Random k-Labelsets
for Multi-Label Classification

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Abstract—A simple yet effective multi-label learning method, called label powerset (LP), considers each distinct combination of labels that exist in the training set as a different class value of a single-label classification task. The computational efficiency and predictive performance of LP is challenged by application domains with large number of labels and training examples. In these cases the number of classes may become very large and at the same time many classes are associated with very few training examples. To deal with these problems, this paper proposes breaking the initial set of labels into a number of small random subsets, called *labelsets* and employing LP to train a corresponding classifier. The labelsets can be either disjoint or overlapping depending on which of two strategies is used to construct them. The proposed method is called RAkEL (RAndom k labELsets), where k is a parameter that specifies the size of the subsets. Empirical evidence indicate that RAkEL manages to improve substantially over LP, especially in domains with large number of labels and exhibits competitive performance against other high-performing multi-label learning methods.

Index Terms—Categorization, Multi-label, Ensembles, Labelset

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1 INTRODUCTION

TRADITIONAL single-label classification is concerned with learning from a set of data that are associated with a single label λ from a set of disjoint labels L of size M, with $M > 1$. If $M = 2$, then the learning task is called binary classification, concept learning, or filtering, while if $M > 2$, then it is called multi-class classification.

In several application domains however, data are associated with a set of labels $Y \subseteq L$. In text categorization for example, a newspaper article concerning the reactions of the Christian church to the release of the "Da Vinci Code" film can be classified into both of the categories *society\religion* and *arts\movies*. Similarly in semantic scene classification [1], [2], [3], a photograph can belong to more than one conceptual class, such as *sunset* and *beach* at the same time. Other interesting applications of multi-label classification include music categorization into emotions [4], [5], [6], semantic video annotation [7], [8], direct marketing [9] and automated tag suggestion [10], [11].

This paper focuses on the label powerset (LP) multi-label learning method [1], [12], which considers each subset of L, hitherto called *labelset*, that exists in the training set as a different class value of a single-label classification task. LP is an interesting approach to study, as it has the advantage of taking label correlations into consideration. This way it can, in some cases, achieve better performance compared to computationally simpler approaches like binary relevance (BR), which learns a binary model for each label independently of the rest [13].

However, LP is challenged by application domains with large number of labels and training examples, due to the typically proportionally large number of labelsets appearing in the training set. The large number of these labelsets (class values for the single-label classifier of LP), raises the computational cost of LP on one hand, and makes its learning task quite hard on the other, as many of these labelsets are usually associated with very few training examples. Moreover, LP can only predict labelsets observed in the training set. This is an important limitation, because new labelsets typically do appear in test sets, which simulate unseen data.

In order to deal with the aforementioned problems of LP, this work proposes randomly breaking the initial set of labels into a number of small-sized labelsets, and employing LP to train a corresponding multi-label classifier. This way, the resulting single-label classification tasks are computationally simpler and the distribution of their class values is less skewed. The proposed method is called RAkEL (RAndom k labELsets) [13], where k is a parameter that specifies the size of the labelsets. Two different strategies for constructing the labelsets are studied. The first one leads to *disjoint*, whereas the second to *overlapping* labelsets.

Empirical evidence indicate that both approaches manage to significantly improve LP, especially in domains with large number of labels. The overlapping strategy achieves higher predictive performance than the disjoint one, as the aggregation of multiple predictions for each label via voting allows the correction of potential uncorrelated errors. Finally, a comparative study against other multi-label learning methods, indicates that RAkEL with overlapping labelsets is highly competitive.

The rest of this paper is structured as follows. The following section presents related work on learning from multi-label data. Section 3 discusses the motivations

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and rationale for using RAkEL and describes the two alternative strategies for creating the labelsets in detail. Section 4 describes the datasets that are involved in the experiments and the evaluation measures, while Section 5 presents and discusses the results. Finally, the last section highlights the main points of this work and presents its conclusions.

2 RELATED WORK

Multi-label learning methods can be grouped into two categories [12]: i) *problem transformation*, and ii) *algorithm adaptation*. Methods of the first group transform the learning task into one or more single-label classification or ranking tasks, for which a large bibliography of learning algorithms exists. The second group of methods extend specific learning algorithms in order to handle multi-label data directly.

