

Original Research Article

Receiver Operating Characteristic Optimization based on Convex Hull and evolutionary algorithm

ABSTRACT

Classification is basically a Multi-objective problem. The efficiency of classification vastly depends on performance of a classifier which can be evaluated on the basis of Receiver Operating Characteristic (ROC) graph, Area under Curve (AUC), and selection of different threshold values are generally used as a tool. In machine learning, generally, 2-D classifiers are available that deal with bi-objective problems where overlapping of class may occur i.e. sensitivity and specificity may overlap. Recently, multi-class classification in which classes are mutually exclusive is in research trends along with the evolutionary algorithm. The application of ROC graph is extended to evaluate multi-dimensional classification as it is cost sensitive learning. The goal of this paper is to gather recent achievements in the field at one place to analyze the classifier performance for multi-dimensional classification problems using convex hull and evolutionary algorithms. In this paper, we tried to cover all the existing recent advance techniques in maximization of ROC and proposed a convex hull and evolutionary algorithm based new model for ROC maximization.

Keywords: AUC, Convex Hull, Evolutionary Algorithm, Genetic Algorithm, Multi-objective Optimization Pareto Approximation, ROC.

1. INTRODUCTION

Classification plays a significant role in machine learning. This is because correct class uses the known example to determine which class the unknown example belongs to [9]. Classifier efficiency is assessed mainly on the basis of Receiver Operating Characteristics (ROC) curve and Area under Curve (AUC). ROC is widely used in the automatic detection of a signal, Data Mining, Medical Diagnosis, and many other disciplines [10]. For a safety perspective, the cost of making false classification has an negligible cost in case of life-threatening [2]. It limits and reduces the number of true classifications. The classifier and its operating parameters are selected in such a way that true positive rate (TPR) gets maximized and false positive rate (FPR) minimized [3]. ROC analysis produces a simple and convenient indication of trade-off between true and false classification rates [12]. Applicable to signal processing, machine learning, medical diagnosis system, and other classifications shows obvious reasons to have ROC analysis to be a prominent method for selecting operating points [1]. The trade-off between TPR and FPR makes ROC analysis could be approached as a Multi-Objective Optimization (MOO) problems.

The ROC graph is analyzed on the basis of confusion matrix representing accuracy, precision, sensitivity, and specificity produced by a classifier for a given dataset. Each classifier is characterized by a TPR and FPR. Representation

of points on the ROC graph where sensitivity plotted along X-axis and specificity as the Y-axis signifies the performance of a classifier.

Convex hull is the smallest convex polygon that encompasses every point in a specific set of points [7]. This algorithm computes the smallest convex polygon that is applied to the points produced by the classifier in the ROC curve. Its application on a set of points produced in the ROC graph poses a set of potential solutions for a given classifier [4]. The set of points on the ROC graph aids in visualizing the classification potential and in deciding which classifier to use, ensuring better classification outcomes. A classifier is assumed to be potentially optimal if all its points in ROC space lie on the convex hull; otherwise, there would be one possible classifier having a lower FPR with the same TPR or more TPR with at most the same FPR [4].

ROCCH (ROC-Convex Hull) poses a collection of optimal solutions in search space. Each solution among them is equally acceptable with a different attainable goal in mind. To address these types of multi-objective problems, we have two goals: One, finding the solution as near as possible to approach the Pareto front (Convex hull needed) and, two, solutions obtained should be as diverse as non-dominated solution possible (Genetic Programming Needed) [9].

We have two approaches: One, a traditional approach where the weighted sum is used to mold it into a single function and solved with a deterministic approach. These weight vectors are used for scaling the problems which influence the solutions. If the decision-maker needs one more resolution, it is unable to produce the second solution with the same efficiency, though, it assures less computational complexity. Two, to solve the population-based optimal solution sets, it is natural to use genetic algorithms to capture the number of solutions simultaneously and optimize them for better classification results [11].

Maximization of ROC is described as an optimization problem that aims to decrease the computational complexity by removing redundant points in calculating the Pareto front and increase the classifier efficiency by optimizing ROC [11]. So, it is essential to develop an efficient algorithm to classify the multi-dimensional data in machine learning as well as in data mining.

In the next section, various research papers applicable to classifier performance are studied. In subsection (a), an application of convex hull in ROC to analyze the Pareto-front of solution space has been studied. In subsection (b), some evolutionary algorithms applicable to the optimization of Pareto-front have been studied. In the next subsection, some important genetic algorithms are studied. Section contains the proposed model for enhancing the classifier and section concludes research with its future scope.

