

Dealing with difficult minority labels in imbalanced multilabel datasets



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ABSTRACT

Multilabel classification is an emergent data mining task with a broad range of real world applications. Learning from imbalanced multilabel data is being deeply studied latterly, and several resampling methods have been proposed in the literature. The unequal label distribution in most multilabel datasets, with disparate imbalance levels, could be a handicap while learning new classifiers. In addition, this characteristic challenges many of the existent preprocessing algorithms. Furthermore, the concurrence between imbalanced labels can make harder the learning from certain labels. These are what we call *difficult labels*. In this work, the problem of difficult labels is deeply analyzed, its influence in multilabel classifiers is studied, and a novel way to solve this problem is proposed. Specific metrics to assess this trait in multilabel datasets, called SCUMBLE (*S*core of *C*onc*U*rrence among *iM*Balanced *L*ab*E*ls) and SCUMBLElbl, are presented along with REMEDIAL (*R*Esampling *M*ultilab*E*l datasets by *D*ecoupling *h*ighly *I*mb*A*lanced *L*abels), a new algorithm aimed to relax label concurrence. How to deal with this problem using the R mldr package is also outlined.

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1. Introduction

Multilabel classification (MLC) [1,2] models are designed to predict the subset of labels associated to each instance in a multilabel dataset (MLD), instead of only one class as traditional classifiers do. It is a task useful in fields such as automated tag suggestion [3], protein classification [4], and object recognition in images [5], among others. Many different methods have been proposed lately to accomplish this problem.

The number of instances in which each label appears is not homogeneous. In fact, most MLDs show big differences in label frequencies. This peculiarity is known as imbalance [6], and it has been profoundly studied in traditional classification. In the context of MLC, several proposals to deal with imbalanced MLDs [7–15] have been made lately. Despite these efforts, there are still some aspects regarding imbalanced learning in MLC that would need additional analysis.

Resampling techniques are commonly used in with traditional (non-multilabel) datasets [16] to balance their class distributions, hence they are an obvious choice to face the same problem with

MLDs. Notwithstanding, the nature of MLDs can be a challenge for resampling algorithms. In this paper, we will show how a specific characteristic of these datasets, the joint presence in the same instance of labels with different frequencies, could prevent the goal of these algorithms.

We hypothesized¹ that this symptom, the concurrence among imbalanced labels, would influence the resampling algorithms behavior. Specifically, the minority labels which jointly appear with majority ones would be difficult labels. In order to deal with this problem we propose to face it in two phases:

- Firstly, the concurrence problem has to be assessed. For doing so, two new metrics, named SCUMBLE (*S*core of *C*onc*U*rrence among *iM*Balanced *L*ab*E*ls) and SCUMBLElbl, designed explicitly to assess this causality, will be proposed. Its effectiveness will be experimentally demonstrated.
- Secondly, an algorithm specifically designed to preprocess MLDs affected by this problem would be needed. A such method, called REMEDIAL (*R*Esampling *M*ultilab*E*l datasets by *D*ecoupling *h*ighly *I*mb*A*lanced *L*abels), will be introduced, and its performance will be empirically tested.

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¹ This paper is an extended version of our previous work [17] from HAIS'14, including additional metrics, a deeper analysis, and an algorithm aimed to solve the described problem. The proposed solutions have been implemented in R, and the software package containing them is also described.

The SCUMBLE measure was conceived aiming to know how difficult would be to work with a certain MLD for resampling algorithms. Its goal is to appraise the concurrence among imbalanced labels, giving as result a score easily interpretable. This score will be in the range [0,1]. A low score would denote an MLD with not much concurrence among imbalanced labels, whereas a high one would evidence the opposite case. Our hypothesis is that the lower the score obtained, the better the resampling algorithms would work. SCUMBLElbl complements the former metric, allowing to know which labels are more affected by this problem. The less frequent labels with a high SCUMBLElbl would be specially difficult cases.

Once the presence of the concurrence problem has been stated, the idea of how to deal with it naturally arises. For this reason the algorithm REMEDIAL, a specific method able to reduce concurrence among imbalanced labels, is also introduced. REMEDIAL works by decoupling imbalanced labels through an editing and oversampling approach. It is a resampling algorithm, since it produces new data samples. At the same time, it also edits existent instances. However, it does not change the number of times that each label appears in the dataset. The details about REMEDIAL and how to use this algorithm along with the proposed metrics, relying on the mldr R package [18], will also be explained.

The rest of this paper is structured as follows. Section 2 offers a brief introduction to MLC, as well as a description on how the learning from imbalanced MLDs has been faced. In Section 3, the problem of concurrence among imbalanced labels in MLDs will be defined, and how to assess this concurrence using the proposed metrics will be explained. The algorithm REMEDIAL is described in Section 4. Section 5 portrays the experimental framework used, as well as the obtained results from experimentation. Finally, Section 6 will offer the conclusions. Appendix A describes how to assess the label concurrence level and how to apply the REMEDIAL algorithm thorough a specific software package developed by the authors.

2. Preliminaries

In this section, a concise introduction to multilabel classification is offered, along with a description on how the learning from imbalanced MLDs has been faced until now.

2.1. Multilabel classification

Currently, there are many domains [4,5,19–22] in which each data pattern is not associated exclusively to one class, but to a group of them. In this context, the classes are named labels, and the set of labels that belongs to a data sample is called labelset. Let D be an MLD, D_i the i th instance, and L the full set on labels on D . The goal of a multilabel classifier is to predict a set $Z_i \subseteq L$ with the labelset for D_i .

Multilabel classification has been traditionally faced through two different approaches [23]. The first one, called data transformation, aims to produce binary or multiclass datasets from an MLD, allowing the use of non-MLC algorithms. The second, known as algorithm adaptation, has the goal of adapting established algorithms to natively work with MLDs. The two most common transformation methods are Binary Relevance (BR) [24] and Label Powerset (LP) [25]. The former produces several binary datasets from an MLD, usually one for each label or one for each label pair [26]. The latter transforms the MLD into a multiclass dataset, taking each labelset as class identifier. Regarding adapted algorithms, the number of proposals is quite high. There are multilabel KNN classifiers such as ML-kNN [27], multilabel trees based on C4.5 [28], and multilabel ANNs such as [29], as well as a profusion of algorithms

based on ensembles of BR and LP classifiers. A recent review on multilabel classification algorithms can be found in [2].

Thus far, most proposed multilabel characterization metrics are focused in assessing the number of labels and labelsets. The most common ones are the total number of labels $|L|$, label cardinality ($Card$), which is the average number of labels per instance, and label density, obtained as $Card/|L|$.

2.2. Learning from imbalanced data

Imbalanced learning is a well-known problem in traditional classification [30–33], having been faced through three main approaches. First, by way of algorithmic adaptations of existent classifiers, the imbalance is taken into account in the classification process. Second, the preprocessing approach aims to balance class distributions by way of data resampling, creating (oversampling) or removing (undersampling) data samples. Third, cost sensitive classification is a combination of the two previous approaches. The data resampling approach has the advantage of being classifier independent, and its effectiveness has been proven in many scenarios.

In the MLC field, both the algorithmic adaptation and the data resampling approaches have been applied. The former is present in [7,8,11], while the latter appears in [10,12–15]. There are also proposals based on the use of ensemble of classifiers, such as [9].

When it comes to assessing the imbalance level in MLDs, the metrics in Eqs. (1) and (2) are proposed in [34]. Let D be an MLD, L the full set of labels in it, y the label being analyzed, and Y_i the labelset of i th instance in D . In Eq. (1) the symbol $\llbracket \cdot \rrbracket$ denotes de Iverson bracket, which returns 1 if the expression inside it is true or 0 otherwise. $IRLbl$ is a measure calculated individually for each label. The higher is the $IRLbl$ the larger would be the imbalance, allowing to know which labels are in minority or majority. $MeanIR$ is the average $IRLbl$ for an MLD. It is useful to estimate the global imbalance level.

$$IRLbl(y) = \frac{\max_{y' \in L} \left(\sum_{i=1}^{|D|} \llbracket y' \in Y_i \rrbracket \right)}{\sum_{i=1}^{|D|} \llbracket y \in Y_i \rrbracket}. \quad (1)$$

$$MeanIR = \frac{1}{|L|} \sum_{y \in L} IRLbl(y). \quad (2)$$

Even though the previously cited proposals for facing imbalanced learning in MLC achieve some good results, their behavior is heavily influenced by MLDs characteristics such as the imbalance levels, measured by means of the previous metrics, or the concurrence among imbalanced labels, which will be described later. In the following we will focus in this topic, specifically in regard to data resampling solutions.

2.3. Related work

In general, resampling methods aimed to work with non-MLDs can be divided into two categories, oversampling algorithms and undersampling algorithms. The former technique produces new samples with the minority class, while the latter removes instances linked to the majority class. The way in which the samples to be removed or reproduced are chosen can also be grouped into two categories, random methods and heuristic methods. Since this kind of datasets use only one class per instance, the previous techniques effectively balance the distribution of classes. However, this is not always true when dealing with MLDs. Moreover, most MLDs have more than one minority and one majority label.

The preceding approaches have been migrated to the multilabel scenario at some extent, giving as result proposals such as the following:

- *Random undersampling*: Two multilabel random undersampling algorithms are presented in [12], one of them based on the LP transformation (LP-RUS) and another one on the *IRlbl* measure (ML-RUS). The latter determines what labels are in minority, by means of their *IRlbl*, and avoids removing samples in which they appear.
- *Random oversampling*: The same paper [12] also proposes two random oversampling algorithms, called LP-ROS and ML-ROS. The former is based on the LP transformation, while the latter relies on the *IRlbl* measure. Both take into account several minority labels, and generate new instances cloning the original labelsets.
- *Heuristic undersampling*: In [14] a method to undersample MLDs following the ENN (*Edited Nearest Network*) rule was presented. The instances are not randomly chosen, as in LP-RUS or ML-RUS, but carefully selected after analyzing their *IRlbl* and the differences with their neighborhood.
- *Heuristic oversampling*: The procedure proposed in [13] is based on the original SMOTE algorithm. First, instances of an MLD are chosen using different criteria, then the selected samples are given as input to SMOTE, producing new samples with the same labelsets. In [15] a more sophisticated approach is presented, with a multilabel version of SMOTE, called MLSMOTE, able to produce synthetic samples whose labelsets are generated from those of the nearest neighbors, instead of cloning them.