2.1 Problem Transformation Methods

The following paragraphs describe a number of problem transformation methods from the literature. For the formal description of these methods, we will use $L = \{\lambda_j : j = 1 \ldots M\}$ to denote the finite set of labels in a multi-label learning task and $D = \{(\vec{x_i}, Y_i), i = 1 \ldots N\}$ to denote a set of multi-label training examples, where $\vec{x_i}$ is the feature vector and $Y_i \subseteq L$ the set of labels of the i-th example.

There exist several transformations that can be used to convert a multi-label dataset into a single-label one, where a single-label classifier that outputs a probability distribution over the classes can be applied in order to learn a label ranker [1], [14]. The *copy* transformation replaces each multi-label example (x_i, Y_i) with $|Y_i|$ examples (x_i, λ_j), for every $\lambda_j \in Y_i$. A variation of this transformation, dubbed *copy-weight*, associates a weight of $\frac{1}{|Y_i|}$ to each of the produced examples. The *select* family of transformations replaces Y_i with one of its members. This label could be the most (*select-max*) or least (*select-min*) frequent among all examples. It could also be randomly selected (*select-random*). Finally, the *ignore* transformation simply discards every multi-label example.

Binary relevance (BR) is a popular problem transformation method that learns M binary classifiers, one for each different label in L. It transforms the original dataset into M data sets $D_{\lambda_j}, j = 1 \ldots M$ that contain all examples of the original dataset, labeled positively if the label set of the original example contained λ_j and negatively otherwise. For the classification of a new instance, BR outputs the union of the labels λ_j that are predicted by the M classifiers.

Label powerset (LP) is a simple but effective problem transformation method that works as follows: It considers each unique set of labels that exists in a multi-label training set as one of the classes of a new single-label classification task. Given a new instance, the single-label classifier of LP outputs the most probable class, which actually represents a set of labels.

Ranking by pairwise comparison (RPC) [15] transforms the multi-label data set into $\frac{M(M-1)}{2}$ binary label datasets, one for each pair of labels $(\lambda_i, \lambda_j), 1 \leq i < j \leq M$. Each dataset contains those examples of D that are annotated by at least one of the two corresponding labels, but not both. A binary classifier that learns to discriminate between the two labels, is trained from each of these datasets. Given a new instance, all binary classifiers are invoked, and a ranking is obtained by counting the votes received by each label. The multi-label pairwise perceptron (MLPP) algorithm [16] is an instantiation of RPC using perceptrons for the binary classification tasks.

Calibrated label ranking (CLR) [17] extends RPC by introducing an additional virtual label, which acts as a natural breaking point of the ranking into a relevant and an irrelevant set of labels. The binary models that learn to discriminate between the virtual label and each of the other labels, correspond to the models of BR. This occurs, because each example that is annotated with a given label is considered as positive for this label and negative for the virtual label, while each example that is not annotated with a label is considered negative for it and positive for the virtual label.

2.2 Algorithm Adaptation Methods

The following paragraphs briefly report a plethora of algorithm adaptation methods grouped by the learning paradigm that they extend.

Decision Trees and Boosting. The C4.5 algorithm was adapted in [18] for the handling of multi-label data. AdaBoost.MH and AdaBoost.MR [19] are two extensions of AdaBoost for multi-label data. A combination of AdaBoost.MH with an algorithm for producing alternating decision trees was presented in [20]. The main motivation was the production of multi-label models that can be understood by humans.

Probabilistic Methods. A probabilistic generative model for multi-label text classification is proposed in [21], according to which, each label generates different words. Based on this model a multi-label document is produced by a mixture of the word distributions of its labels. A similar word-based mixture model is presented in [22]. A deconvolution approach is proposed in [23], in order to estimate the individual contribution of each label to a given item. The use of conditional random fields is explored in [24], where two graphical models that parameterize label co-occurrences are proposed.

