

Exploring the Hidden Challenges Associated with the Evaluation of Multi-class Datasets using Multiple Classifiers

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Abstract – The optimization and evaluation of a pattern recognition system requires different problems like multi-class and imbalanced datasets be addressed. This paper presents the classification of multi-class datasets which present more challenges when compare to binary class datasets in machine learning. Furthermore, it argues that the performance evaluation of a classification model for multi-class imbalanced datasets in terms of simple “accuracy rate” can possibly provide misleading results. Other parameters such as failure avoidance, true identification of positive and negative instances of a class and class discrimination are also very important. We, in this paper, hypothesize that “misclassification of true positive patterns should not necessarily be categorized as false negative while evaluating a classifier for multi-class datasets”, a common practice that has been observed in the existing literature. In order to address these hidden challenges for the generalization of a particular classifier, several evaluation metrics are compared for a multi-class dataset with four classes; three of them belong to different neurodegenerative diseases and one to control subjects. Three classifiers, linear discriminant, quadratic discriminant and Parzen are selected to demonstrate the results with examples.

Index Terms— Classifier evaluation; multi-class dataset; pattern recognition; neurodegenerative diseases; multiple classifiers

I. INTRODUCTION

There are several ways to evaluate the performance of learning algorithms. Most often, the evaluation is based on a *confusion matrix* to represent the results in terms of accuracy and a classifier’s ability to correctly and incorrectly classified instances of a class [1].

This evaluation technique becomes more complex and intricate when multi-class pattern recognition is required. This is because the continuous growth of biomedical data has largely deteriorated the performance and accuracy of many evaluation techniques [2]. These problems are largely seen in our modern life, for instance, web page classification [3], web spam detection [4], and medical diagnosis [5], [6]. Some of the other fields that involve the analysis of enormous multi-class datasets are mobile commerce [7], bankruptcy or credit detection [8], fraud detection, and crime activity analysis.

Moreover, with the traditional empirical measure, “accuracy rate”, it is difficult to distinguish patterns in multi-class datasets. For instance, misclassification of *true positive* instances should not necessarily be considered a *false negative* when a multiclass dataset is being evaluated. More specifically, multi-class datasets offer more complexities and challenges while ranking the reliability of a particular classification model. This paper discusses some of these challenges when multi-class dataset are evaluated.

To demonstrate the uncertainty among results, a 4-class dataset has been selected which belongs to neurodegenerative diseases (NDDs) and control subjects, as a case study. NDDs is an umbrella term used to describe medical conditions that directly affect the neurons within the brain [9]. These include Parkinson’s disease (PD), Alzheimer’s disease (AD), Huntington disease (HD), and Amyotrophic Lateral Sclerosis (ALS) among others. Patients suffering with these kinds of disease, experience a cognitive decline over a long period and symptoms include gait abnormalities, problems with speech, and memory loss due to progressive cognitive deterioration [10]. Analysing gait signals to recognize relevant patterns and correlations with specific neurodegenerative diseases is one of the most challenging tasks that will be considered in this paper using various evaluation techniques. This research work is an extension of previous published work [11], [12], which discussed the classification of gait patterns in neurodegenerative diseases and their relationship with brain activity. A set of 11 well-known classifiers on a dataset of healthy and sick persons is considered. Three classifiers have performed comparatively better than the remaining eight and are used to discuss classification accuracy, Precision, Recall, Sensitivity, Specificity, F-Measure, ROC and Reject Curves [13],[1].

This paper highlights the shortcomings and weaknesses of existing evaluation techniques to evaluate the performance of multi-class datasets. The main idea is to bring forward those attributes that are important to generalize the performance of a particular classification model and to provide a future research direction in this regard. Moreover, it also presents an overview of well-known evaluation measure for multi-class dataset with multiple classifiers.

The rest of the paper is structured as follows; Section II describes the hidden challenges that should be addressed in multi-class pattern recognition. Section III lists the features that are used for classification, followed by the description of classification models that are used for simulation in Section IV. Section V narrates commonly used classifier evaluation measures and their results on a multi-class dataset while the results are discussed in Section VI with conclusion.