A major disadvantage in some of these algorithms is that they always work over full labelsets, cloning the set of labels in existent samples or completely removing them. Although this approach can benefit some MLDs, in other cases the result can be counterproductive depending on the MLD traits.

The aforementioned multilabel resampling algorithms will not have an easy work while dealing with MLDs which have a high *SCUMBLE* level. Undersampling algorithms can produce a loss of essential information, as the samples selected for removal because majority labels appear in them can also contain minority labels. In the same way, oversampling algorithms limited to cloning the labelsets, such as the proposals in [12,13], can be also increasing the presence of majority labels.

3. Imbalanced MLDs and resampling algorithms behavior

Most traditional resampling methods do their job by removing instances with the most frequent class, or creating new samples from instances associated to the least frequent one. Since each instance can belong to one class only, these actions would effectively balance the classes frequencies. However, this is not necessarily true when working with MLDs.

3.1. Concurrence among imbalanced labels in MLDs

The instances in a MLD are usually associated simultaneously to two or more labels. It is entirely possible that one of those labels is the minority label, while other is the majority one. In the most extreme situation, all the appearances of the minority label could be jointly with the majority one, into the same instances. This will make the minority label specially difficult to classify by any MLC algorithm, as most of them tend to be biased to the majority ones. In practice the scenario would be more complicated, as commonly there are more than one minority/majority label in an MLD. Therefore, the potential existence of instances associated to

minority and majority labels at once is very high. This fact is what we call concurrence among imbalanced labels.

A multilabel oversampling algorithm that clones minority labels, such as the proposed in [12], or that generates new samples from existing ones preserving the labelsets, as is the case in [13], could be also increasing the number of instances associated to majority labels. Thus, the imbalance level would be hardly reduced if there is a high level of concurrence among imbalanced labels. In the same way, a multilabel undersampling algorithm designed to remove instances from the majority labels, such as the proposed in [12], could inadvertently cause also a loss of samples associated to the minority ones. In both cases, difficult labels (those which are in minority and have a high concurrence with majority ones) will be the most harmed by the classifier.

The ineffectiveness of these resampling methods, when they are used with certain MLDs, would be noticed once the preprocessing is applied and the classification results are evaluated. This process will need computing power and time. For that reason, it would be desirable to know in advance the level of concurrence among imbalanced labels that each MLD suffers, saving these valuable resources.

3.2. Metrics to assess the concurrence level

The concurrence of labels in an MLD can be visually explored in some cases, as shown in Figs. 1 and 2. Each arc represents a label, being the arc's length proportional to the number of instances in which this label is present. The first (Fig. 1) diagram corresponds to the genbase dataset. At the position of twelve o'clock appears a label called P750 which is clearly a minority label. All the samples associated to this label also contains P271, another minority label. The same situation can be seen with label P154. These minority labels have not necessarily to be difficult labels. By contrast, in the yeast MLD (Fig. 2) is easy to see that the samples associated to minority labels, such as Class14 and Class9, always appear together with one or more majority labels. At first sight, that the concurrence between imbalanced labels is higher in yeast than in genbase, and that the former contains some difficult labels while the latter does not, could be concluded. However, this visual exploratory technique is not useful with MLDs having more than a few dozens labels, because the diagram would be hardly legible.

Existing metrics previously described (see Section 2.2), such as *IRLBL* and *MeanIR*, assess the imbalance level of the labels, i.e., the relative frequency of each label with respect to the most common one and the average frequency. However, none of them allows to know if minority labels appear in their own or jointly with majority ones. The *SCUMBLE* metric proposed here is aimed to evaluate this casuistic, that was not considered in the literature until now.

The *SCUMBLE* metric aims to quantify the imbalance variance among the labels present in each data sample. This metric (Eq. (4)) is based on the Atkinson index [35] and the *IRlbl* measure (Eq. (1)) proposed in [34]. The former is an econometric measure directed to assess social inequalities among individuals in a population. The latter is the metric that lets us know the imbalance ratio of each label in an MLD. The Atkinson index is used to know the diversity among people's earnings, while our objective is to assess the extend to which labels with different imbalance levels appear jointly. Our first hypothesis is that the higher is the concurrence level the harder would be the work for resampling algorithms, and therefore the worse they would perform.

The Atkinson index is calculated using incomes. We used the imbalance level of each label instead, taking each instance D_i in the MLD D as a population, and the active labels in D_i (those which are relevant to D_i and therefore are set to 1) as the individuals. If the label l is present in the instance i then $IRlbl_{il} = IRlbl(l)$, otherwise $IRlbl_{il} = 0$. \overline{IRlbl}_i stands for the average imbalance level

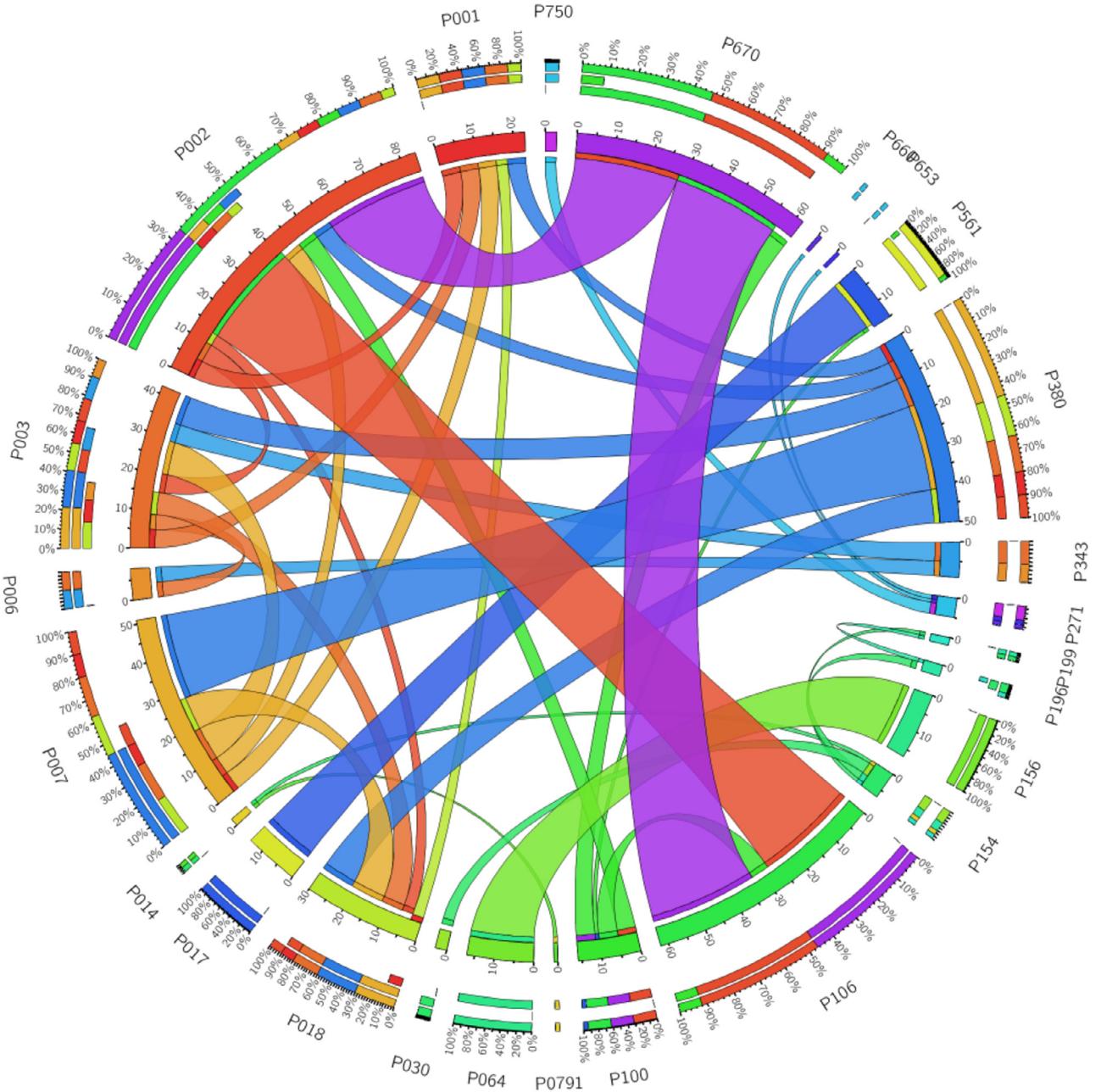


Fig. 1. Label concurrence in genbase MLD.

of the labels appearing in instance i . The scores for every sample are averaged, obtaining the final SCUMBLE value.

$$\text{SCUMBLE}_{\text{ins}}(i) = 1 - \frac{1}{|IRLbl_i|} \left(\prod_{l=1}^{|L|} IRLbl_{il} \right)^{(1/|L|)} \quad (3)$$

$$\text{SCUMBLE}(D) = \frac{1}{|D|} \sum_{i=1}^{|D|} \text{SCUMBLE}_{\text{ins}}(i) \quad (4)$$

Since SCUMBLE is computed as an average of concurrence by instance, it could be influenced by extreme values. A few instances with a very high $\text{SCUMBLE}_{\text{ins}}$ value would introduce a certain deviation into the global SCUMBLE measure. To estimate the importance of this deviation, the SCUMBLE.CV metric (see Eq. (5)) provides the corresponding coefficient of variation. The higher is the SCUMBLE.CV , the larger would be the differences in concurrence

among instances.

$$\begin{aligned} \text{SCUMBLE.CV} &= \frac{\text{SCUMBLE}\sigma}{\text{SCUMBLE}}, \\ \text{SCUMBLE}\sigma &= \sqrt{\sum_{i=1}^{|D|} \frac{(\text{SCUMBLE}_{\text{ins}}(i) - \text{SCUMBLE})^2}{|D| - 1}} \end{aligned} \quad (5)$$

