PROTOTYPE SELECTION IN IMBALANCED DATA FOR DISSIMILARITY REPRESENTATION
A Preliminary Study

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Abstract: In classification problems, the dissimilarity representation has shown to be more robust than using the feature space. In order to build the dissimilarity space, a representation set of *r* objects is used. Several methods have been proposed for the selection of a suitable representation set that maximizes the classification performance. A recurring and crucial challenge in pattern recognition and machine learning refers to the class imbalance problem, which has been said to hinder the performance of learning algorithms. In this paper, we carry out a preliminary study that pursues to investigate the effects of several prototype selection schemes when data set are imbalanced, and also to foresee the benefits of selecting the representation set when the class imbalance is handled by resampling the data set. Statistical analysis of experimental results using Friedman test demonstrates that the application of resampling significantly improve the performance classification.

1 INTRODUCTION

Classification is one of the key tasks in many pattern recognition applications, which mainly consists of predicting the categorical or numerical class of a given input object. Usually, one of the main goals in data classification is to obtain high accuracy, where the object representation and the classification model play an important role.

In traditional pattern recognition approaches, objects are represented in a feature space, i.e. by attribute vectors (Duda et al., 2001). In the dissimilarity space, unlike the feature space, objects are represented by pairwise of dissimilarities. The dissimilarity representation has shown to be more robust to distinguish among classes than in the feature space, since the nearness provides more discriminative information of each object (Pekalska and Duin, 2006).

Additionally, an study (Pekalska et al., 2002) showed that for a complex problem in a 2D space, a non-linear classifier was required in the feature space to reach the same performance obtained by a linear classifier in the dissimilarity space.

In the dissimilarity representation, the classifier is constructed using a training set and a set of prototypes, known as the *representation set*. Then, the dissimilarity space is built by a dissimilarity measure to the set of chosen representation objects. Several methods for prototype selection have been proposed in the literature (Pekalska et al., 2006; Pekalska and Duin, 2002a; Pekalska and Duin, 2002b; Jacobs et al., 2000; Lozano et al., 2006) and the classification accuracy may be affected depending on the method used. In addition, data complexities may also affect the classification performance.

A recurring complex situation in the data sets refers to the presence of severely skewed class priors, which is generally known as the class imbalance problem (Fernández et al., 2011). A data set is said to be imbalanced when one of the classes (the minority one) is heavily under- represented in comparison to the other (the majority) class. It has been observed that class imbalance often leads to poor classification performance in many real-world applications (Blagus and Lusa, 2010; Chandola et al., 2009; Kamal et al., 2009; Liao, 2008), especially for the minority classes. This topic is particularly critical in those applications where it is costly to misclassify minority examples.

Research on this topic has primarily focused on the implementation of solutions for handling the imbalance both at the data and algorithmic levels. Other investigations have addressed the problem of measuring the classifier performance in imbalanced domains. Also, the relationship between class imbalance and other data complexity characteristics has been analyzed. From these three general topics in class im-

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balance, data level methods are the most investigated. These methods consist of balancing the original data set, either by over-sampling the minority class and/or by under-sampling the majority class, until the problem classes are approximately equally represented.

Although class imbalance has been extensively studied for binary classification problems, very few approaches explore the class imbalance problem in the dissimilarity space (Koknar-Tezel and Latecki, 2011; Sousa et al., 2008b; Sousa et al., 2008a). In this particular context, some works have used dissimilarity based-classification as a tool to deal with imbalanced data sets (Sousa et al., 2008b; Sousa et al., 2008a).

In the present work, we study the effectiveness of some prototype selection methods required for selection or creation of the representation set when the data set is imbalanced. We also explore on the combined use of some of them and resampling techniques to enhance the classification results. To this end, we will carry out several experiments over real data sets using four prototype selection methods taken from the literature, when employing the Nearest Neighbor rule (1NN) and the Fisher classifier. The significance of classification performance will be analyzed by means of Friedman's Test.

The remainder of the paper is organized as follows. In Section 2, a summary of classification in dissimilarity representation is presented together with the prototype selection methods chosen for our study. An introduction to resampling algorithms is provided in Section 3. Section 4 reports the experiments and the related results are discussed, ending up the paper with some conclusions and proposals for further work in Section 5.

2 DISSIMILARITY SPACE

In the dissimilarity space, objects are represented by pairwise dissimilarities values, where each object is related with other objects by a vector of dissimilarities (Pekalska and Duin, 2002a).

