit it, evaluating the rationale behind the inference. In that sense, the FIS can be a suitable choice for not only accurately modeling the problem but also providing an interpretation of its results.

Despite its inherent interpretability and achieving competitive results in a wide range of applications, FIS can be a challenging to adjust. Differently from

other Machine Learning approaches, traditional FIS generally requires manual adjustments, which may involve expert knowledge to generate appropriate fuzzy rules and fuzzification sets, for example. To better understand the complexity of adjusting such parameters manually, Fig. 1 shows the traditional FIS and the related manual design.

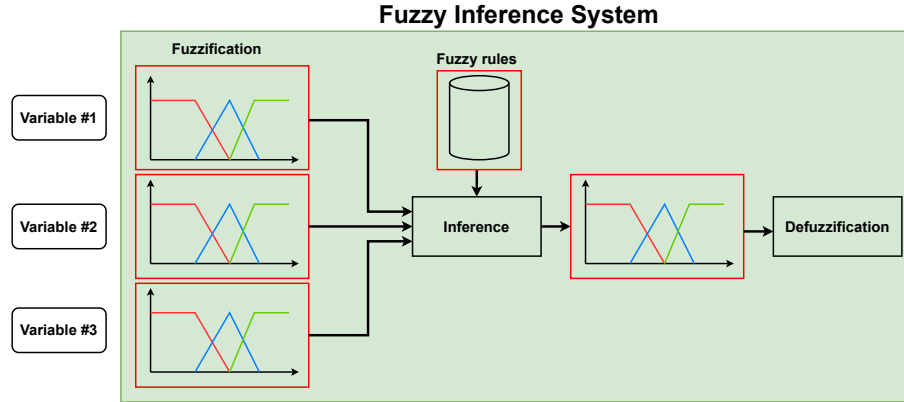


Fig. 1. Overview of the Fuzzy Inference System. Steps that require manual adjustment are highlighted in red.

The automatic design of FIS is usually applied to circumvent the problems related to adjusting such parameters manually, transforming it into a data-centric approach. This strategy can be optimized based on statistical approaches, but usually, the FIS is coupled with an optimization strategy. Among all options, one of the most common approaches is based on combining FIS and evolutionary algorithms, by either optimizing the fuzzy base rules or all of the parameters of the FIS.

In this work, we follow a fuzzy-genetic approach for the automatic design of FIS. In this case, we use the Genetic Algorithm (GA) to optimize both fuzzy sets and the fuzzy rules associated with the problem. For the modeling of the GA, it is necessary to adequately represent the solution to the problem by defining the structure of the individuals, defining the selection methods and appropriate crossings for the solution search process, in addition to the objective function, which will guide the algorithm in the search for the optimal solution.

For modeling the problem in the automatic design FIS approach, Fig. 2 presents the proposed chromosome representation for this problem. The individual can be conceptually divided into two parts: the first with information about the FIS rules and the second with information about the parameters that define the membership functions of each linguistic variable, considering the points listed from two to four in the base of the fuzzy sets in Fig. 1.

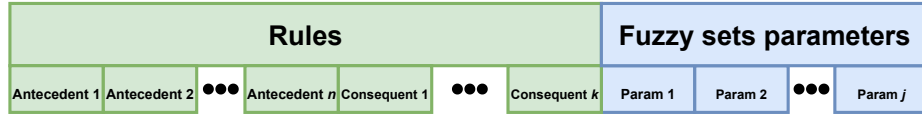


Fig. 2. Individual modeling for the rule search problem and fuzzy set tuning for prostate cancer classification. In this example, the chromosome contains j parameters to compose the fuzzy sets for all variables and k rules, each one containing n maximum antecedents.

The part of the individual that is responsible for the rules has the following order of formation: the genes that represent the antecedents of the rules, composed by the maximum of existing variables in the problem, which in this case are eighteen, and can have a value ranging from zero, which means not using the antecedent, and the other defined fuzzy sets (from one to three) and the rule's consequent that is only allowed to have values corresponding to the problem's classes.