II. CHALLENGES WITH MULTI-CLASS SKEWED DATASETS EVALUATION

Evaluation of a classifier is considered important for making decisions in data mining [14]. There are many classifier performance metrics that claim to be better than other evaluation techniques [13]. One particular performance measure may evaluate a classifier from a single perspective and often fail to measure others [15]. Consequently, there is no single rule that successfully covers all performance issues regarding a classifier's evaluation.

In practice, there are several multi-class domains that belong to real world applications [16]. For instance, text categorization, and protein fold classification where a protein may retain more than one subcellular locations [17], [18], [19] *etc.* These multiclass datasets pose new challenges compared to simple two-class problems. Zhou *et al.* [20] argue that handling multi-class datasets is much harder than handling two-class problem domains. Furthermore, almost all classifier evaluation techniques are designed for two-class problems that cannot be used in multi-class problems. They are less effective and in some cases show negative impact on multi-class data evaluations.

Furthermore, learning from skewed dataset distributions, where one class has more subjects (majority class) as compared to the other class (minority class) produce misleading results [21], [22], [14]. In this case the classification model becomes more sensitive to recognize the majority class patterns as compared to the minority class patterns. These kinds of results ultimately cause more destruction if data comes from real time environments, such as biomedical, genetics, radar signals, intrusion detection, risk management and credit card scoring [23], [24]. Especially, in the field of bioinformatics where patient's class usually has less data as compared to the class of control subjects [25].

Instead of providing comprehensive solutions for multi-class imbalanced datasets, most attention in the literature focuses on class decomposition [26]. In this case ($K > 2$) class problems are solved by generating all possible pairwise binary class classifiers between K classes [19]. Eventually, the final

decision of a class is made by following one-against-all or by one-vs.-others rule [27]. This approach does not provide the desired output because votes of the correct class are randomly distributed among other classes due to imbalanced distributions. Moreover, results derived from sub-classes can cause potential classification errors [28, 29].

Compounding the problem further, in the realm of all the issues related to classifier evaluation, existing evaluation measures do not fully explain the hidden facts of the results. A common practice that has been considered to generalize the reliability of a classifier is *accuracy rate*; this offers serious shortcomings because it does not take misclassification cost into consideration [15]. This paper argues that while evaluating a multi-class dataset, results could not simply be presented in terms of true class identification. Further investigations are important to identify the mislabelling of a single instance and its final class decision before concluding the authentication of a particular classifier.

III. DATASETS AND DATA PREPROCESSING

The dataset is a collection of prior knowledge (age, gender, height, weight, BMI, walking speed and time) with empirical knowledge (sensory measurements for right and left foot signals) to get a posterior knowledge to recognize gait patterns of a disease as shown in the Figure 1.

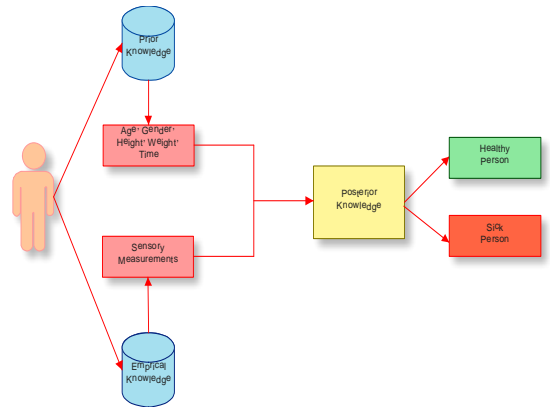


Figure 1: Extraction of Posterior Knowledge from Prior and Empirical Knowledge

Table I shows a set of eight (8) features that are used as an input for classification. We have a dataset of right and left feet gait signal values for control subjects and those that are sick. Within the dataset other clinical information for each subject, including age, gender, height, weight, walking speed, disease severity or duration and BMI are considered to improve the accuracy and reliability of the classification results. Additional

TABLE I: A SET OF EIGHT FEATURES USED FOR CLASSIFICATION

Right Feet Signals	Left Feet Signals	Age	Height	Weight	Time	Walking Speed	BMI
Motion Vectors in Millisecond	Motion Vectors in Millisecond	20-80 (Years)	1.57-2.13 (Meters)	40.82-117.5 (Kg)	10 Sec	0.5-1.82 (m/sec)	14.4-37.1 (weight(kg) / height ² (m ²))

data is simulated to solve the problem of skewed datasets (*Oversampling* for the minority class where we, at first, determine the maximum and minimum values of each feature set and then randomly generate more data between these two data points for the minority class [12]). The resulting dataset is an 80x8 matrix where we have 20 subjects in each class.