The SCUMBLE measure for an MLD would provide a glimpse at how much concurrence between imbalanced labels there is in it. It also would be interesting to know which labels are more affected by this problem. This is the aim of the SCUMBLElbl metric (Eq. (6)). The SCUMBLElbl.CV metric can also be obtained, following the same procedure described above for SCUMBLE.CV . Since the number of instances in which the assessed label appears is used as denominator, dividing the sum of SCUMBLE , that SCUMBLElbl will be lower for majority labels is something intuitively deductible. Majority labels usually will interact with minority ones only in a

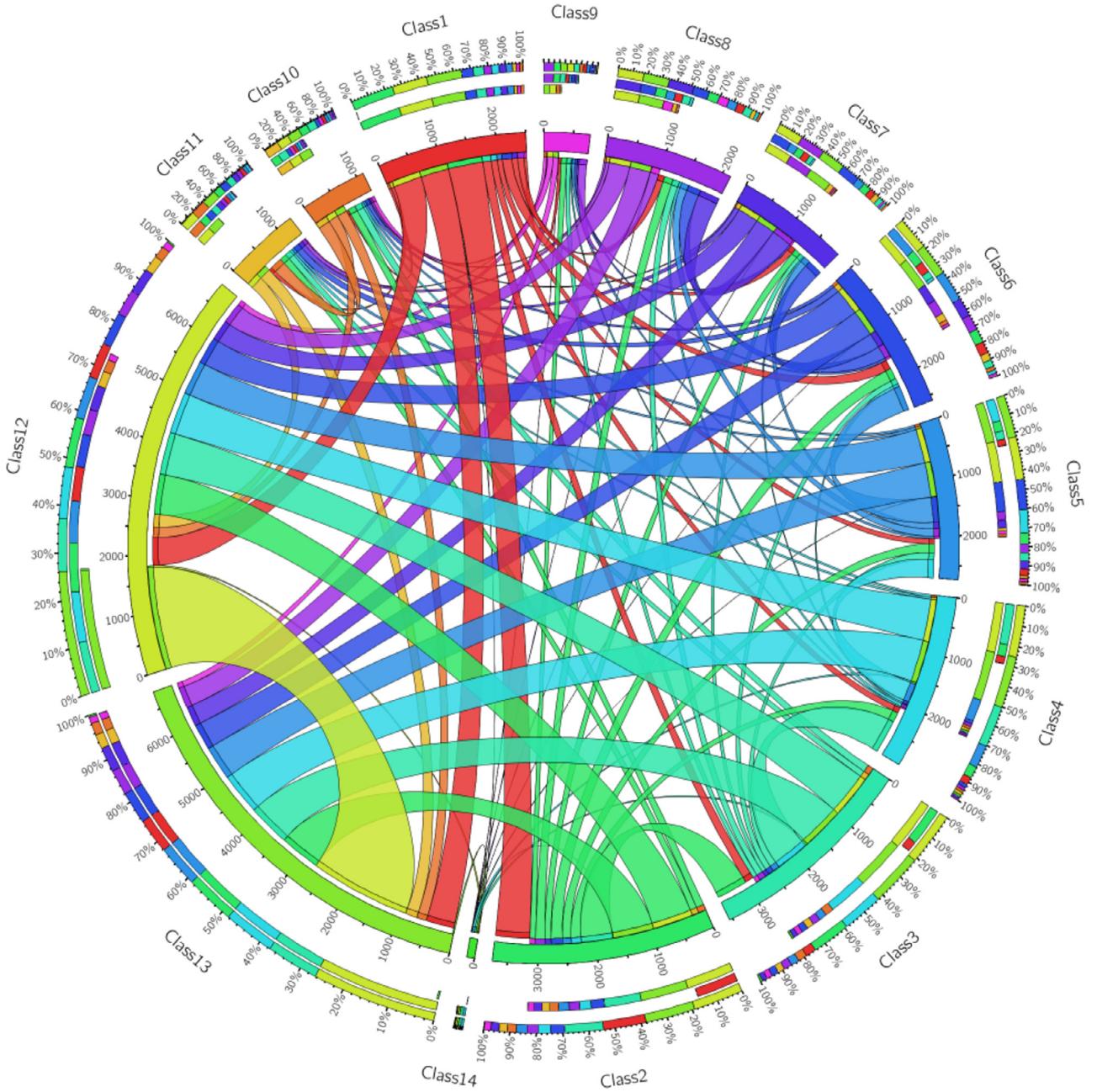


Fig. 2. Label concurrence in yeast MLD.

few instances, those containing the minority label. Therefore, this metric would allow comparisons between labels with a similar frequency in the MLD. Our second hypothesis is that this information would be useful to know which of the minority labels are in fact heavily related to majority ones. In other words, which of them are difficult labels.

$$\text{SCUMBLElbl}(y) = \frac{\sum_{i=1}^{|D|} [y \in Y_i] \cdot \text{SCUMBLE}_{\text{ins}}(i)}{\sum_{i=1}^{|D|} \|y \in Y_i\|} \quad (6)$$

Whether our initial hypothesis are correct or wrong, and therefore these metrics are able to predict the difficulty that an MLD implies for resampling algorithms or not, is something to be proven experimentally.

4. The algorithm REMEDIAL

In this section the algorithm REMEDIAL, firstly introduced in [36] as a specific method for MLDs with concurrence of highly imbalanced labels, is described. How REMEDIAL has been implemented into the mldr package, and how to use it, is also explained in Appendix A.

As its name suggests, REMEDIAL (*REsampling MultilabEl datasets by Decoupling highly ImbalAnced Labels*) is a method specifically designed for MLDs that suffer from concurrence between imbalanced labels. In this context, *highly imbalanced labels* has to be understood as labels with large differences in their *IRLbls*. This is a fact assessed with the *SCUMBLE* measure, thus REMEDIAL is directed to MLDs with a high *SCUMBLE* level.

When the few samples in which a minority label is present also contain one or more majority labels, whose frequency in the

Table 1
Main characteristics of the datasets.

Dataset	Instances	Attributes	Labels	Labelsets	Card	Dens	MeanIR	MaxIR	SCUMBLE	Ref.
Corel5k	5000	499	374	3175	3.522	0.009	189.568	1 120.000	0.394	[37]
Mediamill	43,907	120	101	6555	4.376	0.043	256.405	1 092.548	0.355	[38]
Cal500	502	68	174	502	26.044	0.150	20.578	88.800	0.337	[19]
Enron	1702	1001	53	753	3.378	0.064	73.953	913.000	0.303	[20]
Corel16k	13,618	500	144	4692	2.815	0.020	32.998	116.407	0.279	[39]
Cs	9270	635	274	4749	2.556	0.009	85.002	226.700	0.272	[3]
Tmc2007	28,596	49,060	22	1341	2.158	0.098	15.157	41.980	0.175	[40]
Yeast	2417	103	14	198	4.237	0.303	7.197	53.412	0.104	[21]
Bibtex	7395	1836	159	2856	2.402	0.015	12.498	20.431	0.094	[41]
Medical	978	1449	45	94	1.245	0.028	89.501	266.000	0.047	[22]
Genbase	662	1186	27	32	1.252	0.046	37.315	171.000	0.029	[4]

MLD is much higher, the power of the input features to predict the labels might be biased to the majority ones. Our hypothesis is that, in a certain way, majority labels are masking the minority ones when they appear together, a problem that could be solved to some extent by decoupling the labels in these instances.

REMEDIAL is kind of a resampling algorithm. It could be seen as an oversampling method, since it produces new instances in some cases. At the same time it also modifies existent samples. However, REMEDIAL never changes the number of samples associated to each label, i.e., the absolute frequency of the labels in the MLD. In short, REMEDIAL is an editing plus oversampling algorithm, and it is an approach which has synergies with traditional resampling techniques. The method pseudo-code is shown in [Algorithm 1](#).

Algorithm 1 REMEDIAL algorithm.

```

1: function REMEDIAL(MLD  $D$ , Labels  $L$ )
2:    $\triangleright$  Calculate imbalance levels
3:    $IRLbl_l \leftarrow \text{calculateIRlbl}(l \text{ in } L)$ 
4:    $IRMean \leftarrow IRLbl$ 
5:    $\triangleright$  Calculate SCUMBLE
6:    $SCUMBLEIns_i \leftarrow \text{calculateSCUMBLE}(D_i \text{ in } D)$ 
7:    $SCUMBLE \leftarrow \overline{SCUMBLEIns}$ 
8:   for each instance  $i$  in  $D$  do
9:     if  $SCUMBLEIns_i > SCUMBLE$  then
10:       $D'_i \leftarrow D_i$   $\triangleright$  Clone the affected instance
11:       $\triangleright$  Maintain minority labels
12:       $D_i[\text{labels}_{IRlbl \leq IRMean}] \leftarrow 0$ 
13:       $\triangleright$  Maintain majority labels
14:       $D'_i[\text{labels}_{IRlbl > IRMean}] \leftarrow 0$ 
15:       $D \leftarrow D + D'_i$ 
16:    end if
17:   end for
18: end function

```

The $IRlbl$, $IRMean$ and $SCUMBLE$ measures are computed in lines 2–7. $SCUMBLEIns_i$ is the concurrence level of the instance D_i . The mean $SCUMBLE$ for the MLD is obtained by averaging the individual $SCUMBLE$ for each sample.

Taking the mean $SCUMBLE$ as reference, only the samples with a $SCUMBLEIns_i > SCUMBLE$ are processed. Those instances, which contain minority and majority labels, are decoupled into two instances, one containing only the majority labels and another one with the minority labels. In line 10 D_i , a sample affected by the problem at glance, is cloned in D'_i . The formula in line 12 edits the original D_i instance by removing the majority labels from it. Majority labels are considered as those whose $IRlbl$ is equal or below to $IRMean$. Line 14 does the opposite, removing from the cloned D'_i the minority labels. D_i belongs to the D MLD, but D'_i has to be added to it (line 15).