2. MATERIALS AND METHODS

We searched the classification maximization techniques with convex hull and genetic algorithms. Reviewing all related literature and analysing the results in them. We proposed an algorithm theoretically which may provide better results and hence maximize the classifier performance.

2.1. Literature Review

Pareto Front-based algorithms that are aspired to find the best solutions of a trade-off for the Receiver operating curve optimization problem. Convex Hull (CH) and Genetic algorithms (GA) are two important categories of algorithms to optimize the performance of a classifier. Convex Hull algorithm is used in selecting the solution points in ROC space. Evolutionary

algorithm, Genetic algorithm, Genetic Programming are applied in the sorting of a potential solution and finding an optimal solution.

2.1.1 Convex Hull

Convex Hull is used to enclosing ROC points with minimum connecting points which increase processing efficiency. It is a well-known computational geometry algorithm which is known for the application of geometry to solve computational problems. Here, we present a review of the application of the convex hull in the ROC curve.

Jiaqi Zhao et al.[11] proposed a 3D convex hull that produces convex hull volume that contains three objectives to be optimized. They used CCR (classifier complexity ratio) as the third constraint besides sensitivity and specificity. It works effectively in 3D ROC space also. Pu Wang et al.[12] presented a method for the selection of points on the ROC curve using the convex Hull algorithm in a binary classifier. It selects all front points which give a set of solutions for a given classifier. This method works effectively in selecting the Pareto front points.

Pietro Ducange et al.[13] used the convex hull in selecting a solution in classifier with three-objectives. Selected points are then optimized with a genetic algorithm. This method works effectively even on the optimization of the classifier with three-objectives.

Oswaldo Cadenas et al.[14] presented a parallel pre-processing method for reducing a set of n (2-Dimensional) points to a smaller set of S points with properties that allow the smaller data set to produce the same convex hull as the larger data set. The reduction in points was nearly ninety percent. The computational efficiency of convex hull computation is improved by using this method.

Peter A. Flach et al.[15] presented hybrid method for detection and repairing of concavity present in ROC curve by manipulating the predictions. To repair the concavity of a point in the ROC curve, each point is mirrored and calculated till the entire concave region below the convex hull gets mirrored. It ultimately improves the performance of a classifier.

Zhao et al. [17] reduced the computational costs by calculating redundant convex hull area or volume which helps in the calculation of non-dominated sorting. Incremental convex hull calculation with fast removal of non-dominated sorting has been introduced without affecting the result with less complexity.

Some important techniques which calculate the convex hull more efficiently are shown in Table 1.

Table 1. Some Important Techniques for Calculation of Convex Hull-based ROC.

Author	Application	Techniques	Results
Jiaqi Zhao et al.[11]	3D classifier.	3D Pareto Front Approximation.	It shows high performance in designing spam filters and finding a sparse neural network.
Pu Wang et al.[12]	2D classifier with Two Objectives.	Sorting based on Convex Hull without redundancy	It performs better than other non-dominating sorting algorithms.
Pietro Ducange et al.[13]	2D classifier with Three Objectives.	Fuzzy Rule Base Classifier.	It performs better in terms of AUCH except for the linear discriminant classifier for an Unbalanced Dataset.

Oswaldo Cadenas et al.[14]	Pre-processing of Data sets.	Parallel Processing.	It reduces time complexity to $O(n)$ without sorting.
Peter A.Flach et al.[15]	2D classifier with concavity removal.	Hybrid Model.	It produces encouraging results, particularly with the Naïve Bayes algorithm.
Zhao et al.[17]	3D classifier with incremental calculation.	Incremental Convex Hull Calculations.	It calculates convex hull approximately thirty times faster.

From the above discussions, it is obvious that the calculation of the convex hull affects classifier performance. It shows that the minimum number of points to be chosen to produce the same convex hull to decrease computational complexities lead to finding out the Pareto optimal solution efficiently in ROC space.

2.2.2 Evolutionary Algorithm Based Optimization

Here, we present a review of many different evolutionary algorithms based on MOO techniques to maximize the ROC curve of classifier.