IV. CLASSIFIERS AND THEIR IMPLEMENTATION

Using the defined feature set, eleven classifiers have been implemented for a comparison of evaluation techniques. The principle goal is to use classifiers that perform the best. The classifiers considered are the Linear Discriminant Classifier (ldc), Quadratic Discriminant Classifier (qdc) and the Quadratic Bayes Normal Classifier (udc) based on Bayes Normal classification. For Linear Classification, an additional four classifiers are selected, that are Logistic linear (logic), Fisher's (fisherc), Nearest Means (nmc) and the Polynomial (polyc). A linear classifier predicts the class labels based on a weighted linear combination of features or the pre-defined variables. The Parzen (parzenc), Decision Tree (treec), Support Vector Machine (svc) and k-Nearest Neighbour (knnc) classifiers have been selected for non-linear classification of our datasets.

The results produced by all eleven classifiers are illustrated in Figure 2. These results were evaluated using a confusion matrix table to determine the performance of each classifier. In this instance, the Confusion Matrix technique was used to determine the distribution of errors across all classes.

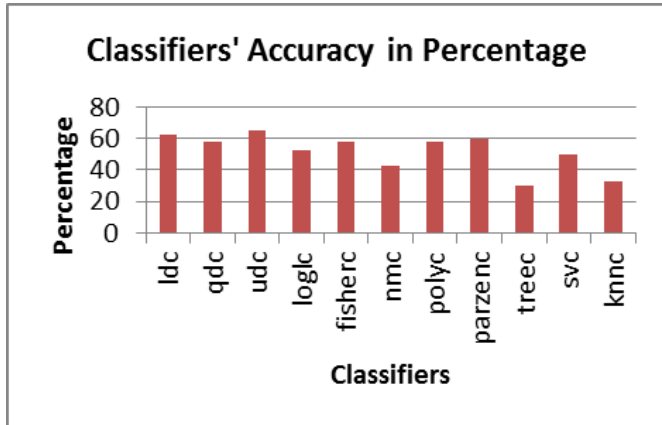


Figure 2: Classification Accuracy for 11 classifiers

Three classifiers that have given comparatively better results are selected for a comparison of evaluation techniques. Those classifiers are Bayes Quadratic classifier (udc), Linear Discriminant Classifier (ldc) and Parzen Classifier (parzenc) with accuracies of 65%, 62.5%, and 60% respectively.

V. CLASSIFIER PERFORMANCE METRICS

The performance evaluation of a classifier is mostly done by a parameter called the decision threshold, t ($0 \leq t \leq 1$), which decides the final class membership of a given object [13, 30]. A class with a higher posterior probability of this

threshold is assigned to a particular object. This threshold value may vary for imbalanced and multiclass datasets.

Two different kinds of measures are used to compare the performance evaluation results of all these classifiers:

1. *Visualization*: representing the possible outcome of true and false values of a classifier in the form of graphs; Reject and ROC curves
2. *Statistical Analysis*: to compare the evaluation results by mathematical formulas such as classification accuracy (Confusion Matrix), Precision, Recall, Sensitivity, Specificity and F-Measure

Here is a brief description of the above mentioned performance evaluation measures that have been articulated in this research work.

A. Confusion Matrix

The Confusion Matrix determines the distribution of errors across all classes [31]. The estimate of the classifier is calculated as the trace of the matrix divided by the total number of entries.

$$\text{Confusion Matrix} = \frac{TP+TN}{TP+FP+TN+FN} \quad (1)$$

B. Precision

Precision is a function of true positive values and the objects that are misclassified as positive i.e. false positive.

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

C. Recall/Sensitivity and Specificity

Recall presents a function of correctly classified objects i.e. true positives and false negatives while *specificity* describes the results in terms of true negative values.