The modeling of the individual allows the discovered rules to have antecedents of the with value zero; that is, this antecedent is removed from the rule. For this reason, there is only one alternative to not using a fuzzy rule, when all the antecedents have a value of zero. In addition, it is important to define that rules considered invalid have the same antecedent with a different consequent. To better understand the chromosome representation, Fig. 3 exemplifies a possible rule during the optimization step.

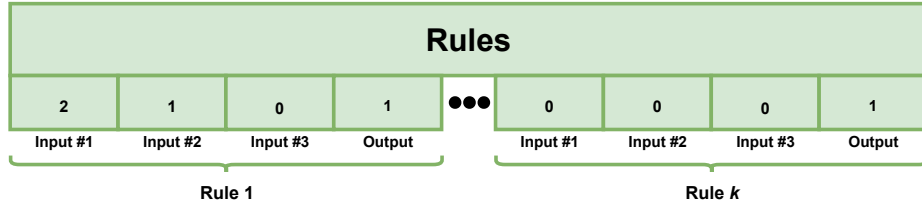


Fig. 3. Example of rules in an individual.

The first n genes of this example represent the antecedents associated with all linguistic variables and, in this example, only the two variables are being used, because they are the only genes with values other than zero. The consequent that is represented by the gene in the last position represents the class, which designates one of the classes of the problem.

The second part of the individual represents the parameters of fuzzy sets of each linguistic variable, considering that the universe of discourse of each variable varies between zero and one since each input variable was normalized in this same interval.

In this problem, we follow a Strong Fuzzy Partition (SFP), which brings benefits in terms of interpretability and optimization [17]. In fact, using the SFP allows that, for every value of the universe of discourse, the sum of the membership degrees is always 1, thus generating potentially more coherent fuzzy sets and enhancing the interpretability [7]. Also, from an optimization modeling perspective, the SFP lowers the number of required genes to optimize the fuzzy sets associated with a linguistic variable. Thus, for each linguistic variable, using only three genes in the fuzzy set optimization presented in Fig 4 will be necessary.

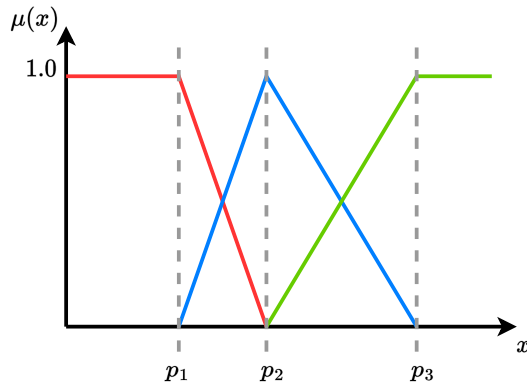


Fig. 4. Fuzzy partition adopted in this article. Only p_1 , p_2 , and p_3 are adjusted in the optimization process.

The data presented in Fig. 5 are the possible parameter values of the fuzzy set for the first linguistic variable that can be interpreted as follows: For the first fuzzy set, the function will be trapezoidal will be defined with the parameters [0; 0; 0.15; 0.22]; for the fuzzy set, the function will be triangular with the parameters [0.15; 0.22; 0.26] and for the third (and last) fuzzy set the function will be trapezoidal with the parameters [0.26; 0.45; 1; 1].

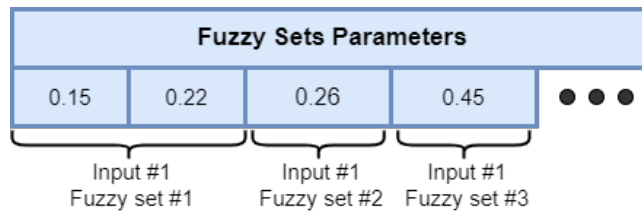


Fig. 5. Example of a fuzzy set parameters in an individual.

With the modeling of the individual defined, it will be necessary to define the objective function that will guide the evolutionary process. The problem to be solved comprises multiple objectives, covering both accuracy and explainability terms, presented in Table 1. Invalid rules are those with all antecedents disabled or those with the same antecedent with a different consequent.