What differentiates REMEDIAL from existing resampling methods, such as the ones enumerated in [Section 2.3](#), is that it does not change the label frequencies in the MLD. All existent proposals increase the number of instances associated to minority labels or decrease the amount of samples linked to majority ones. On the other hand, the goal of REMEDIAL is to look for instances where minority and majority labels appear together, splitting them if it is necessary, but without deleting or adding labels. As far as we are concerned, there is not a comparable method to REMEDIAL proposed in the literature.

5. Experimentation and analysis

The conducted experimentation has been structured into two phases. First, the interest is in checking how the $SCUMBLE$ level impacts the performance of some resampling methods. Second, how the proposed REMEDIAL algorithm influences the MLDs, and the classification behavior, is analyzed. The test bed framework is described in the next subsection, the obtained results and corresponding analysis of the two aforementioned phases are provided in the following ones.

5.1. Experimental framework

In the first phase of the experimentation, to determine the usefulness of the $SCUMBLE$ metric, six of the MLDs shown in [Table 1](#), corel5k, cal500, enron, yeast, medical and genbase, were used. They have been chosen as representatives of different $SCUMBLE$ values, including the extreme levels, corel5k (highest) and genbase (lowest), and four values which are in between. The rightmost column indicates each dataset's origin. All of them are imbalanced, so theoretically they could benefit from applying a resampling algorithm. Aside from the $SCUMBLE$ measure, the $MaxIR$ and $MeanIR$ values are also shown. These measurements correspond to whole datasets. The values taken as reference point to the posterior analysis will be average values from training partitions² using a 2×5 folds scheme. The datasets appear in [Table 1](#) sorted by $SCUMBLE$ value, from higher to lower. According to this measure, corel5k and cal500 would be among the most difficult MLDs in the first group, since they have a high level of concurrence among labels with different imbalance levels. On the other hand, medical and genbase would be the most benefited from resampling, as most of the majority/minority labels in them do not appear together.

Regarding the resampling algorithms, the two proposed in [\[34\]](#) have been applied. Both are based on the LP transformation. LP-ROS does oversampling by cloning instances with minority labelsets, whereas LP-RUS performs undersampling removing samples associated to majority labelsets. All the dataset partitions

² The dataset partitions used in this experimentation, as well as color version of all figures, are available to download at <http://simidat.ujaen.es/SCUMBLE>.

were preprocessed, and the imbalance measures were calculated for each algorithm.

In the second phase of the experimentation, to check the influence of REMEDIAL in classification results, the eleven MLDs shown in Table 1 have been given as input, before and after preprocessing them with REMEDIAL, to six different MLC algorithms:

- BR (*Binary Relevance*) [25]. Ensemble of binary classifiers. It is a transformation based method. A binary classifier is generated for each label and the individual predictions are joined to obtain the final prediction.
- HOMER (*Hierarchy of Multilabel Classifiers*) [42]. Ensemble of multiclass classifiers. It is a transformation method based on the label powerset approach, thus each label combination is interpreted as a label class.
- IBLR (*Instance-Based Learning by Logistic Regression*) [43]. Instance based classifier. IBLR is an improved version of ML-kNN [27], the best-known instance based multilabel classifier.
- CLR (*Calibrated Label Ranking*) [44]. Ensemble of binary classifiers based on pair-wise comparisons. A binary classifier is generated for each label pair, instead of each label as in BR. The classifier produces a ranking of labels, from which the predicted labelset is obtained after applying a threshold.
- ECC (*Ensemble of Classifier Chains*) [45]. Ensemble of binary classifiers based on chaining each model with the next one. The ensemble generates several chains setting the classifiers for each label at random locations in their respective chain.
- EPS (*Ensemble of Pruned Sets*) [46]. Ensemble of multiclass classifiers with pruned labelsets. Each classifier relies on the PS [47] method to prune infrequent labelsets, easing the work of the underlying multiclass classifier.

The C4.5 tree induction algorithm has been used as base classifier where an underlying binary or multiclass classifier is needed. Default parameters were used in all cases.

As stated in [48], the performance of a multilabel classifier should be always assessed by means of several evaluation metrics. In this case, classification results are evaluated using five usual multilabel measures: Hamming Loss (HL), Precision, MacroFMeasure (MacroFM), One Error (OE), and Ranking Loss (RL). HL (see Eq. (7)) is a global sample-based measure. It assesses differences between Z_i , the predicted labelset, and Y_i , the real one, without distinction among labels. The Δ operator returns the symmetric difference between both labelsets. The lower the HL the better the predictions are. Precision (8) is also example-based, and it is among the most usual performance metrics when it comes to evaluate a classifier. MacroFM is the label-based version of the usual F-Measure (see Eqs. (8)–(10)). As can be seen in Eq. (11), in MacroFM F-Measure is evaluated independently for each label and then it is averaged. In the latter equation TP stands for *True Positives*, FP for *False Positives*, TN for *True Negatives*, and FN for *False Negatives*. OE (12) and RL (13) are ranking-based evaluation metrics. In these equations, $rk(x_i, l)$ is a function that returns the confidence degree for the label l in the prediction Z_i provided by the classifier for the

instance x_i . Additional information about all these metrics can be found in [1].

$$HL = \frac{1}{|D|} \sum_{i=1}^{|D|} \frac{|Y_i \Delta Z_i|}{|L|}. \quad (7)$$

$$Precision = \frac{1}{|D|} \sum_{i=1}^{|D|} \frac{|Y_i \cap Z_i|}{|Z_i|} \quad (8)$$

$$Recall = \frac{1}{|D|} \sum_{i=1}^{|D|} \frac{|Y_i \cap Z_i|}{|Y_i|} \quad (9)$$

$$F\text{-Measure} = 2 * \frac{Precision * Recall}{Precision + Recall} \quad (10)$$

$$MacroFM = \frac{1}{|L|} \sum_{i=1}^{|L|} F\text{-Measure}(TP_i, FP_i, TN_i, FN_i) \quad (11)$$

$$OE = \frac{1}{n} \sum_{i=1}^n \sum_{y \in Z_i} \llbracket \text{argmax}_{y \in Z_i} \langle rk(x_i, y) \rangle \notin Y_i \rrbracket. \quad (12)$$

$$RL = \frac{1}{n} \sum_{i=1}^n \frac{1}{|Y_i| \cdot |\bar{Y}_i|} |y_a, y_b : rk(x_i, y_a) > rk(x_i, y_b)|, \\ (y_a, y_b) \in Y_i \times \bar{Y}_i \quad (13)$$

5.2. SCUMBLE influence in preprocessing and classification algorithms

Once the LP-ROS and LP-RUS resampling algorithms were applied, the imbalance levels on the preprocessed MLDs were reevaluated. Table 2 shows the new *MaxIR* and *MeanIR* values for each dataset. Comparing these values with the original ones, it can be verified that a general improvement in the imbalance levels has been achieved. Although there are some exceptions, in most cases both *MaxIR* and *MeanIR* are lower after applying the resampling algorithms.

It would be interesting to know if the imbalance reduction is proportionally coherent with the values obtained from the SCUMBLE measure. The graphs in Figs. 3 and 4 are aimed to visually illustrate the connection between SCUMBLE values and the relative variations in imbalance levels. For each MLD, their SCUMBLE value is represented along with the percentage change in *MaxIR* and *MeanIR* after applying the LP-ROS/LP-RUS resampling methods. The tendency for the three values among the six MLDs is depicted by three logarithmic lines. As can be seen, a clear parallelism exists between the continuous line, which corresponds to SCUMBLE, and the dashed lines. This affinity is specially remarkable with the LP-RUS algorithm (Fig. 4).

Although the previous figures allow to infer that an important correlation between the SCUMBLE measure and the success of the resampling algorithms exists, this relationship must be formally

Table 2
Imbalance levels after applying resampling algorithms (average values on training partitions).

Dataset	LP-ROS				LP-RUS			
	MaxIR		MeanIR		MaxIR		MeanIR	
	Before	After	Before	After	Before	After	Before	After
Corel5k	896.000	969.400	166.057	140.743	896.000	817.100	166.057	155.032
Cal500	133.192	179.358	21.274	25.468	133.192	133.192	21.274	21.274
Enron	657.050	710.967	72.552	53.255	657.050	620.050	72.552	68.672
Yeast	53.689	15.418	7.218	2.612	53.689	83.800	7.218	19.884
Medical	212.800	39.963	68.388	10.556	212.800	46.570	68.388	6.371
Genbase	136.800	13.703	31.665	4.500	136.800	150.800	31.665	51.157