Neural Networks and Support Vector Machines. BP-MLL [25] is an adaptation of the popular backpropagation algorithm for multi-label learning. The main modification to the algorithm is the introduction of a new error function that takes multiple labels into account. This error function is similar to the ranking loss [19]. ML-RBF [26] is a recent approach for adapting

radial basis function networks to multi-label data. The multi-class multi-label perceptron (MMP) [27] is a family of online algorithms for label ranking from multi-label data based on the perceptron algorithm. MMP maintains one perceptron for each label, but weight updates for each perceptron are performed so as to achieve a perfect ranking of all labels. An SVM algorithm that minimizes the ranking loss is proposed in [28].

Lazy and Associative Methods. A number of methods [29], [5], [30], [2], [31] are based on the popular k Nearest Neighbors (kNN) lazy learning algorithm. The first step in all these approaches is the same as in kNN, i.e. retrieving the k nearest examples. What differentiates them is the aggregation of the label sets of these examples. MMAC [32] is an algorithm that follows the paradigm of associative classification, which deals with the construction of classification rule sets using association rule mining. Finally, an approach that combines lazy and associative learning is proposed in [33], where the inductive process is delayed until an instance is given for classification.

3 RANDOM k-LABELSETS

Label powerset (LP) is a relatively simple method with the advantage of taking label correlations into account. However, as briefly mentioned in the introduction of this article, it is challenged by domains with large number of labels, M, and training examples, N.

The computational complexity of LP with respect to M and N depends on the computational complexity of the underlying single-label classification algorithm with respect to the number of examples N and the number of classes, which is equal to the number of labelsets that are used as annotations for the instances of the training set. This number is upper bounded by $\min(N, 2^M)$, but is usually much smaller in practice. Columns *bound* and *actual* of Table 2 show the bound of the number of labelsets and their actual number, for the datasets that are used in the experiments. Note that apart from the dataset with the fewest number of labels (6), in the rest the bound is equal to N. The actual number of labelsets in a dataset ranges from 5% to 44% of this bound, as indicated by column *diversity*, which measures the diversity of the labelsets that exist in a dataset. Despite being smaller than the bound, the high number of these labelsets can constitute an important scalability problem for LP, especially for large values of N and M.

In addition, the fact that many of these labelsets are associated with very few examples, makes the learning process difficult as well. As an example, consider the *mediamill* dataset [8], which is described in more detail in Section 4.1 along with the rest of the datasets that are used in the experiments. Figure 1 shows a histogram of the number of appearances of the 6555 different labelsets that exist in this dataset. The total number of appearances (examples in the dataset) is 43907. The y axis (logarithmic scale with base 10) shows the number

of labelsets, whose number of appearances falls into the corresponding bin of the x axis (logarithmic scale with base 2). It can be seen that most of the labelsets are very infrequent. In fact, 4104 labelsets appear just once in this dataset, while those that appear up to 8 times account for 92% of all 6555 distinct labelsets.
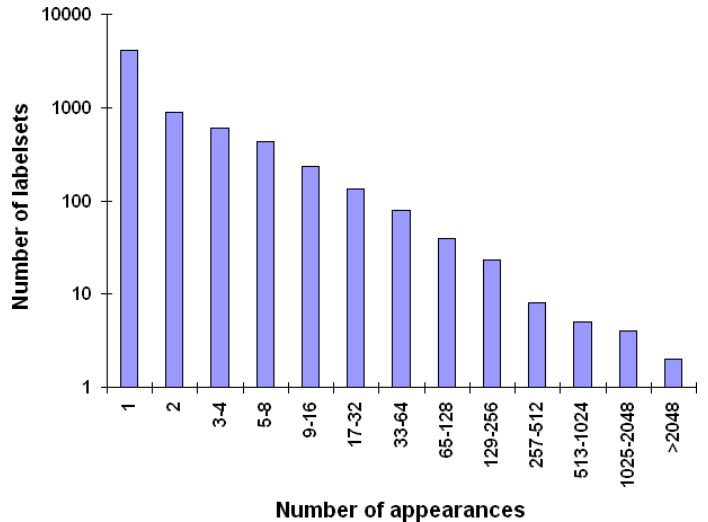

Fig. 1. Histogram of the number of appearances of the 6555 different labelsets in the mediamill dataset. The counts in the y axis (logarithmic scale with base 10) correspond to the number of labelsets that exhibit the corresponding bin of appearances in the x axis (logarithmic scale with base 2).