2.1 Dissimilarity-based Classification

The dissimilarity space is built using a representation set $R = \{p_1, \ldots, p_r\}$ of r objects, called prototypes. Given a dissimilarity measure, the representation is obtained as the proximity to prototypes in R. Then, the dimension of this new space is determined as the amount of prototypes.

Let X be the training set of n objects in the feature space, $X = \{x_1, \ldots, x_n\}$, the classifier in dissimilarities is built from the proximities between training set objects and prototypes, i.e. on the distance matrix $D(X,R)$. Usually, $R \subseteq X$ covering all classes. Consequently, $D(X,R)$ is a dissimilarity matrix of size $n \times r$, where the object x_i is associated with all prototypes in R and described in the i-th row by a r-dimensional dissimilarity vector $D(x_i,R) = \{d(x_i, p_1), \ldots, d(x_i, p_r)\}$, being d the proximity measure (e.g., the Euclidean distance). When the object x_i and p_h are identical $d(x_i, p_h) = 0$, this distance gets to be higher in so far as x_i and p_h become more different.

In the same way, given a test set S of s objects in the feature space, it may be represented in dissimilarities by pairwise proximities between objects in S and prototypes, $D(S,R)$. This representation space has the advantage that any conventional classifier operating in vector space can be used (Pekalska and Duin, 2005; Pekalska et al., 2002)

2.2 Prototype Selection Methods

The main problem in the dissimilarity space is the possible high dimensionality of the representation of data in pairwise proximities, which is determined by the size of R. For this reason, many works focus on investigating different methods for prototype selection, with the aim of finding a small representation set that reduces the computational effort while preserving the accuracy in the classification (Pekalska and Duin, 2002a; Lozano et al., 2006).

In this work, we analyze the effect of the representation set when data are imbalanced. To this end, we employed four prototype selection methods:

- *R*50: This method consists on randomly choose a fifty percent of objects ($n/2$) in T, keeping the a priori probabilities of each class.
- *R*100: The representation set contains all training set objects, i.e. $R = T$. It has the disadvantage that the computational cost may be high since the dimension of the space is equal to the number of objects in the training set.
- *RCNN*: The representation set is constructed by applying the conventional algorithm of condensed Nearest Neighbor rule (CNN), introduced by (Hart, 1968), to the training set with the aim to retain a consistent subset of the original T. This method has the undesirable property that the consistent subset depends on the order in which data are processed.
- *RMSS*: It builds the representation set based on the Modified Selective Subset method (MSS), proposed by (Barandela et al., 2005), which reduces

the training set size while preserving the original decision boundaries as much as possible.

3 DATA-LEVEL METHODS

Data-driven methods consist of artificially balancing the original data set, either by over-sampling the minority class and/or by under-sampling the majority class, until the problem classes are approximately equally represented. Both strategies can be applied in any learning system, since they act as a preprocessing phase, allowing the learning system to receive the training instances as if they belonged to a well-balanced data set. Thus, any bias of the system towards the majority class due to the different proportion of examples per class would be expected to be removed. The simplest method to increase/reduce the minority/majority class corresponds to non-heuristic methods that aim at balancing the class distribution through the random replication/elimination of positive/negative examples. Nevertheless, these methods have shown important drawbacks. Random over-sampling may increase the likelihood of overfitting, since it makes exact copies of the minority class instances. On the other hand, random under-sampling may discard data potentially important for the classification process. Despite this problem, it has empirically been shown to be one of the most effective resampling methods. In order to overcome these drawbacks, several authors have developed *focused resampling* algorithms that produce balanced data sets in an intelligent way.

(Chawla et al., 2002) proposed an over-sampling technique that generates new synthetic minority instances by interpolating between several positive examples that lie close together. This method, called SMOTE (Synthetic Minority Oversampling TEchnique), allows the classifier to build larger decision regions that contain nearby instances from the minority class. From the original SMOTE algorithm, several modifications have been proposed in the literature, most of them pursuing to determine the region in which the positive examples should be generated. For instance, Borderline- SMOTE (Han et al., 2005) consists of using only positive examples close to the decision boundary, since these are more likely to be misclassified.

Unlike the random method, many proposals are based on a more intelligent selection of negative examples to be eliminated. For example, (Kubat and Matwin, 1997) proposed an under-sampling technique, called obe-sided selection, that selectively removes only those negative instances that are "redundant" or that "border" the minority class examples (they assume that these bordering cases are noise). In contrast to the one-sided selection technique, the so-called neighborhood cleaning rule emphasizes more on data cleaning than on data reduction. To this end, Wilsons editing is used to identify and remove noisy negative instances. Similarly, (Barandela et al., 2003) introduced a method that eliminates not only noisy instances of the majority class by means of Wilsons editing (WE), but also redundant examples through the MSS condensing algorithm.