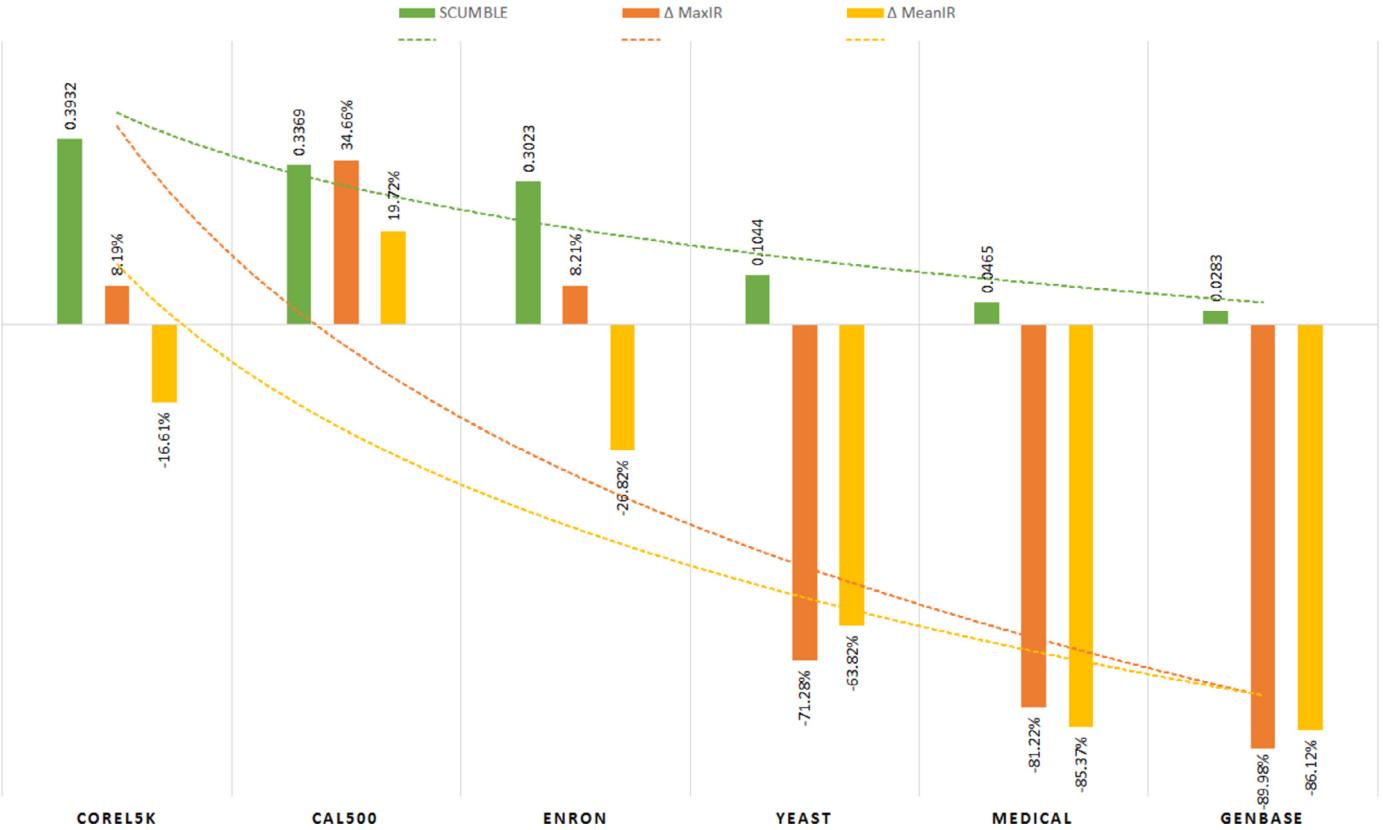


Fig. 3. SCUMBLE vs. changes in imbalance level after applying LP-ROS.

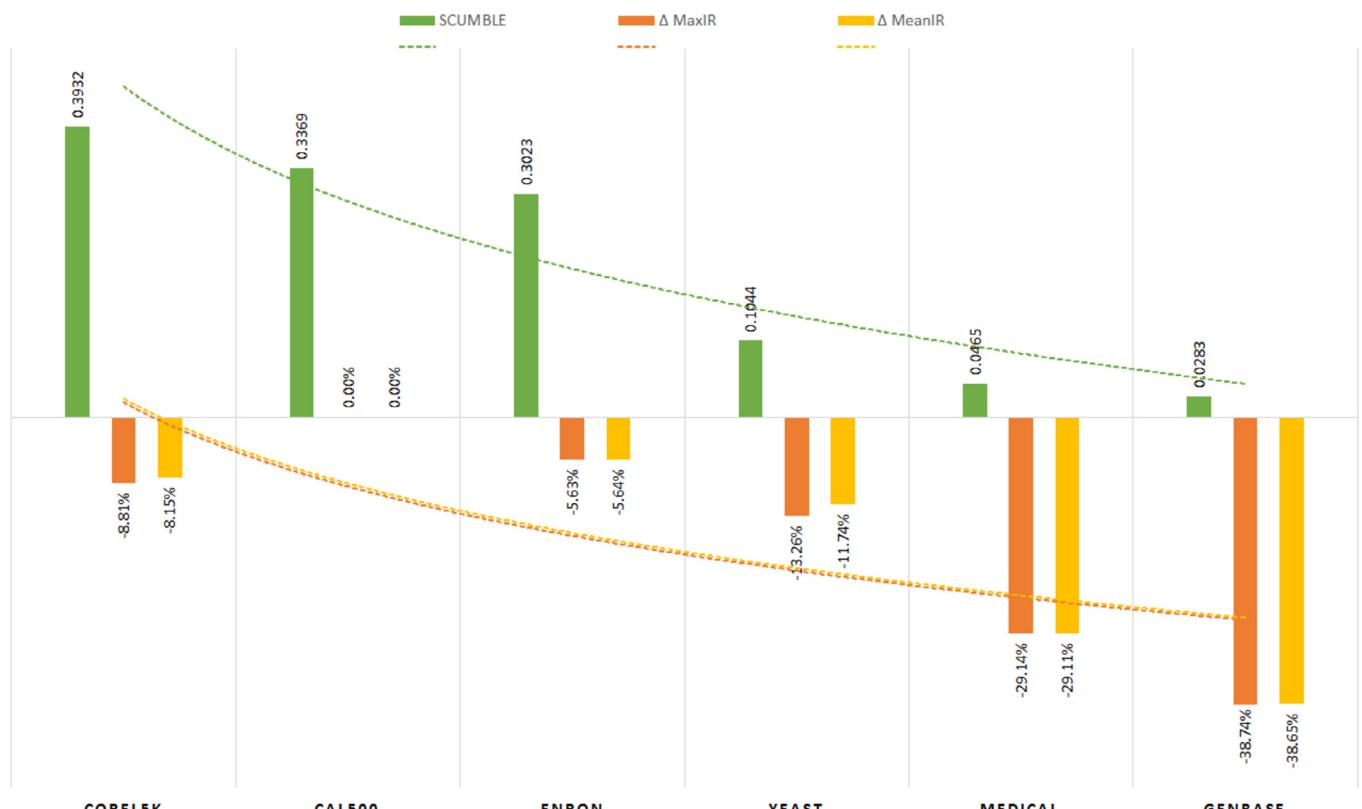


Fig. 4. SCUMBLE vs. changes in imbalance level after applying LP-RUS.

Table 3
Results from the Pearson correlation tests.

Algorithm	SCUMBLE vs. Δ MaxIR		SCUMBLE vs. Δ MeanIR	
	Cor	p-value	Cor	p-value
LP-ROS	0.8120	0.0497	0.9189	0.0096
LP-RUS	0.8607	0.0278	0.8517	0.0314

analyzed. To this end, a Pearson correlation test was applied over the SCUMBLE values and the relative changes in imbalance levels for each resampling algorithm. The resulting correlation coefficients and p-values are shown in Table 3. It can be seen that all the coefficients are above 80%, and all the p-values are under 0.05. Therefore, a statistical correlation between the SCUMBLE measure and the behavior of the tested resampling algorithms can be concluded.

Following this analysis, it seems reasonable to avoid resampling algorithms when the SCUMBLE measure for an MLD is well above 0.1, such as is the case with corel5k, cal500 and enron. In this situation the benefits obtained from resampling, if any, are very small. The result can even be a worsening of the imbalance level. In average, the MeanIR for the three MLDs with $SCUMBLE > 0.3$ has been reduced only by 6%, while the MaxIR is actually increasing in the same percentage. By contrast, the average MeanIR reduction for the other three MLDs, with $SCUMBLE \leq 0.1$, reaches 52% and the MaxIR reduction 54%.

Aiming to know how these changes in the imbalance levels would influence classification results, and if a correlation with SCUMBLE values exists, the HOMER [42] algorithm was used. It must be highlighted that the interest here is not in the raw performance values, but in how they change after a resampling algorithm has been applied and how this change correlates with SCUMBLE values. Therefore, the HOMER algorithm is used only as a tool to obtain classification results before and after applying the resampling. Any other MLC algorithm could be used for this task. Additionally, the proposed SCUMBLE measure is not used in the experimentation to influence the behavior of LP-ROS, LP-RUS or HOMER by any means. The goal is to explore the correlation between changes in classification results and SCUMBLE values.

Table 4 shows these results assessed with F-measure, the harmonic mean of precision and recall measures. It can be seen that with the three MLDs which show high SCUMBLE values, the pre-processing has produced a remarkable deterioration in classification results. Among the other three MLDs the resampling has improved them in some cases, while producing a slight worsening (less than 1%) in others. Therefore, even though the MLC algorithm behavior would be also affected by other dataset characteristics, that the SCUMBLE metric would offer valuable information to

Table 4
F-measure values obtained by HOMER MLC algorithm (average values over test partitions).

Dataset	Base	LP-RUS	LP-ROS	Δ RUS	Δ ROS
Corel5k	0.3857	0.2828	0.2920	-26.6788	-24.2935
Cal500	0.3944	0.3127	0.3134	-20.7150	-20.5375
Enron	0.5992	0.5761	0.5874	-3.8551	-1.9693
Yeast	0.6071	0.6950	0.6966	14.4787	14.7422
Medical	0.9238	0.9158	0.9162	-0.8660	-0.8227
Genbase	0.9896	0.9818	0.9912	-0.7882	0.1617

determine the convenience of applying a resampling method can be concluded.

5.3. REMEDIAL experimental results

Once the usefulness of the SCUMBLE metric has been demonstrated, the next experimental phase has been applying the algorithm REMEDIAL to the eleven datasets previously shown in Table 1, then learning from them using six multilabel classifiers. The results obtained from each one of them over the datasets, before and after preprocessing, are provided in Tables 5–9. Each table correspond to one evaluation metric. Best results are highlighted in bold. EPS was not able to process a couple of datasets.

The analysis of these results can be structured into three parts depending on where we put the focus, the classifiers, the datasets or the evaluation metrics.