The main idea in this work is to randomly break a large set of labels into a number of small-sized labelsets, and for each of them train a multi-label classifier using the LP method. For the multi-label classification of an unlabeled instance, the decisions of all LP classifiers are gathered and combined. For simplicity, we only consider labelsets of the same size, k. A labelset $R \subseteq L$ with $k = |R|$ is called k-labelset. Therefore, the proposed approach is dubbed RAkEL (RAndom k labELsets). This paper examines the construction of two different types of labelsets: a) disjoint (RAkEL$_d$), and b) overlapping (RAkEL$_o$). In the following two sections we describe the functionality of both variations of RAkEL in more detail.

RAkEL offers advantages over LP for the following reasons. First of all, the resulting single-label classification tasks are computationally simpler. To see why this occurs, consider the case of the *mediamill* dataset again. If we break the set of 101 labels of *mediamill* into a number of labelsets of size $k = 3$, then each LP model will have to predict 8 (2^3) classes in the worst case. If we construct 200 such models, training each of them using a one-vs-rest support vector machine, then 1600 ($200 * 8$) binary models will be built in the worst case, which is much less compared to the 6555 binary models required by the full LP using the same underlying learning algorithm. On the other hand, using a decision tree learning algorithm underneath will probably lead RAkEL to a larger overall

computational cost, as decision tree learners are sublinear with respect to the number of classes. A complexity analysis is presented in Section 3.3.

In addition, the resulting single-label classification tasks are characterized by a much more balanced distribution of class values. Using the same example as above, we can see that the distribution of the 8 class values of each simpler problem, will not be as skewed as that of the 6555 class values that we have seen in Figure 1. This in turns means an easier single-label learning problem to deal with. Note that this benefit is independent of the single-label learning algorithm used underneath.

Finally, in the case of overlapping labelsets, RAkEL can gather multiple predictions for the same label by the different LP models that include this label in their labelset. As the different LP models are trained on a different output space (different class labels), they offer a diverse view of the task of predicting the value for specific labels. Therefore combining their output through a voting process, offers the chance of correcting potential uncorrelated errors, and improving the overall performance. In this respect, RAkEL reminds ensemble methods, like ECOC (error correcting output codes) [34], that construct multiple single-label models by manipulating the output space [35].

3.1 RAkEL$_d$

Given a size of labelsets k, RAkEL$_d$ initially partitions L randomly into $m = \lceil M/k \rceil$ disjoint labelsets R_j, $j = 1 \ldots m$, $\bigcap_{j=1}^{m} R_j = \emptyset$. Labelsets R_j, $j = 1 \ldots m - 1$ are k-labelsets. If M/k is an integer, then labelset R_m is also a k-labelset, otherwise R_m contains the remaining M mod k labels. Then RAkEL$_d$ learns m multi-label classifiers h_j, $j = 1 \ldots m$ using LP. Each classifier h_j confronts a single-label classification task having as class values all the subsets of R_j that are found in the training set.

The training set for h_j, denoted as D_j, contains all examples of the original training set annotated with the intersection of their original annotations and R_j: $D_j = \{(\vec{x_i}, Y_i \cap R_j), i = 1 \ldots N\}$. Note that this may lead to the empty set appearing as an annotation for an example. This doesn't mean that these examples are excluded from D_j. The empty set is just another class of the single-label classification task of h_j. Actually, the empty set is an acceptable annotation based on the definition of a multi-label dataset ($Y_i \subseteq L$) and most multi-label learners (including LP) handle it without any special consideration. Figure 2 offers an algorithmic presentation of the training process of RAkEL$_d$.