S.Mane et al.[10] To solve the classification problem, a multi-objective evolutionary algorithm was used to optimize the neural network. To optimize the neural network, the Pareto approach is used. To optimize accuracy with mean squared error and local search at the same time, a non-dominated sorting genetic algorithm is used. The hybrid technique is used to overcome slow convergence in producing optimal solutions by augmenting an evolutionary algorithm with local search. Accuracy and mean squared error are considered as optimization goals. A hybrid evolutionary multi-objective framework is also introduced, which aids in faster convergence to Pareto optimal solutions using local search techniques. This framework could also be used for unbalanced data sets.

Marco Barreno et al.[13] presented a systematic analysis of a combination of binary classifiers has been done on the theoretical basis of Neyman-Pearson lemma which is a hypothesis testing of two simple hypotheses with some threshold value which rejects H_0 in favor of H_1 at a given significance level of α with a given likelihood ratio. Then, the lemma states that is the most powerful test for its size. It gives a method to find the optimal decision rule of a combined classifier and generated ROC is proved to be optimal.

Pietro Ducange et al.[14] proposed an evolutionary algorithm for optimization of classifier with three objectives. It is applied for approximating of Pareto front composed of the fuzzy rule-based classifier. The trade-off occurs among three objectives namely sensitivity, specificity, and complexity which is expressed as the sum of the conditions in the antecedents of classifier rules. To elect the potentially optimal classifier in Pareto front approximation, ROCCH method is employed. Wilcoxon test shows, this method produces a second good result with unbalanced datasets after AUC in the calculation of misclassification cost.

Jiaqi Zhao et al.[17] proposed three dimensional-ROC with three objectives namely false positive rate (FPR), false negative rate (FNR) and classifier complexity ratio (CCR) as the additional third objective. On contrary to use ROC to optimize classification costs, Detection error Trade-off (DET) has been used here to optimize the misclassification costs. DET is the space encompassed between the ROC curve and the convex hull based Pareto Front. To make non-dominated sorting more efficient, convex hull based multi-objective programming applied. A sparse neural network has been applied to optimize the network structure as well as a classifier.

Marco Cococcioni et al.[18] A population-based multi-objective evolutionary algorithm (MOEA) with TPR and FPR was proposed as a measure for comparing classifier performance for binary classifier optimization. MOEAs select the fuzzy rule-based classifier by balancing FPR and TPR. There are two approaches for solving multi-objective optimization (MOO). The first is the preference-based approach, which requires the decision-maker (DM) to provide comprehensive information about the problem. DM weights the function based on prior knowledge. This problem information causes the solution to converge to a function of weighted sum, which can be solved using any other method, such as direct, iterative deterministic, or stochastic. Two, in an Ideal approach, DM does not use weight, so all solutions are equally optimal. The Pareto Front is the collection of all equally optimal solutions. However, it is more time consuming. To overcome time complexities, hybrid approach which combines the above two approaches is to detect the class and for automatically classification, fuzzy rule has been implemented. And to analyze the ROC curve, DM uses a weighted sum of FPR and TPR to calculate error cost of binary classifiers. Since the optimal solution belongs to the superior part of the convex hull and others are sub-optimal, Pareto front approximation reproduced by this hybridized approach. These two approaches outshine the state of art NSGA-2 algorithms in the detection of Lung Nodule from Non-Lung Nodule.

Michael C. Mozer et al. [19] designed a classifier to maximize the ability to discriminate two classes with an additional constraint with correct acceptance and correct rejection. A classifier is applied in predicting the churn (moving from one service provider to others) in the telecommunication industry. It proposes four algorithms for training of classifiers based on their constraints. One, it emphasizes critical training of datasets where classifier gets trained with positive and negative and classifiers to assign a posterior probability of membership class. Each member is arranged according to a posterior probability value. This step makes classification work easy for classifiers. Two, it de-emphasizes irrelevant data. In this algorithm, data with more difficulty in classify them correctly, that data could be left out to achieve the correct acceptance rate and correct rejection rate. Three, for optimizing the constraint to maximize the correct acceptance rate while maintaining the threshold acceptance to acceptance rate. Four, Steady-state Genetic search is used algorithms are used to find the fitness of classifiers. This shows the real-world problem of telecommunication and its specific nature. Although the Churning problem has been assumed as static this is not in reality.

V. Mingote et al.[20] presented signal representation of face verification with the help of deep learning and is used to verify speaker. This paper deals with the generation of signal for subject identity and uttered the phrase. The matrix produced is better suited to train a system for detection tasks. It proposed three objectives in ROC i.e. sensitivity, specificity, and loss function. The loss function is maximize and minimize inter-speaker and intra-speaker similarity respectively. The goal of keeper speaker and phrase information is to attain the correct verification process. For the creation of a super vector, Gaussian mixture model is used which provides better performance in speaker verification.