- Going through the results by classifier, that REMEDIAL works better with BR and HOMER than with IBLR and CLR can be easily observed. The results for ECC and EPS are not conclusive, with almost as many cases with improvements and worsenings. Binary relevance based algorithms train a classifier for each label, taking as positive the instances containing it and as negative the remainder samples. When a majority label is being processed, all the instances in which it appears jointly with a minority label are processed as positive, disregarding the fact that they contain other labels. The decoupling of these labels tends to balance the bias of each classifier, something that also influences the behavior of ECC. LP based algorithms, such as HOMER, surely are favored by REMEDIAL, since the decoupling produces simpler labelsets. Moreover, the number of distinct labelsets is reduced after the resampling. The influence of REMEDIAL on instance based classifiers, such as IBLR, is easy to devise. The attributes of the decoupled samples do not change, so they will occupy exactly the same position with respect to the instance which is taken as reference for searching nearest neighbors. Therefore, the classifier will get two samples at the same distance but with disjoint labelsets, something that can

Table 5
Results before and after applying REMEDIAL assessed with Hamming Loss (↓).

Dataset	BR		CLR		ECC		EPS		HOMER		IBLR	
	Before	After										
Bibtex	0.0147	0.0132	0.0127	0.0130	0.0126	0.0135	–	–	0.0185	0.0166	0.0165	0.0155
Cal500	0.1630	0.1497	0.1381	0.1442	0.1422	0.1490	–	–	0.1875	0.1815	0.2341	0.2125
Corel16k	0.0206	0.0196	0.0198	0.0195	0.0387	0.0195	0.0196	0.0268	0.0271	0.0228	0.0199	0.0198
Corel5k	0.0098	0.0094	0.0095	0.0094	0.0094	0.0089	0.0173	0.0101	0.0132	0.0118	0.0242	0.0148
Cs	0.0094	0.0089	0.0088	0.0088	0.0086	0.0578	0.0133	0.0112	0.0117	0.0104	0.0182	0.0143
Enron	0.0522	0.0540	0.0476	0.0517	0.0484	0.0086	0.0733	0.0601	0.0574	0.0555	0.0571	0.0593
Genbase	0.0012	0.0084	0.0014	0.0080	0.0014	0.0386	0.0028	0.0040	0.0016	0.0064	0.0022	0.0092
Mediamill	0.0343	0.0331	0.0291	0.0321	0.0288	0.0118	0.0524	0.0377	0.0384	0.0355	0.0291	0.0338
Medical	0.0107	0.0131	0.0109	0.0132	0.0100	0.0717	0.0141	0.0143	0.0109	0.0118	0.0198	0.0198
Tmc2007	0.0568	0.0684	0.0538	0.0658	0.0507	0.2316	0.0872	0.0693	0.0607	0.0647	0.0646	0.0775
Yeast	0.2505	0.2347	0.2202	0.2228	0.3594	0.0094	0.2042	0.2853	0.2601	0.2476	0.1941	0.2264

Table 6Results before and after applying REMEDIAL assessed with Precision (\uparrow).

Dataset	BR		CLR		ECC		EPS		HOMER		IBLR	
	Before	After	Before	After	Before	After	Before	After	Before	After	Before	After
Bibtex	0.5770	0.7451	0.8267	0.9173	0.7385	0.8023	–	–	0.4701	0.5356	0.4920	0.5004
Cal500	0.4397	0.5326	0.6363	0.8327	0.5636	0.6848	–	–	0.3842	0.3983	0.2859	0.2743
Corel16k	0.3610	0.4682	0.4455	0.6056	0.1944	0.6913	0.4697	0.2010	0.2475	0.2921	0.3623	0.3079
Corel5k	0.3643	0.4781	0.4621	0.5983	0.5465	0.6868	0.1938	0.2906	0.2232	0.2438	0.0598	0.0602
Cs	0.5174	0.6239	0.6297	0.7247	0.6211	0.7611	0.3366	0.3632	0.3884	0.4394	0.1076	0.0919
Enron	0.6391	0.7063	0.7047	0.7813	0.6681	0.9960	0.4873	0.5592	0.5893	0.6269	0.6151	0.6519
Genbase	0.9947	0.9977	0.9946	0.9977	0.9950	0.8877	0.9950	0.9942	0.9932	0.9961	0.9899	0.9890
Mediamill	0.6683	0.8091	0.7959	0.8707	0.7986	0.8740	0.4827	0.6271	0.6177	0.6805	0.7758	0.8388
Medical	0.8633	0.8680	0.8699	0.8725	0.8636	0.8701	0.7813	0.7837	0.8639	0.8648	0.7272	0.7552
Tmc2007	0.7675	0.8334	0.7855	0.8539	0.8056	0.7370	0.6079	0.6903	0.7389	0.7829	0.7309	0.8031
Yeast	0.6020	0.6647	0.6768	0.7323	0.4777	0.6899	0.6960	0.5422	0.5876	0.6169	0.7110	0.7442

Table 7Results before and after applying REMEDIAL assessed with Macro F-Measure (\uparrow).

Dataset	BR		CLR		ECC		EPS		HOMER		IBLR	
	Before	After										
Bibtex	0.3368	0.3604	0.3342	0.3518	0.3750	0.3763	–	–	0.2984	0.2985	0.2140	0.1950
Cal500	0.2933	0.2286	0.3323	0.2436	0.3058	0.0670	–	–	0.3301	0.3372	0.2772	0.2527
Corel16k	0.1550	0.1266	0.1084	0.0707	0.1477	0.1056	0.1223	0.1401	0.1510	0.1377	0.1146	0.0956
Corel5k	0.1774	0.1827	0.1330	0.1073	0.1666	0.2922	0.1860	0.1767	0.1963	0.1860	0.1060	0.1432
Cs	0.3457	0.3795	0.2801	0.2606	0.3617	0.2760	0.3044	0.2992	0.2999	0.2922	0.1355	0.1341
Enron	0.4029	0.4189	0.4199	0.3755	0.4324	0.8970	0.3828	0.3933	0.3836	0.3828	0.3458	0.2755
Genbase	0.9890	0.9923	0.9848	0.9415	0.9906	0.1741	0.9775	0.9527	0.9806	0.9662	0.9655	0.8449
Mediamill	0.2836	0.2959	0.2307	0.2011	0.2445	0.8085	0.3382	0.2657	0.2492	0.2147	0.2818	0.1820
Medical	0.8165	0.8013	0.7942	0.7864	0.8179	0.3318	0.7283	0.7292	0.7981	0.7855	0.6404	0.6189
Tmc2007	0.6015	0.4243	0.6073	0.3578	0.5966	0.4063	0.5802	0.5951	0.5981	0.4551	0.4667	0.2786
Yeast	0.4341	0.5204	0.4480	0.4075	0.4782	0.1356	0.4629	0.4428	0.4363	0.4400	0.4945	0.3901

Table 8Results before and after applying REMEDIAL assessed with One Error (\downarrow).

Dataset	BR		CLR		ECC		EPS		HOMER		IBLR	
	Before	After	Before	After	Before	After	Before	After	Before	After	Before	After
Bibtex	0.5060	0.4648	0.4110	0.4120	0.3886	0.4018	–	–	0.6040	0.6040	0.6043	0.6651
Cal500	0.7202	0.6963	0.1254	0.1245	0.1504	0.3735	–	–	0.8167	0.7660	0.8756	0.8885
Corel16k	0.6964	0.7289	0.6650	0.6696	0.7138	0.7036	0.6809	0.7906	0.7712	0.8065	0.7106	0.7359
Corel5k	0.7067	0.7134	0.6716	0.6753	0.6828	0.5181	0.7853	0.9070	0.7994	0.8165	0.9401	0.9066
Cs	0.5690	0.5679	0.5112	0.5130	0.4833	0.3144	0.5596	0.6629	0.6680	0.7042	0.9041	0.8711
Enron	0.3922	0.3554	0.2350	0.2311	0.2700	0.0037	0.3044	0.4168	0.4456	0.4360	0.3805	0.3734
Genbase	0.0052	0.0060	0.0022	0.0030	0.0022	0.1769	0.0037	0.0068	0.0114	0.0106	0.0098	0.0384
Mediamill	0.3943	0.2093	0.1125	0.1155	0.1153	0.1616	0.1155	0.1651	0.3839	0.3479	0.1215	0.1351
Medical	0.1906	0.1984	0.1559	0.1544	0.1534	0.1716	0.1830	0.1917	0.2107	0.2224	0.3190	0.3175
Tmc2007	0.2374	0.2137	0.1575	0.1544	0.1603	0.2685	0.1855	0.2122	0.2788	0.2836	0.2298	0.2345
Yeast	0.4181	0.3856	0.2399	0.2366	0.2574	0.7249	0.2520	0.2873	0.4268	0.3885	0.2255	0.2441

- be confusing depending on how the algorithm predicts the labelset of the reference sample.
- Analyzing the results by dataset, two thirds of the best values for enron, corel5k and cal500 are obtained after applying REMEDIAL. As can be checked, these are the datasets with highest SCUMBLE levels. On the other hand, the results that correspond to the genbase, medical and tmc2007 have not improvements. As shown in Table 1, these are three datasets with low SCUMBLE values. Although some differences are quite small, in general the decoupling of labels has worsened classification performance. The remainder five MLDs get mixed results, although this trend (the higher the SCUMBLE level the more the result is improved) is similar. As a consequence a clear guideline follows from the analysis of these results, REMEDIAL should not be used with MLDs with low SCUMBLE levels, since it is an algorithm specifically designed to face the opposite casuistic.
 - Lastly, focusing on the evaluation metrics, that Precision is higher after applying REMEDIAL for most of the datasets and classifiers, with only 9 out of 64 (14%) cases without improvements, can be observed. According to the other four evaluation

metrics, HL, MacroFM, OE and RL, there is almost a tie between cases whose results have been improved and those which have not achieved this goal. The view changes drastically depending on each classifier/metric combination. For instance, the HL and Precision values for HOMER state that REMEDIAL improves results in 19 out of 22 cases (86%), but MacroFM and RL indicates the same only for 5 out of 22 (23%).

The statistical significance of the differences in the results just pointed out has been assessed by means of a paired Wilcoxon statistical test. The exact p -values for each metric/classifier are shown in Table 10. Those preceded with a * symbol can be considered as significant from a statistical point of view, applying the usual 0.05 threshold. Most of the differences are not statistically significant. However, Precision and MacroFM show important differences in half or more of the cases. The former metric reveals statistically significant improvements with BR, CLR, ECC and HOMER. On the contrary, MacroFM indicates that the worsening of results is remarkable for CLR, HOMER and IBLR.