Both Recall and Precision are relevant to each other. Precision is the fraction of retrieved information relevant to the search while Recall is the fraction of the information related to the search query that is retrieved successfully [14, 32]. The formulas for Sensitivity and Specificity are given below:

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

$$\text{Specificity} = \frac{TN}{TN+FP} \quad (4)$$

TABLE II: RESULTS OF EVALUATION TECHNIQUES ON MULTI-CLASS DATASET

	UDC	LDC	PARZEN

Confusion Matrix	65%	62.5%	60%
Precision	86.36%	85.71%	85%
Recall/Sensitivity	63%	60%	56%
Specificity	70%	70%	40%
F-Measure	72.72%	70%	67%
Type I Error	36.6%	40%	43.3%
Type II Error	30%	30%	60%

D. F-Measure

F-Measure is another common evaluation metric that combines precision and recall into a single value. In other words it provides the percentage of the instances that are truly classified by a classification model [33], [34]. The formula is:

$$F - Measure = 2X \frac{Recall \times Precision}{Recall + Precision} \quad (5)$$

Table II describes the results of the above mentioned evaluation techniques, in percentages, for three selected classifiers.

E. ROC and Reject Curves

In this paper we visualize the Receiver Operating Curve (ROC) for Error Type I and Error Type II [35]. The curve is drawn for “False Positive” and “False Negative” values as Error Type I represents the “false positive” values while Error Type II represents the “false negative” values that a classifier predicts during the classification of a dataset. Results in terms of ROCs curve are presented in Figure 3.

$$Type\ I\ Error = \frac{FN}{TP + FN} \quad (6)$$

$$Type\ II\ Error = \frac{FP}{TN + FP} \quad (7)$$

Another common approach is the Reject curve which works on reducing the error cost by turning them into a rejection [36]. In this case the objects close to the decision boundaries are not classified. Reject curve for all three classifiers is presented in Figure 4.

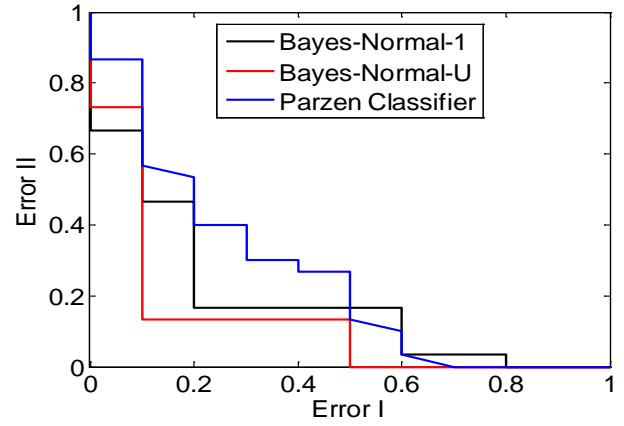


Figure 3: Receiver Operating Curve for Classifier's Evaluation

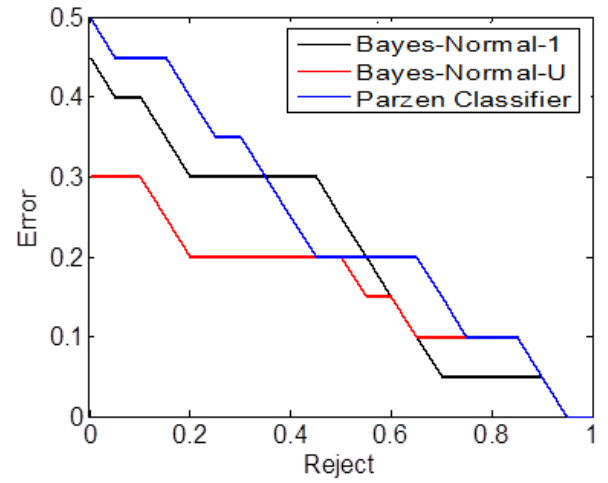


Figure 4: Rejection Curve for Classifier's Evaluation

VI. DISCUSSION AND CONCLUSION

All the above mentioned evaluation techniques have their own importance in analysing a classifier's performance. All different techniques have confirmed that the best classifier for analysing gait patterns for NDDs patients is Bayes Normal Density based classifier with un-correlated variables (*UDC*) due to a quadratic decision boundary. Table II shows that the percentage of *recall* for the Quadratic classifier is higher than precision. This indicates that 95% of patterns in the dataset are recognized as related to some disease or control subject while 86.36% are correctly classified to its specific class. In case of curve analysis the Bayes classifier (red line) is showing the least error compare to others, both for the ROC and Rejection curve.