Given a new multi-label instance $\vec{x}$, the binary predictions $h_i(\vec{x}, \lambda_j)$ of all classifiers h_i for all labels $\lambda_j \in R_i$ are gathered in order to build the final multi-label classification vector (see Figure 3). Note that it is possible for RAkEL$_d$ to predict a labelset that has not appeared in the training set, as its final prediction is assembled from different parts of existing labelsets.

Input: Set of labels L of size M, training set D, labelset size k
Output: Number of models m, k-labelsets R_i, corresponding LP classifiers h_i
$m = \lceil M/k \rceil$;
for i=1 to m **do**
  $r_i \leftarrow \emptyset$;
  for j=1 to k **do**
    if $L = \emptyset$ **then**
      break;
    $\lambda_j \leftarrow$ randomly selected label from L;
    $R_i \leftarrow R_i \cup \{\lambda_j\}$;
    $L \leftarrow L \setminus \{\lambda_j\}$;
  train an LP classifier h_i based on D and R_i;

Fig. 2. The training process of RAkEL$_d$.

Input: Number of models m, new instance $\vec{x}$, k-labelsets R_i, corresponding LP classifiers h_i
Output: Multi-label classification vector $Result$
for i=1 to m **do**
  forall $\lambda_j \in R_i$ **do**
    $Result_j \leftarrow h_i(x, \lambda_j)$;

Fig. 3. The classification process of RAkEL$_d$.

3.2 RAkEL$_o$

We first introduce some additional notation. Let the term L^k denote the set of all distinct k-labelsets of L. The size of L^k is given by the binomial coefficient: $|L^k| = \binom{M}{k}$. Given a size of labelsets k and a number of desired classifiers $m \le |L^k|$, RAkEL$_o$ initially selects m k-labelsets R_i, $i = 1 \ldots m$ from the set L^k via random sampling without replacement. Note that in this case the labelsets may overlap, while the overlap is certain when $mk > M$. Then RAkEL$_o$ learns m multi-label classifiers h_i, $i = 1 \ldots m$ using LP, as in the case of RAkEL$_d$. Figure 4 presents the training process of RAkEL$_o$ in pseudocode.

Input: Set of labels L of size M, training set D, labelset size k, number of models $m \le \binom{M}{k}$
Output: k-labelsets R_i, corresponding LP classifiers h_i
$S \leftarrow L^k$;
for $i \leftarrow 1$ **to** $\min(m, |L^k|)$ **do**
  $R_i \leftarrow$ a k-labelset randomly selected from S;
  train an LP classifier h_i based on D and R_i;
  $S \leftarrow S \setminus \{R_i\}$;

Fig. 4. The training process of RAkEL$_o$.

For the multi-label classification of a new instance $\vec{x}$, each model h_i provides binary predictions $h_i(\vec{x}, \lambda_j)$ for each label λ_j in the corresponding k-labelset R_i. Subse-

quently, RAkEL$_o$ calculates the mean of these predictions for each label $\lambda_j \in L$ and outputs a final positive decision if it is greater than a 0.5 threshold. This intuitive threshold corresponds to the majority voting rule for the fusion of classifier decisions. It has been used for deriving a final decision in the problem transformation method RPC [15] as well. The pseudocode of the classification process of RAkELo is given in Figure 5, while Table 1 exemplifies it for a run with $k = 3$ and $m = 7$ on a multi-label training set with 6 labels $\{\lambda_1, \lambda_2, \ldots, \lambda_6\}$. Similarly to RA$kEL_d$, RA$kEL_o$ can also predict a labelset that is not present in the training set, as its final prediction is obtained through a voting process, based on predictions that correspond to different overlapping parts of existing labelsets.