4 EXPERIMENTAL SETUP AND RESULTS

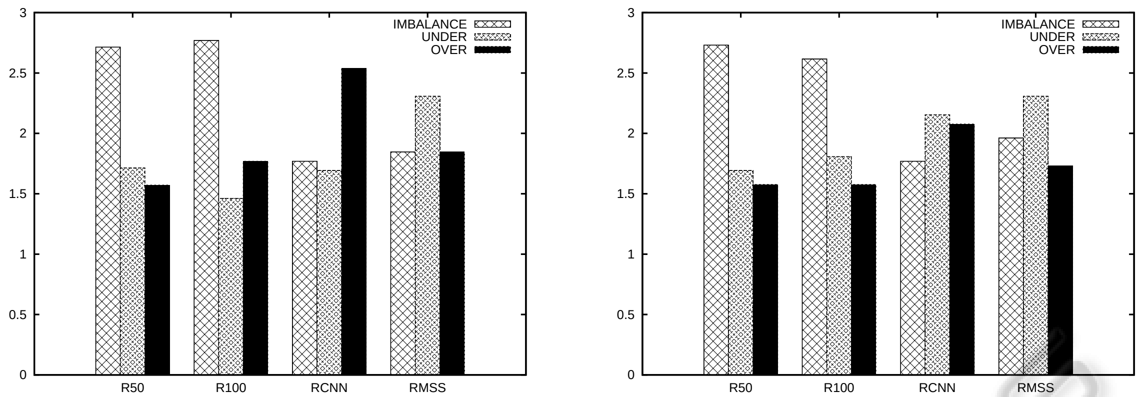
Experiments were carried out over 13 data sets taken from the UCI Machine Learning Database Repository (Frank and Asuncion, 2010) and a private library (http://www.vision.uji.es/∼sanchez/Databases/). All data sets have been transformed into two-class problems by keeping one original class (the minority class) and joining the objects of the remaining classes (giving the majority class). For example, in Segmentation database the objects of classes 1, 2, 3, 4 and 6 were joined to shape a unique majority class and the original class 5 was left as the minority class (see a summary in Table 1).

Table 1: Data sets used in the experiments

Data Set	Positive Examples	Negative Examples	Classes	Majority Class
Breast	81	196	2	1
Ecoli	35	301	8	1,2,3,5,6,7,8
German	300	700	2	1
Glass	17	197	9	1,2,4,5,6,7,8,9
Haberman	81	225	2	1
Laryngeal$_2$	53	639	2	1
Phoneme	1586	3818	2	1
Pima	268	500	2	1
Scrapie	531	2582	2	1
Segmentation	330	1980	6	1,2,3,4,6
Spambase	1813	2788	2	1
Vehicle	212	634	4	2,3,4
Yeast	429	1055	10	1,3,4,5,6,7,8,9,10

For each data set, we have used a stratified 5-fold cross-validation, obtaining 65 new problems. SMOTE and random under-sampling were applied to the training data (in the feature space), and four different prototype selection techniques were used on imbalanced and resampled data sets: R50, R100, RCNN and RMSS. Two learners, Fisher and 1-NN classifiers, were constructed from the original and transformed data sets.

In total, 65 different training data sets, two resampling methods and no sampling, results in $65 \times 3 = 195$ transformed data sets. Since there are four prototype selection methods and two learning algorithms,



(a) (b)

Figure 1: Friedman rankings for four different prototype selection methods over imbalanced and resampled data sets. (a) Fisher and (b) 1NN classifiers.

a total of $1,560$ classifiers were trained and evaluated in our experiments.

Typical metrics for measuring the performance of learning systems are classification accuracy and error rates. However, as pointed out by many authors (Fatourechi et al., 2008; Gu et al., 2009; Huang and Ling, 2005) these performance measures show a biased behavior in the presence of skewed distributions. In this paper, we will use the geometric mean of accuracies (Kubat and Matwin, 1997), which is defined as $Gm = \sqrt{a^+ \times a^-}$, where a^+ denotes the accuracy on the positive class, and a^- is the accuracy on the negative class. This measure can be seen as a kind of correlation between both rates, because a high value occurs when they both are also high, while a low value is related to at least one low rate.