Given the nature of the multiclass datasets it is difficult to compare the results with the previous findings, where most of the time, the analysis is for 2-class datasets. However, the results can be elaborated from a different perspective. The accuracy rate (calculated from confusion matrix) is 65%, 62.5% and 60% for *UDC*, *LDC* and *Parzen* classifiers, respectively.

In term of *sensitivity* and *specificity*, it is actually quite difficult to calculate *true positive* and *false positive* values because of three different NDDs. The *sensitivity* of *UDC* in terms of (CO-HD), (CO-PD), and (CO-ALS) is 90%, 50% and 50%, respectively. While the overall *sensitivity* for all 4-class datasets is 63%. Similarly, for *LDC* it is 40%, 80% and 60% for (CO-HD), (CO-PD), and (CO-ALS), respectively. Nonetheless, the overall percentage is 60%. In the case of *Parzen*, the overall *sensitivity* is 56%. Working on the same line, the *specificity* for individual diseases can be calculated. However, the overall percentage is 70%, 70% and 40% for *UDC*, *LDC*, and *Parzen* separately.

Similarly, the precision of *UDC*, *LDC*, and *Parzen* is 86.36%, 85.71%, and 85%, respectively. F-measure is calculated through *sensitivity* and *specificity*, which is 72.72%, 70% and 67% for *UDC*, *LDC*, and *Parzen* respectively. Furthermore, Table II also reveals the *false negative* and *false positive* values for all classifiers in term of Error type I and Error type II.

As a preamble to our argument, a conjecture has already been postulated in the beginning that “a misclassification of true positive instance should not necessarily be considered a false negative when it comes to multi-class pattern recognition”. This indicates that all classes are of equal importance and yet must be distinguished. This has been clearly evident in the screen short of a *confusion matrix* (Figure 5) where 1 indicates CO, 2, 3 and 4 indicate HD, PD and ALS respectively.

For instance, while recognizing the gait patterns of HD subjects (column 2 in Figure 5), 5 out of 10 are distinguished as *true positive* and the remaining 5 are misclassified. But interestingly, the rest of the 5 are not categorized as *false negative* rather 3 of them miss-classified to PD, 1 as ALS (other NDDs) while only 1 is *false negative*.

True Labels	1	2	3	4	Totals
1	7	1	2	0	10
2	1	5	3	1	10
3	0	1	9	0	10
4	0	2	3	5	10
Totals	8	9	17	6	40

Figure 5: Screen Short of Confusion Matrix for UDC

Working on the same line, while classifying Parkinson patients, 9 out of 10 are classified as PD while none of the instances is classified as *false negative*, as shown in the column 3 of Figures 5. Similarly, only 5 ALS patients are positively classified (*true positive*) while the rest of the five are either misclassified as HD or PD, and none of the instances is classified as *false negative* as shown in the column 4 of Figure 5. This has clearly given a new dimension to our results.

This is further verified from the *confusion matrix* results of *LDC* and *Parzen* classifiers as shown in the Figure 6 and Figure 7 respectively.

True Labels	1	2	3	4	Totals
1	7	1	1	1	10
2	3	4	2	1	10
3	0	1	8	1	10
4	1	1	2	6	10
Totals	11	7	13	9	40

Figure 6: Screen Short of Confusion Matrix for LDC

True Labels	1	2	3	4	Totals
1	7	2	0	1	10
2	3	5	1	1	10
3	1	0	8	1	10
4	2	3	1	4	10
Totals	13	10	10	7	40

Figure 7: Screen Short of Confusion Matrix for Parzen Classifier

According to this justification, the new calculation says that *sensitivity* of the *UDC* classifier is $(19/19+1) \times 100 = 95\%$ which is highest comparing to the literature so far. Similarly, for *LDC* and *Parzen* is 81.8% and 74%, respectively.

Even the ROC curves are hard to compare using different classifiers for different misclassification costs and class distributions. Here, we have analysed an equal number of objects for each class to avoid misclassification and bias results due to skewed datasets.

In this paper we have discussed the challenges and complexities related to performance evaluation techniques for multi-class pattern recognition with multiple classifiers. We have demonstrated using a *confusion matrix* how some important features get neglected while evaluating the performance of a classification model based on a simple *accuracy rate*. In future work, we intend to consider new measures that best evaluate a multi-class dataset such as *Youden's index*, *likelihood* and *discrimination power* focusing on failure avoidance or class discrimination.

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