TABLE 1
An example of the classification process of RAkEL$_o$ run with $k = 3$ and $m = 7$ on a multi-label training set with 6 labels.

		predictions					
model	labelset	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6
h_1	$\{\lambda_1, \lambda_2, \lambda_6\}$	1	0	-	-	-	1
h_2	$\{\lambda_2, \lambda_3, \lambda_4\}$	-	1	1	0	-	-
h_3	$\{\lambda_3, \lambda_5, \lambda_6\}$	-	-	0	-	0	1
h_4	$\{\lambda_2, \lambda_4, \lambda_5\}$	-	0	-	0	0	-
h_5	$\{\lambda_1, \lambda_4, \lambda_5\}$	1	-	-	0	1	-
h_6	$\{\lambda_1, \lambda_2, \lambda_3\}$	1	0	1	-	-	-
h_7	$\{\lambda_1, \lambda_4, \lambda_6\}$	0	-	-	1	-	0
	average votes	3/4	1/4	2/3	1/4	1/3	2/3
	final prediction	1	0	1	0	0	1

Input: Set of labels L of size M, number of models m, k-labelsets R_i, corresponding LP classifiers h_i, new instance $\vec{x}$
Output: Multi-label classification vector $Result$
for $j \leftarrow 1$ **to** M **do**
    $Sum_j \leftarrow 0$;
    $Votes_j \leftarrow 0$;

for $i \leftarrow 1$ **to** m **do**
    forall *labels* $\lambda_j \in R_i$ **do**
        $Sum_j \leftarrow Sum_j + h_i(\vec{x}, \lambda_j)$;
        $Votes_j \leftarrow Votes_j + 1$;

for $j \leftarrow 1$ **to** M **do**
    $Avg_j \leftarrow Sum_j / Votes_j$;
    if $Avg_j > 0.5$ **then**
        $Result_j \leftarrow 1$;
    else $Result_j \leftarrow 0$;

Fig. 5. The classification process of RAkEL$_o$.

Note that user-specified parameters m (number of classifiers) and k (size of labelsets) determine the expected number of predictions for each label, which is equal to $\frac{km}{M}$. We hypothesize that the larger the expected number of predictions per label, the larger the predictive accuracy of RAkEL$_o$, due to the fusion of more predictions. Given that k should be small to avoid the problems

of LP, then in order to increase km, one should select a large value for the number of models, m. The empirical study that follows, studies the relationship of m and k and provides guidelines for appropriate values.

3.3 Complexity Analysis

If the complexity of the algorithm employed to learn the transformed single-label classification task is $O(g(C, N, A))$ for a dataset with C class values, N examples and A predictive attributes, then the computational complexity of RAkEL is $O(mg(min(N, 2^k), N, A))$, where $m = \lceil M/k \rceil$ in the case of disjoint labelsets. It is linear with respect to the number of LP classifiers and it further depends on the complexity of the single-label classification algorithm.

The number of LP classifiers, m, is linear with respect to M in the case of disjoint labelsets. The empirical study that follows, indicates that in the case of overlapping labelsets a value of m that is linear with respect to M (e.g. $2M$) suffices for reaching a high level of predictive performance. Finally, note that the exponential factor 2^k does not pose a problem, as k will be set to a small value.

4 EXPERIMENTAL SETUP

This section provides details on the experimental setup. More specifically, Section 4.1 describes the datasets and Section 4.2 the measures that were used to empirically evaluate the performance of the proposed approach.

4.1 Datasets

Experiments were conducted on 8 multi-label datasets[1]. Table 2 includes basic statistics, such as the number of examples and labels, along with statistics that are relevant to labelsets, such as their bound, actual number and diversity. Short descriptions of these data sets are given in the following paragraphs.

TABLE 2
Multi-label datasets and their statistics sorted by increasing order of number of labels.

name	examples	labels	bound of labelsets	actual labelsets	labelset diversity
scene	2407	6	64	15	23%
yeast	2417	14	2417	198	8%
tmc2007	28596	22	28596	1341	5%
medical	978	45	978	94	10%
enron	1702	53	1702	753	44%
mediamill	43907	101	43907	6555	15%
reuters	6000	101	6000	1028	17%
bibtex	7395	159	7395	2856	39%

The *scene* dataset contains 2407 images annotated with up to 6 concepts such as *beach*, *mountain* and *field* [1]. Each image is described with 294 visual features.

The *yeast* dataset [28] contains micro-array expressions and phylogenetic profiles for 2417 yeast genes. Each gene

1. Available at http://mlkd.csd.auth.gr/multilabel.html

is annotated with a subset of 14 functional categories (e.g. *metabolism*, *energy*, etc) from the top level of the functional catalogue (FunCat).