To simplify the composition of these objectives, we used the Mean Squared Error function (MSE), which calculates the error between the individual's value and the desired value, described in Eq. 1. Therefore, each objective is transformed into its minimization of the target values. In Table 1 it is possible to briefly identify the multiple objectives, the desired target value, and the weight of each objective.

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (x_i - t_i)^2 \quad (1)$$

Table 1. Objectives to finding rules and parameters for the membership functions of fuzzy sets.

Objective (%)	Target value	Weight
Accuracy	1	3
Number of rules	0.05	1
Average Antecedents	0.125	1
Invalid rules enabled	0	1
Repeated rules enabled	0	1

where n is the number of objectives, x_i is the i -th objective value in the optimization step, and t_i is the target value. To complete the settings of the genetic algorithm, we used the binary crossover function in the crossover step, the polynomial mutation function in the mutation step [4]. In the selection step elitism of 10% of the population and a tournament function between three individuals with 90% of the population is implemented.

3.1 Fuzzy Inference System and Interpretability

After the optimization strategy, the fuzzy system behaves like a traditional FIS. Therefore, all of the characteristics of a Mamdani FIS remain, including ease of interpretation of results from a human perspective. However, although we highlight that a Mamdani FIS is more suitable for explaining of results, there is no guarantee that such systems are always interpretable [19]. In fact, it is reasonable to understand that a FIS with multiple simultaneously activated rules can be considered a system barely understandable for humans, despite using the Mamdani rules.

To guide the optimization strategy in both the accuracy and interpretable design of the FIS, we adjust the objective function to match the following interpretability criteria:

1. **Rule length:** This metric evaluates the average number of antecedents used in the fuzzy rules. The lower its values, the better the legibility of the rule by the human. To achieve this criterion, we use the average antecedents to benefit shorter rules.
2. **Complementarity:** Evaluates the distribution of the fuzzy sets in the universe of discourse. Generally, the sum of activated membership functions is always expected to be 1. This interpretability measure is obtained using the SFP, which guarantees the aforementioned condition.
3. **Base rule size:** This metric evaluates the generalization capability of the SIF and its complexity. A lower dimensional base rule indicates a more intelligible one by humans. We use the enabled rules to guide the optimization into a more concise base rule, while not compromising the accuracy.
4. **Consistency:** Determine the number of rules with the same antecedents and different consequents. Ideally, there would be no conflicting rules in the system. Our approach uses the invalid rules-enabled objective term to obtain a more consistent SIF.

4 Experiments

4.1 Dataset

The work aims to provide a model with the best trade-off between accuracy, and explainability for breast cancer recurrence and for that purpose, we used a dataset that contains data from 344 patients, of which 199 with recurrence and 145 without recurrence. The dataset contains 11 categorical and seven continuous features with two classes (with and without recurrence), it is also important to point out that all categorical feature is considered as a singleton set in the FIS. All collected features are shown in Table 2.

4.2 Machine Learning Models

To evaluate our proposed approach in terms of accuracy, we tested the modeling capability using traditional ML methods, namely Logistic Regression, Naive Bayes, K-Nearest Neighbors, Support Vector Machine, and neural Network. Also, we selected some state-of-the-art ML models for structured data. To this end, we evaluated the results obtained by XGBoost, CatBoost, and Random Forest. To get a fair comparison, we performed a grid search to obtain the best hyperparameters for each model on the validation set.

4.3 Experimental Protocol for the proposed approach

Searches for the best fuzzy system were performed through the Genetic Algorithm, considering the smallest base rule with the smallest number of antecedents being used in the rules. The maximum number of rules to be searched was set arbitrarily with the value of 20, since the object is to find the best minimum set of rules to solve the problem of breast cancer classification.