Lars Graving et al.[21] improved multi-objective learning with the help of multi-objective optimization algorithm to optimize the structure and weight of Neural Network classifier based ROC to solve binary classifier tasks. The objective is to maximize TPR and minimize FPR. A multi-objective framework with an evolutionary algorithm improved the efficiency of generalization ability as compared to the single objective optimization algorithm. Although existing generalization improving techniques are like early stopping, regularization network pruning, and weight decay are some of them for single objective optimization algorithms. Almost all the existing method works on single objective learning like gradient-based

algorithm, cannot be ideal with the multiple learning, but most of the machine learning problems are multi-objective.

Pu Wang et al.[22] introduced a multi-objective genetic programming method based on convex hulls without redundancy (CWR-Sorting) and area base contribution indication to obtain the Pareto front and maximize the CH-ROC. Multi-objective programming seeks the Pareto front to maximize the accuracy of each data sample. The results show that NSGA-II (Non-Dominating Sorting Genetic Algorithm) combined with GP and information entropy-based local search operators is the best MOGP for maximizing ROCCH so far. Regardless of the fact that it is not a reliable method for dealing with skewed class distributions and various misclassification costs. The Pareto front resembles ROCCH but not evolutionary multi-objective algorithms. Some ROCCH features, such as point lie in concavity, provide accurate approximation values, whereas combining two classifiers results in a virtual dominating point. As a result, the computational resources spent on approximating the concave parts are better spent on approximating only the convex hull parts of the Pareto front. When combined with an area-based contribution selection scheme that improves classifier performance, CWR- Sorting improves CH-MOGP for maximum ROCCH performance.

The application of Genetic Algorithms in a multi-dimensional classifier to achieve different objectives is shown in table 2.

Table 2. Some Important Genetic Algorithms For Solving Multi-Objective Optimization Problems.

Reference	Techniques	Remarks
S.Mane et al.[10]	A combination of the Genetic Algorithm and the Local Search Algorithm.	It brings faster convergence to Pareto optimal solution.
Marco Barreno et al.[13]	Combining Two Classifiers	It shows better performance than base classifiers theoretically.
Pietro Ducange et al.[14]	Pareto-Front Approximation Method	Wilcoxon signed-Rank test shows better results for all known techniques except the AUC of the ROC curve with three objectives.
Jiaqi Zhao et al.[17]	Sparse Neural Network Algorithm.	It shows promising results in Spam filtering and multi-objective optimization of a sparse neural network, although more time-consuming.
Marco Cococcioni et al.[18]	Hybrid of preference and Ideal based Approach	CHEA(Convex Hull based Evolutionary Algorithm) performs better than NSGA- II in terms of front Generation.
Michael C.Mozer et al. [19]	Steady-State Genetic Search Algorithm	It shows modest improvement in performance but impressive results in financial return in Telecommunication.
V.Mingote et al.[20]	Deep Neural Network Model	It shows a competitive result for text-dependent speaker verification to global average pooling.
Lars graining et al.[21]	Optimized Structure and weights of Neural Network	It suggests that for optimization, Pareto-based multi-objective learning should be preferred over single-objective learning.
Pu Wang et al.[22]	Convex Hull based Multi-objective genetic programming.	It outperforms than a fast non-dominating approach while maintaining diversity in the search process.

From the above discussions, It is obvious that the selection of optimal solution points in ROC space affects the classifier accuracy. It shows points that approximate the Pareto optimal solutions for a given dataset. It assures better accuracy in classification.

Discussing the above algorithms, we try to tabulate the algorithms below to analyze the performance of a classifier by optimizing ROC. We split the classifier analysis into two parts, in which the first part points are plotted in the ROC plane. Points on the convex hull give empirical solutions. In the second part, these points on the convex hull act as population. Genetic algorithms are applied to find either approximate or best solutions for a given problem.

3. PROPOSED MODEL AND ALGORITHM

We propose CRESNA (**C**onvex **H**ull **R**OC **E**volutionary **S**parse **N**eural **A**lgorithm) a **R**apid **P**rototypical **D**esign for optimization of ROC curve.