The *tmc2007* dataset is based on the data of the competition organized by the text mining workshop of the 7th SIAM international conference on data mining[2]. The original data contained 28596 aviation safety reports in free text form, annotated with one or more out of 22 problem types that appear during flights [36]. Text representation follows the boolean bag-of-words model. Feature selection was then in order to reduce the computational cost of training. We used the χ^2 feature ranking method separately for each label in order to obtain a ranking of all features for that label. We then selected the top 500 features based on the their maximum rank over all labels. A similar approach was found to have high performance in previous experimental work on textual datasets [37].

The *medical* dataset[3] is based on the data made available during the Computational Medicine Center's 2007 Medical Natural Language Processing Challenge[4]. The dataset consists of 978 clinical free text reports labeled with one or more out of 45 disease codes.

The *enron* dataset is based on a collection of email messages exchanged between the Enron Corporation employees, which was made available during a legal investigation. It contains 1702 email messages that were categorized into 53 topic categories, such as *company strategy*, *humor* and *legal advice*, by the UC Berkeley Enron Email Analysis Project[5].

The *mediamill* dataset was part of the Mediamill challenge for automated detection of semantic concepts in 2006 [8]. It contains 43907 video frames annotated with 101 concepts (e.g. *military*, *desert*, *basketball*, etc). The specific dataset we used corresponds to experiment 1 (visual feature extraction) as described in [8]. Each video frame is characterized by a set of 120 visual features.

The *bibtex* dataset [10] is based on the data of the ECML/PKDD 2008 discovery challenge. It contains 7395 bibtex entries from the BibSonomy social bookmark and publication sharing system, annotated with a subset of the tags assigned by BibSonomy users (e.g. *statistics*, *quantum*, *datamining*). The title and abstract of bibtex entries were used to construct features using the boolean bag-of-words model.

The *reuters* (rcv1) dataset is a well known benchmark for text classification methods. We have used an existing subset of this dataset (subset1) that contains 6000 news articles assigned into one or more out of 101 topics. In order to reduce the feature space we have kept only words that appear at least 50 times in the corpus leading to a reduced feature space of 1654 features. An extensive description of this dataset can be found in [38].

4.2 Evaluation Measures

The evaluation of multi-label learning methods requires different measures than those used in the case of single-label data. A unified presentation and categorization of existing evaluation measures for multi-label classification is given in [13]. The evaluation in this work is based on the popular and indicative micro F_1 and macro F_1 measures.

The F_1 measure is the harmonic mean of precision and recall and is a popular evaluation measure in the research area of information retrieval. Formally, given the number of true positives (tp), true negatives (tn), false positives (fp) and false negatives (fn), F_1 is defined as follows:

$$F_1 = \frac{2 * tp}{2 * tp + fp + fn} \tag{1}$$

Micro F_1 and macro F_1 are the micro-averaged and macro-averaged versions of F_1 respectively. Micro-averaging as well as macro-averaging [39] are ways to calculate binary evaluation measures across several labels. Consider a binary evaluation measure $B(tp, tn, fp, fn)$. Let tp_λ, fp_λ, tn_λ and fn_λ be the number of true positives, false positives, true negatives and false negatives after binary evaluation for a label λ. The micro-averaged and macro-averaged versions of B, are calculated as follows:

$$B_{\text{micro}} = B\left(\sum_{\lambda=1}^{M} tp_\lambda, \sum_{\lambda=1}^{M} fp_\lambda, \sum_{\lambda=1}^{M} tn_\lambda, \sum_{\lambda=1}^{M} fn_\lambda\right) \tag{2}$$

$$B_{\text{macro}} = \frac{1}{M} \sum_{\lambda=1}^{M} B(tp_\lambda, fp_\lambda, tn_\lambda, fn_\lambda) \tag{3}$$

5 RESULTS AND DISCUSSION

This section presents the results obtained from our empirical study and concludes on the applicability and performance of RA*k*EL. The first part studies the performance of RA*k*EL$_d$ and RA*k*EL$_o$ with respect to their parameters and compares them with LP and each other. Then they are compared against baseline and high-performing multi-label classifiers. Finally, three different single-label classification algorithms are used to study their effect on the performance of RA*k*EL$_o$.