Table 2. Collected features

Feature	Data type
Cancer Type Detailed	Categorical
Subtype	Categorical
Race	Categorical
Neplasm Disease Stage	Categorical
In PanCan Pathways Analysis	Categorical
New Neoplasm Event Post Initial Therapy Indicator	Categorical
Pior Diagnosis	Categorical
Radiation Therapy	Categorical
Tissue Prospective Collection Indicator	Categorical
Ethnicity	Categorical
Sex	Categorical
Diagnosis Age	Continuous
Aneuploidy Score	Continuous
Buffa Hypoxia Score	Continuous
Ragnum Hypoxia Score	Continuous
Winter Hypoxia Score	Continuous
Fraction Genome Altered	Continuous
Mutation Count	Continuous

Several searches were performed 20 experiments with the population number of 300 individuals evolving over 300 generations without early stopping. The crossover probability was 0.65 and the mutation probability was 0.05. These values were chosen to ensure the convergence of the system to the end of the evolutionary process during the searches, but no search of configuration parameters for the Genetic Algorithm was performed.

During the evolutionary process, as shown in Fig. 6, it was identified that after the 50th generation, the improvement of the fitness is lower than the beginning of the process and the individuals are not changing much when comparing the area until the end of 300 generations.

For solution development, the database was separated into a train, validation, and a test set with percentages being 60%, 20%, and 20%, respectively. This approach was used because, during the evolution process, the parameters of the membership functions and the rules were chosen based on the training data. As problems of over-specialization in the data can occur, the accuracy in the validation set was used to guarantee the selection of the best individual found in the performed searches.

5 Discussion and Results

The best individual in the performed searches reached an accuracy of 95.00% training set, 92.72% in the validation set, and 91.30% test set with the distance between the best individual and the target goal of 0.0326, calculated through the MSE. This individual does not have any repeated or invalid rules, does

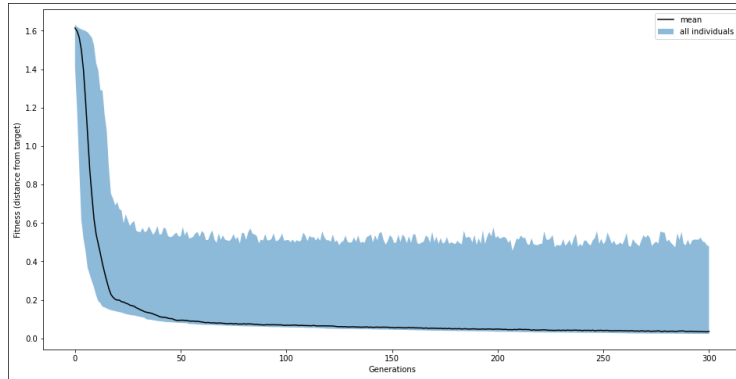


Fig. 6. Fitness of all individuals each generation with the mean fitness curve.

not have any invalid membership function parameter, and does not exist in the training and test data set samples that did not activate any rule. Fig. 7 shows the confusion matrix of test data for the best individual's train.

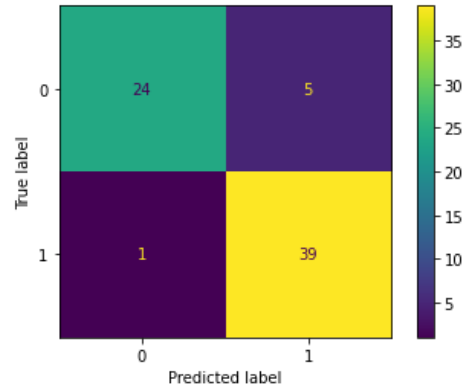


Fig. 7. Confusion matrix of test data for the best individual's train.

The Table 3 presents all the rules enabled in the best individual, so is easy to visualize the number of antecedents used and the linguistic terms of each active antecedent for each class of the problem. In addition, it also presents a selection of input variables during the search for the smallest number of rules and the smallest number of antecedents, and Sex, Ethnicity, Race, Aneuploidy Score, In PanCan Pathway Analysis and Prior Diagnosis was never used in any of eleven rules discovered, which means that this information does not provide any valuable information for the system to identify cancer recurrence of an individual with the data provided in the dataset.