Table 9

Results before and after applying REMEDIAL assessed with Ranking Loss (↓).

Dataset	BR		CLR		ECC		EPS		HOMER		IBLR	
	Before	After										
Bibtex	0.1635	0.1986	0.0620	0.0622	0.0950	0.1206	–	–	0.3295	0.3382	0.1742	0.1824
Cal500	0.3159	0.2086	0.1809	0.1805	0.1975	0.2343	–	–	0.3911	0.3775	0.3790	0.3226
Corel16k	0.1857	0.1848	0.1335	0.1335	0.2907	0.1840	0.1772	0.3367	0.3973	0.4228	0.1687	0.1733
Corel5k	0.1474	0.1416	0.1176	0.1176	0.1414	0.1295	0.4807	0.6748	0.4387	0.4690	0.2754	0.2620
Cs	0.1996	0.1703	0.0672	0.0672	0.1118	0.0911	0.2604	0.3409	0.3532	0.3770	0.2234	0.2271
Enron	0.1746	0.1409	0.0737	0.0736	0.0852	0.0062	0.1667	0.2333	0.2502	0.2759	0.1066	0.1066
Genbase	0.0030	0.0137	0.0088	0.0089	0.0036	0.0534	0.0078	0.0096	0.0060	0.0240	0.0040	0.0326
Mediamill	0.1742	0.0761	0.0336	0.0338	0.0439	0.0394	0.0738	0.1154	0.2162	0.2236	0.0391	0.0404
Medical	0.0703	0.0785	0.0297	0.0297	0.0357	0.0547	0.0686	0.0664	0.0999	0.1045	0.0653	0.0640
Tmc2007	0.1139	0.1271	0.0347	0.0338	0.0444	0.1895	0.0631	0.0956	0.1547	0.1852	0.0558	0.0589
Yeast	0.3156	0.2536	0.1799	0.1785	0.2021	0.1442	0.1854	0.2241	0.3407	0.3213	0.1643	0.1768

Table 10

Exact p-values produced by the Wilcoxon statistical test for each classifier/metric.

Classifier	Hamming Loss	Precision	Macro F-Measure	One Error	Ranking Loss
BR	0.824098	*0.003857	0.893904	0.142368	0.266402
CLR	*0.016316	*0.003857	*0.006692	0.893904	0.824098
ECC	0.689084	*0.029383	0.398305	0.449804	0.964541
EPS	0.150786	0.352542	0.932647	0.150786	0.150786
HOMER	0.168167	*0.003857	*0.029383	0.893904	*0.045447
IBLR	0.683481	0.266402	*0.018408	0.398305	0.414823

Overall, REMEDIAL would be a recommended resampling for MLDs with high *SCUMBLE* levels and when BR or LP based classifiers are going to be used. In these cases the prediction of minority labels would be improved, and the global performance of the classifiers would be better. MLDs such as genbase, medical and tmc2007, as their intrinsic traits have demonstrated, should not be processed with REMEDIAL. The same would be applicable to classifiers such as IBLR, as putting two data samples at the same location but having disjoint labelsets tend to confuse this kind of algorithms. Excluding these cases, the global evaluation of the results produced by REMEDIAL would be much more positive.

The already described before are the benefits brought by REMEDIAL on their own, but this algorithm could be used as a first step aimed to ease the work of traditional resampling techniques. Mixing REMEDIAL with standard oversampling and undersampling techniques would be an interesting further study.

6. Conclusions

From the conducted experimentation and further analysis it can be inferred that, while working with imbalanced MLDs, standard resampling methods should be avoided when the *SCUMBLE* level is well above 0.1. In this situation the benefits from resampling are almost negligible, or even detrimental.

In the described scenario, with MLDs suffering from high concurrence among imbalance labels, the proposed REMEDIAL algorithm has proven to be effective. The algorithm looks for instances with a high *SCUMBLE* level and decouples minority and majority labels, producing new instances. The conducted experimentation has proven that REMEDIAL is able to improve classification results when applied to MLDs with a high *SCUMBLE*.

How to assess the concurrence problem, and how to deal with it in practice, has been explained by means of the mlDr R package (see Appendix A). This software has been extended by the authors to include the metrics and algorithms described in this paper. The goal is to help anyone interested in this topic to conduct their personal analysis.

It could be concluded that basic resampling algorithms, which clone the labelsets in new instances or remove samples, are not a general solution in the multilabel field. More sophisticated ap-

proaches, which take into account the concurrence among imbalanced labels, would be needed. A potential way for designing these new algorithms would be joining REMEDIAL with some of the existent resampling methods. Once the labels have been decoupled, traditional oversampling and undersampling algorithms would find less obstacles to do their work.

Acknowledgments

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Appendix A. SCUMBLE and REMEDIAL implementations in the mlDr package

This appendix describes how to obtain the *SCUMBLE* measurement for any MLD, as well as how to apply the REMEDIAL algorithm proposed in this study to any MLD, by means of a software package developed by the same authors.

A1. Assessing label concurrence with the mlDr package

The mlDr package [18] provides an easy way to make exploratory analysis over MLDs from R, one of the best known tools for machine learning tasks. A quick tutorial describing how to install and use this package can be found in [49]. The capabilities of the mlDr package have been extended to include functions aimed to ease the concurrence analysis in MLDs. These new capabilities, developed ad hoc for the present work, are described below.

Once the package has been loaded into R, the first step will be reading the MLD to analyze. MULAN [50] and MEKA [51] file formats are supported. In order to load an MLD, the mlDr function has to be called providing the file name. The returned result is an S3 R object containing the data (instances with attribute values) and also a plethora of characterization metrics.