Results obtained in terms of *Gm* were evaluated by the multiple comparison Friedman test (Alcalá-Fdez et al., 2011; Demšar, 2006), which is a non-parametric test equivalent to repeated measures of ANOVA. It ranks the algorithms in such a way that the best performing method gets the rank 1. In the case of ties, averaged ranks are assigned.

4.1 Analysis of the Results

Figure 1 shows rank values for the four prototype selection techniques (R50, R100, RCNN and RMSS) when the classification model is (a) Fisher and (b) 1NN. For each technique, the ranking method is applied over the three cases, both when the representation set is imbalanced and when it is balanced. Lower values correspond to the best overall performances for technique-classifier combinations.

For both classifiers, it is observed that when the representation set is R50 or R100, it is worth applying any resampling technique before using the representation space by means of dissimilarities. This may suggest that when the representation set is selected from balanced data sets, the dissimilarity-based classifier learns to distinguish between the classes.

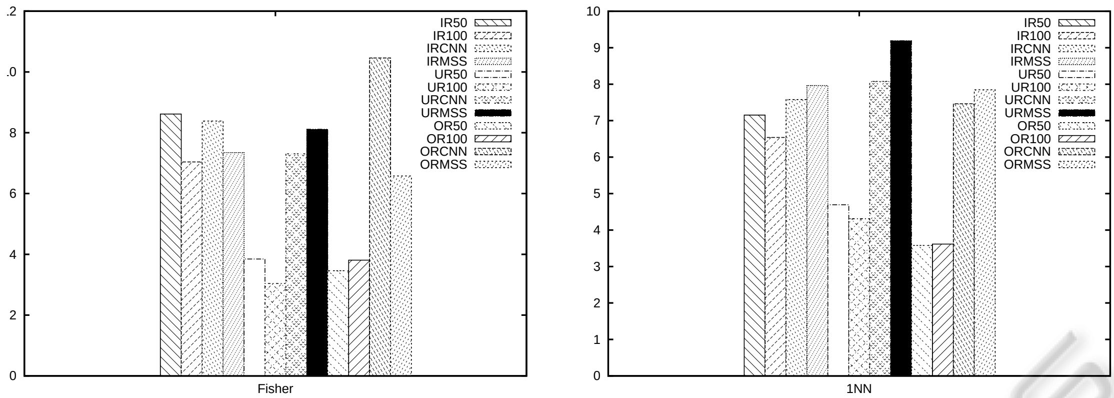
However, this behavior is not observed for the RCNN and RMSS methods, since in some cases the classification of imbalanced data improves the results when they are balanced. It seems that the application of condensed techniques are discarding objects with relevant information of the classes, and possibly the minority class is being more affected. Additionally, when the representation set is undersampled after being condensed, more objects are discarded in the representation set, resulting in a decrease in performance.

Figure 2 shows results when the ranking method is applied over all methods, when data is imbalanced (IR50, IR100, IRCNN and IRMSS), under-sampled (UR50, UR100, URCNN and URMSS) and over-sampled (OR50, OR100, ORCNN and ORMSS), for (a) Fisher and (b) 1NN classifiers.

In general, for both classifiers the best results are observed with the R50 and R100 methods when data sets are resampled. This may indicate that in the dissimilarity space the classification performance is improved if the training set is balanced before building the dissimilarity classifier.

For Fisher classifier, the best performance is achieved with R100 when data are under-sampled. However, with R50 a slightly lower performance is obtained, whereas the difference of computational effort is significant. This may suggest that the R50 technique could be used for keeping a good cost-performance ratio when data are resampled.

On the other hand, the best result for the 1NN classifier is reached for the R50 and R100 methods when data are over-sampled. This confirms the conclusions previously drawn by (Pekalska and Duin, 2002a) in



(a) (b)

Figure 2: Friedman rankings for all prototype selection considering a total of 13 data sets. (a) Fisher and (b) 1NN classifiers.

the sense that *k*-NN classifiers require a much larger representation set to achieve a higher accuracy.

5 CONCLUSIONS

In this paper, we analyze the effect of the representation set in the dissimilarity space when data are imbalanced. For this purpose, we evaluate four prototype selection methods. In addition, the under-sampling and over-sampling techniques are also applied to data before representing them by dissimilarities, with the aim of analyzing how a balanced representation set affect the performance classification. The Fisher and 1-Nearest Neighbor classifier were used to evaluate each method.

In general, for both classifiers, results show that the best performance was obtained for the simplest methods (R50 and R100), what indicates that it is worth applying any resampling technique before building the dissimilarity classifier.

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