The working of a classifier is could be analyzed into two steps: One, Formation of convex hull based ROC and Two, an approximation of solutions. In the proposed method, the selection of a potential solution is done by the convex hull algorithm, and the selection of the Pareto optimal solution is done by a genetic algorithm. The working steps are as follows:

- Three features are selected of each entity from a dataset collected from the data center so that each feature represents a different dimension of the problem.
- Features are represented in the 3D- ROC plane for each entity. Points representing features are pre-processed such that a minimum number of points could form the convex hull equivalent to the convex hull without minimization as suggested by [14].
- The Pareto Front produced by the convex hull is taken as input to the sparse neural network (genetic algorithm).
- Sparse neural network-based genetic algorithm to approximate and produce the Pareto optimal solutions.

The overall methods of the proposed system for classifier performance enhancement are shown in Figure 1.

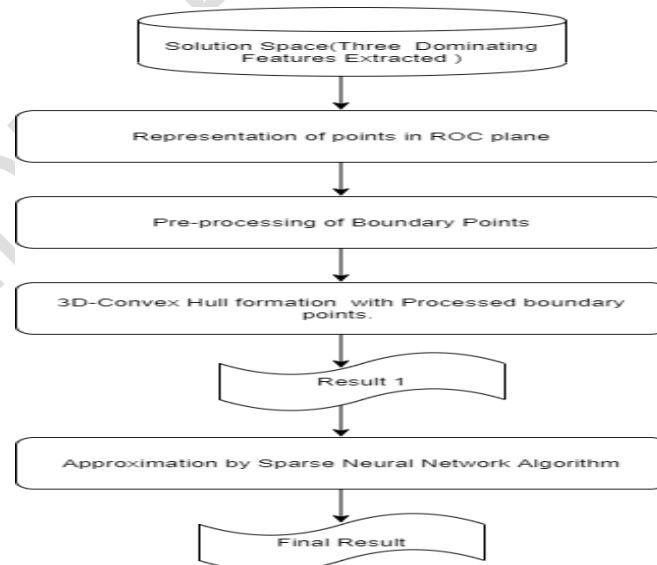


Figure 1. Proposed Method for Classifier Enhancement.

Result-1 is the outcome from the 3D-Convex Hull, which takes a minimum number of pre-processed points with all three features. Whereas the final result shows the approximate or the best solution to the problems among the solution set obtained in result 1.

3.1 Algorithm

The following are the steps of the proposed CRESNA.

1. Create an ROC of certain values defining actual and predicted values of a classifier.
2. Create a convex hull of the points of an ROC.
3. Pass the convex hull as an input to a sparse neural network.
4. Predict a distance measure of the convex hull as per the sparse neural network.
5. Maximize the distance measure of convex hull of a set of collection of points through iteration.

3.2 Pseudo code for algorithm

1. curr_dim_max = 0.0
2. num_intelligent_iterations = 10
3. false_positive_nums, true_positive_nums = calculate_roc
4. For i = 1 ... number_of_intelligent_iterations
 - a. false_positive_nums_new, true_positive_nums_new = calc_roc_from_false_true(false_positive_nums, true_positive_nums)
 - b. pts = get_roc_points(false_positive_nums_new, true_positive_nums_new)
 - c. cch = calculate_convex_hull(pts)
 - d. curr_esna = ESNA(chh)
 - e. curr_esna.select()
 - f. curr_esna.crossover()
 - g. curr_esna.mutate()
 - h. if (curr_esna.dim > curr_dim_max)
 - i. curr_dim_max = curr_esna.dim
5. print("Max dim: " + str(curr_dim_max))

4. RESULTS AND DISCUSSION

We used Google Colab, python 3.7 and a set of user input data for the application and primarily tested CRESNA for maximizing the ROC curve. We take input data and plot, and a convex hull algorithm is applied. The following is a plot of the convex hull of some random points which is taken as input for CRESNA.

Convex hull computation

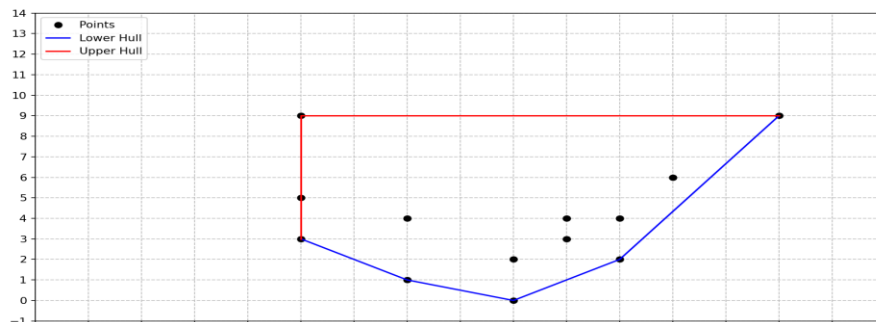


Figure 2. Sample Convex Hull

The application of CRESNA algorithm on a set of random user points that is visualized in figure 2 with application of convex hull on a given set of points. In the next figure a plot of ROC (Receiver Operating Characteristics) for sample data is shown