Table 3. Rules discovered by the fuzzy-genetic system

Rules discovered

IF *Subtype* Small **AND** *Winter Hypoxia Score* Small **AND** *Tissue Prospective Indicator* is True **THEN** Recurrence
IF *Mutation Count* Medium **AND** *Post Initial Therapy* is True **THEN** Recurrence
IF *Diagnosis Age* Medium **THEN** Recurrence
IF *Neoplasm Cancer Code* Medium **THEN** Recurrence
IF *Subtype* Small **AND** *Ragnum Hypoxia Score* Small **THEN** Recurrence
IF *Cancer Type Detailed* Medium **AND** *Radiation Therapy* is True **THEN** Recurrence
IF *Cancer Type Detailed* Medium **AND** *Subtype* Medium **AND** *Fraction Genome Altered* Small **THEN** Recurrence
IF *Diagnosis Age* Medium **AND** *Radiation Therapy* is True **THEN** Recurrence
IF *Fraction Genome Altered* Small **AND** *Mutation Count* Small **AND** *Post Initial Therapy* is True **THEN** No Recurrence
IF *Buffa Hypoxia Score* Medium **THEN** Recurrence
IF *Neoplasm Cancer Code* Small **AND** *Buffa Hypoxia Score* Small **AND** *Winter Hypoxia Score* Small **THEN** Recurrence

As shown in Table 4 it is possible to notice that our model reaches a very similar accuracy to ML algorithms with feature selection and more explainability during the evolutionary process. Although the accuracy metric was not the highest, our model has one of the highest recall values, which can be desired in this kind of application. When the model fails with False Positive (Recurrence), it is possible to double-check either by the doctor or the patient. On the other hand, when the model fails with False Negative, a person with recurrence would be erroneously classified, which could lead to no further investigation related to its diagnosis. Therefore, our model prioritizes the False Negative due to the discovered rules, which is a better choice in the medical field.

Table 4. Comparison with ML algorithms

Method	Accuracy	Precision	Recall	AUROC
Random Forest	0.9420	0.9545	0.9310	0.9879
Logistic Regression	0.9710	0.9762	0.9655	0.9991
Support Vector Machine	0.9275	0.9444	0.9138	0.9948
Naive Bayes	0.9855	0.9878	0.9828	0.9914
K-Nearest Neighbors	0.9130	0.9232	0.9013	0.9500
Neural Network	0.9420	0.9385	0.9453	0.9966
CatBoost	0.9275	0.9444	0.9138	0.9806
XGBoost	0.9275	0.9444	0.9138	0.9357
Fuzzy-genetic (ours)	0.9130	0.8864	0.9750	

6 Conclusion and Future Work

According to the experiments, it is possible to notice that the best system found reached an accuracy of 91.30% in testing, using only eleven rules. One of the rules for no recurrence and 10 for a recurrence and all the rules uses 12 from the 18 attributes, and each rule uses a maximum set of 3 of those 12 selected by the evolutionary algorithm, which allows more confidence and ease for the system user when an inference is made.

In addition, the proposal performs a selection of input variables, as it seeks the least number of antecedents and the least number of rules for classifying prostate cancer. In the evolutionary process, it was found that the linguistic variables Sex, Ethnicity, Race, Aneuploidy Score, In PanCan Pathway Analysis and Prior Diagnosis was never used in any discovered rules, which means that it is not important to predict cancer recurrence.

The proposed model reaches a very similar accuracy to ML algorithms with more explainability and also has one of the highest recall value, which means that when the model usually fails with a false positive it provides a second chance for the patient to do a double check of the result.

In future work, the goal is to improve the result by trying other multi-objective techniques, using, for example, Pareto frontier [18]. Another approach is to use another evolutionary algorithm, such as Particle-Swarm Optimization, Ant Colony Optimization, Bee Colony Algorithm, and Bacterial Evolutionary Algorithm [14, 23] to search for a SIF with better interpretability in problems of higher complexity and a large number of input variables.

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