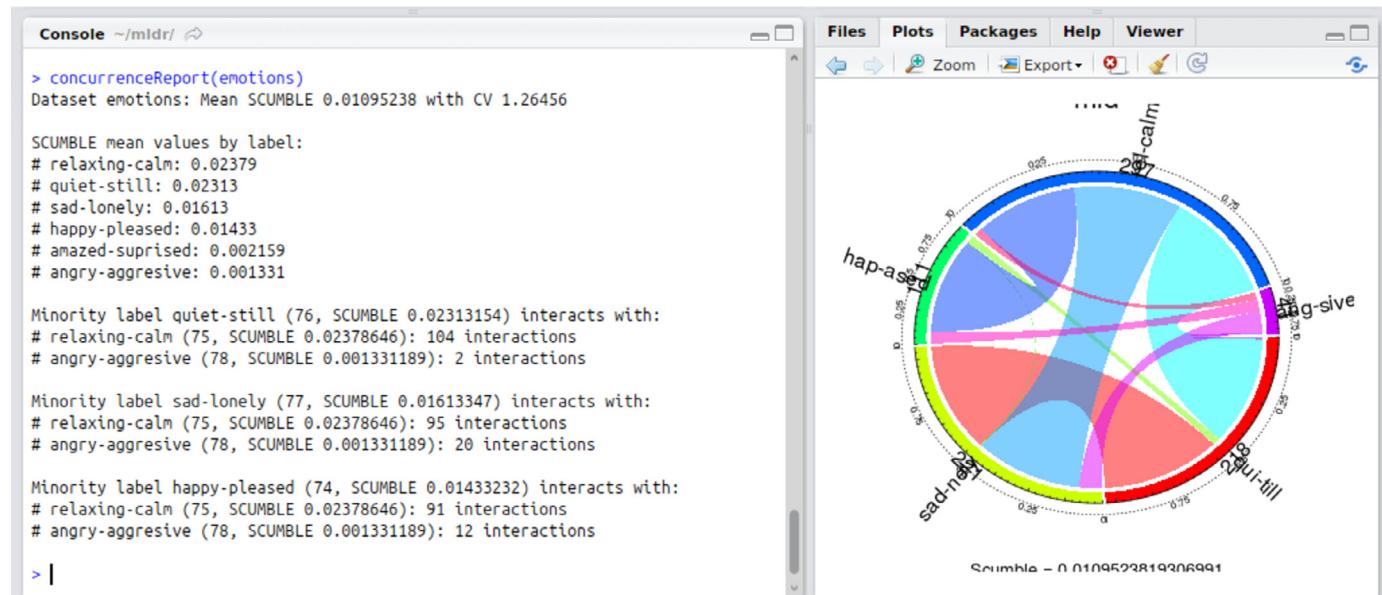
The group of metrics that are general to the whole MLD can be retrieved with the summary function, as shown in the upper part of Fig. A.5. In this example the measures belonging to the genbase

```

> library(mldr)
Enter mldrGUI() to launch mldr's web-based GUI
> summary(genbase)
  num.attributes num.instances num.inputs num.labels num.labelsets num.single.labelsets
max.frequency cardinality   density   meanIR    scumble scumble.cv
1           1213        662     1186       27        32          10
170      1.252266 0.04638022 37.31458 0.0287591  3.614486
> emotions$labels
  index count   freq   IRLbl   SCUMBLE SCUMBLE.CV
amazed-surprised 73 173 0.2917369 1.526012 0.002159173 2.4711227
happy-pleased    74 166 0.2799325 1.590361 0.014332319 0.8889398
relaxing-calm     75 264 0.4451939 1.000000 0.023786461 0.4839719
quiet-still       76 148 0.2495784 1.783784 0.023131538 0.6290932
sad-lonely        77 168 0.2833052 1.571429 0.016133470 0.8069413
angry-aggressive  78 189 0.3187184 1.396825 0.001331189 2.4881141
```

```

**Fig. A5.** Obtaining basic concurrence metrics using the mldr R package.



**Fig. A6.** The concurrence report provides information about label interactions, both textually and visually.

MLD have been obtained. By querying the `labels` member of the object the information relative to each label is retrieved, including the `SCUMBLElbl` and its corresponding coefficient of variation as shown in the bottom part of the same Fig. A5.

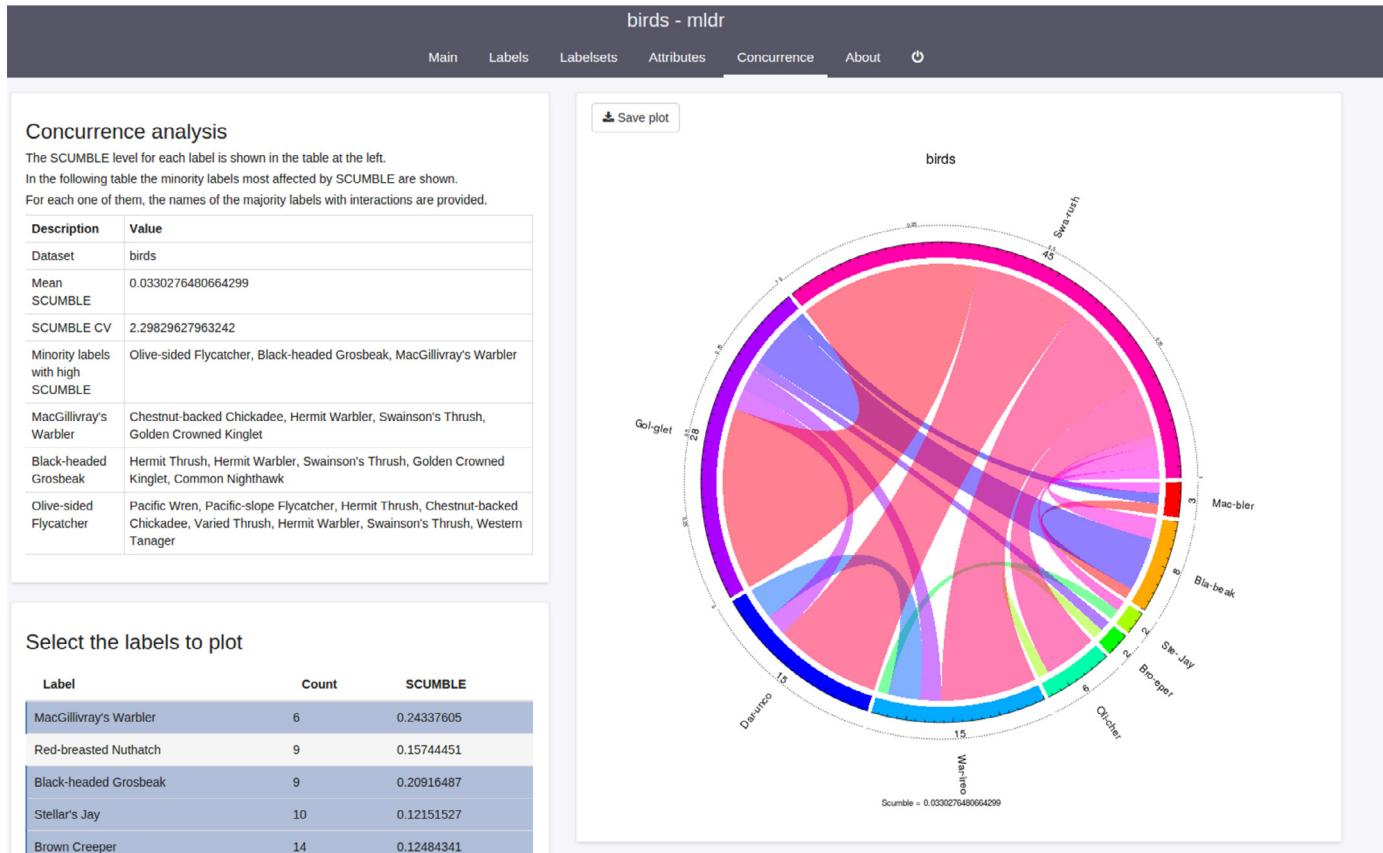
Relying on the measures obtained with the previous methods, essentially the `IRLbl`, `SCUMBLElbl` and name of each label, it is possible to infer which are the minority labels and which of those are more affected by the concurrence problem. However, it would not be easy to know what majority labels are interacting with each minority one. This information can be visually explored using the specific `plot` function provided by the `mldr` package, able to generate interaction plots similar to the ones shown in Figs. 1 and 2.

Another alternative would be calling the `mldr`'s function `concurrenceReport`. It generates a full report stating what are the `SCUMBLE` levels for the MLD and each of its labels, as well as a summary of label interactions and a plot of them. This report is sent to the console by default (see Fig. A6), but it can also be

saved as a PDF document by providing the `pdfOutput` parameter with the `TRUE` value. The report will include the minority labels most affected by the concurrence problem, sorted by their `SCUMBLElbl` value. It will be, in fact, a list of difficult labels, along with the majority labels each one of them interacts with.

In addition to the aforementioned functions, which are only a small sample of the set provided by the `mldr` package, a web GUI is also available. This can be launched from the R command line with the `mldrGUI`<sup>3</sup> function. It is structured into several pages, accessible by the tags located at the top. In the Concurrence page the same information provided by the `concurrenceReport` can be found, along with a customizable plot showing label interac-

<sup>3</sup> An online version of the `mldr`'s web interface, accessible from any browser without needing to install R or the `mldr` package, is available at <https://fdavidc.shinyapps.io/mldr/>. Although the bandwidth provided by shinyapps.io is limited, the application can be used to test the functionality described in this section.



**Fig. A7.** The mldr GUI eases the process of obtaining customized concurrence information.

```
Console ~/mldr/
> library(mldr)
Enter mldrGUI() to launch mldr's web-based GUI
>
> genbase.decoupled <- remedial(genbase)
> summary(genbase)
 num.attributes num.instances num.inputs num.labels num.labelsets num.single.labelsets max.frequency cardinality density meanIR scumble scumble.cv
1 1213 662 662 27 32 10 170 1.252266 0.04638022 37.31458 0.0287591 3.614486
> summary(genbase.decoupled)
 num.attributes num.instances num.inputs num.labels num.labelsets num.single.labelsets max.frequency cardinality density meanIR scumble scumble.cv
1 1213 752 752 27 32 7 171 1.102394 0.04082939 37.31458 0.01395751 3.483609
~ genbase.decoupled <- remedial(genbase.decoupled)
```

**Fig. A8.** MLD basic traits before and after applying the REMEDIAL preprocessing algorithm.

tions. This page is partially visible in Fig. A7. The list below the report allows the interactive selection of labels to be shown in the plot. The result can be saved to a file.

Overall, the exploratory tools implemented into the mldr package will provide all the information needed to analyze how the concurrence among imbalanced labels affects a certain MLD, as well as which of the labels could be considered difficult labels.

## A2. The mldr package's REMEDIAL implementation

Along with the exploratory functionality previously described, the mldr package has been also extended by including a reference implementation of the algorithm REMEDIAL. The function containing this implementation is called `remedial`. To use it an mldr object has to be given as input, obtaining as output the preprocessed version of the same object. In Fig. A8 how to use this function is shown. The algorithm is applied to the genbase MLD, storing the result into the `genbase.decoupled` variable.

From the information provided by the `summary` function, corresponding to the MLD before and after the preprocessing, the following facts can be observed:

- The number of instances grows, as REMEDIAL produces new data samples.
- Since the number of active labels in the MLD does not change, neither do the number of labels and the imbalance related metrics, such as *MeanIR*.
- Because the same number of active labels are split into a larger number of instances, label cardinality and density decrease.
- In general, the decoupling of labels tend to produce simpler and more frequent labelsets.
- The global *SCUMBLE* and the *SCUMBLElbl* are reduced.

As the algorithm REMEDIAL takes as reference the mean *SCUMBLE* to determine which samples are going to be decoupled, and this measure is reduced as a result of applying REMEDIAL, it can be run several times over the same data to progressively reduce the concurrence problem. In Fig. A9 the emotions MLD is used to show a simple example. The main metrics of the MLD and its labels are displayed after calling the `remedial` function once and twice. The differences are remarkable as can be seen.

```

Console ~/mldr/ ↵
> summary(emotions)
num.attributes num.instances num.inputs num.labels num.labelsets num.single.labelsets max.frequency cardinality density meanIR scumble scumble.cv
1 78 593 72 6 27 4 81 1.868465 0.3114109 1.478068 0.01095238 1.26456
> summary(remedial(emotions))
num.attributes num.instances num.inputs num.labels num.labelsets num.single.labelsets max.frequency cardinality density meanIR scumble scumble.cv
1 78 815 72 6 19 2 257 1.359509 0.2265849 1.478068 0.0005623093 2.566903
> summary(remedial(remedial(emotions)))
num.attributes num.instances num.inputs num.labels num.labelsets num.single.labelsets max.frequency cardinality density meanIR scumble scumble.cv
1 78 1043 72 6 13 1 257 1.06232 0.1770534 1.478068 0.0003179895 3.98286
> emotions$labels
 index count freq IRLbl SCUMBLE SCUMBLE.CV
amazed-surprised 73 173 0.2917369 1.526012 0.002159173 2.4711227
happy-pleased 74 166 0.2799325 1.590361 0.014332319 0.8889398
relaxing-calm 75 264 0.4451939 1.000000 0.023786461 0.4839719
quiet-still 76 148 0.2495784 1.783784 0.023131538 0.6290932
sad-lonely 77 168 0.2833052 1.571429 0.016133470 0.8069413
angry-aggressive 78 189 0.3187184 1.396825 0.001331189 2.4881141
> remedial(remedial(emotions))$labels
 index count freq IRLbl SCUMBLE SCUMBLE.CV
amazed-surprised 73 173 0.1658677 1.526012 7.523092e-05 1.3107425
happy-pleased 74 166 0.1591563 1.590361 1.413782e-04 2.3392930
relaxing-calm 75 264 0.2531160 1.000000 3.659295e-04 6.0592314
quiet-still 76 148 0.1418984 1.783784 1.500168e-03 0.5692001
sad-lonely 77 168 0.1610738 1.571429 1.259564e-03 0.7641657
angry-aggressive 78 189 0.1812081 1.396825 5.111396e-04 5.0990195
>

```

**Fig. A9.** The algorithm can be applied several times to progressively reduce the concurrence problem.

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