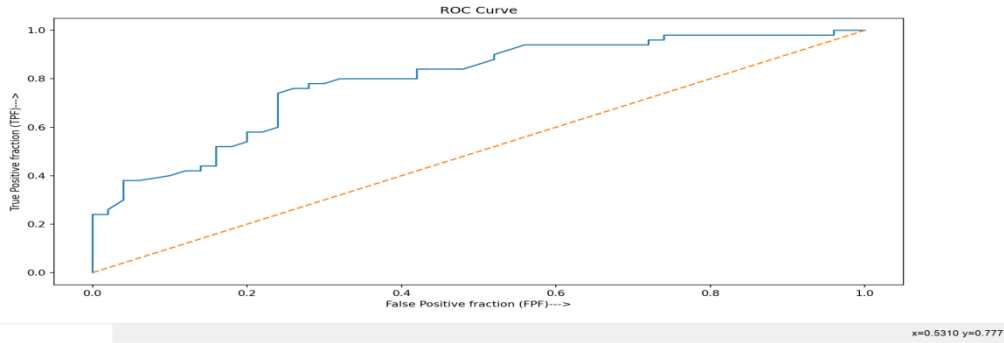


Figure 3. Sample ROC

The following are output from the running of the algorithm. The convex hull depicts the points on the current convex hull in the current iteration of the algorithm. curr dim is a measure of the current ROC and Max dim is the maximum of measure of all the ROCs.

Convex Hull:

0.0,0.0

0.8466781553257862, 0.033932858015801926

0.8466781553257862, 0.033932858015801926

0.2641281379865426, 0.7633895371157465

0.129266446936988, 0.7936198309318685

0.034825420536414284, 0.686166189223361

0.0, 0.18746674852676878

0.0, 0.0

currdim : 0.4020392550336473

Convex Hull:

0.0, 0.0

0.07839162398765578, 0.0011330295192540252

0.33889936313025815, 0.14120946975979282

0.877947580954117, 0.9725877939685567

0.877947580954117, 0.9725877939685567

0.0012526508839545425, 0.8128082316208435

0.0, 0.09273541699749133

0.0, 0.0

currdim : 0.4193444358465877

Max dim: 0.7045540334798165

The convex hull depicts the points on the current convex hull in the current iteration of the algorithm. curr dim is a measure of the current ROC and Max dim is the maximum of

measure of all the ROCs. currdim : 0.4193444358465877,Max dim: 0.7045540334798165 respectively with percentage increase of 0.6801320662749163663.

4.1 Discussion:

The CHRESNA algorithm gives all round fast performance when measuring the following

- ROC
- Convex Hull
- Maximum of the ROC

Improvements to the algorithm can be done by introducing moderate to medium and large level of complexity in terms of calculation of a measure of the ROC.

Suitable measures for the calculation of the ROC might include intricate statistical measures.

5. CONCLUSION AND FUTURE SCOPE

This paper aims to gather recent achievements to augment the classifier performance with a convex hull-based selection of potential solutions set in the ROC curve and optimize the possible solution by a genetic algorithm to maximize ROC, eventually enhancing classifier performance. Although, the result obtained is based on user random input. In the subsequent publication, we use proper data and ROC maximization results based on the CHRESNA algorithm. We want to extend this concept to solve classification problems in the future.

CONSENT (WHEREEVER APPLICABLE)

We declare that 'written informed consent was obtained from the patient (or other approved parties) for publication of this case report and accompanying images. A copy of the written consent is available for review by the Editorial office/Chief Editor/Editorial Board members of this journal.

ETHICAL APPROVAL (WHEREEVER APPLICABLE)

We hereby declare that "Principles of laboratory animal care" (NIH publication No. 85-23, revised 1985) were followed, as well as specific national laws where applicable. All experiments have been examined and approved by the appropriate ethics committee.

We hereby declare that all experiments have been examined and approved by the appropriate ethics committee and have therefore been performed in accordance with the ethical standards laid down in the 1964 Declaration of Helsinki.

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