In all experiments, RA*k*EL$_d$ and RA*k*EL$_o$ are run 10 times using different seed values for the initialization of the pseudo-random number generator that guides the selection of the labelsets, in order to obtain more representative results on one hand and assess the effect of the stochastic component of the algorithm on the other.

5.1 Empirical Evaluation of RA*k*EL

In this section, the evaluation is based on the micro F_1 measure, estimated via the holdout method using the original train and test subsets provided with the releases of the 8 datasets.

The first two parts of this section examine the performance of the two RA*k*EL variations with respect to their parameters, which for RA*k*EL$_d$ is the size of the labelset, k, while for RA*k*ELo is both k and the number of models, m. Instead of absolute micro F_1 values, the percentage of improvement over LP is shown. This improves the legibility of the figures and simplifies the interpretation of the results across several different datasets. The last part compares the absolute micro F_1 performance of RA*k*EL$_d$ and RA*k*EL$_o$ using specific parameters against LP and each other.

The C4.5 decision tree learning algorithm was used as the base-level single-label classification algorithm of LP and the LP classifiers of RA*k*EL. We used the implementation of C4.5 within Weka [40] and our implementations of LP and RA*k*EL within Mulan [13].

5.1.1 Evaluation of RA*k*EL$_d$

Figure 6 presents the percentage of improvement of RA*k*EL$_d$ over LP in terms of micro F_1 measure with respect to the size of the labelset (k) in all datasets. The values of k correspond to different fractions of the total number of labels (from $k = \lceil M/10 \rceil$ to $k = \lceil 9M/10 \rceil$), so that the effect of k is studied for a broad range of values and at the same time results are comparable across all datasets. When $k = M$, RA*k*EL$_d$ becomes equivalent to LP.
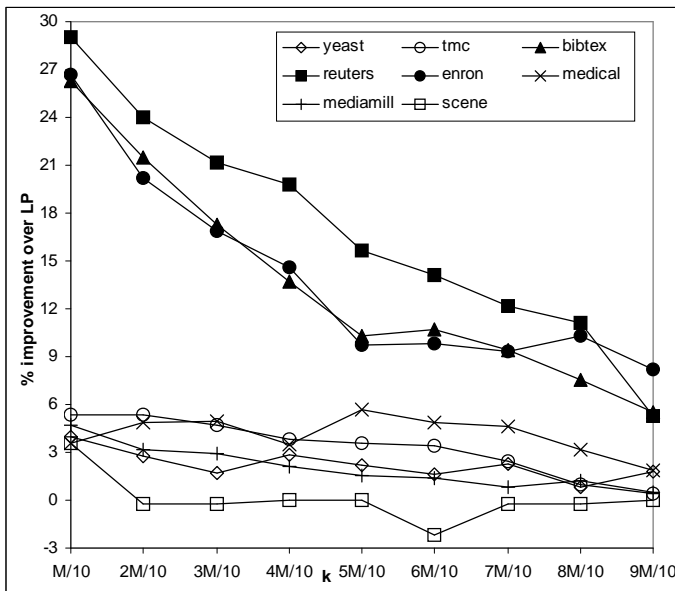

Fig. 6. Percentage of micro F_1 measure improvement of RA*k*EL$_d$ over LP with respect to k

A first observation is that RA*k*EL$_d$ provides a substantial improvement over the LP classifier for all datasets

with the exception of *scene*, where it leads to worse performance for $k = \lceil 6M/10 \rceil = 4$. However, this was an expected result due to the small number of labels in this dataset (6).

Concerning the effect of k on the predictive performance of RA*k*EL$_d$, we could argue that in general smaller values of k usually lead to better results. This confirms the hypothesis made earlier that splitting the initial multi-label problem into a number of simpler and smaller subproblems will improve the performance of LP. On the other hand, greater values of k allow the LP models of RA*k*EL$_d$ to take larger labelsets (and potentially more correlations) into account. This is a plausible explanation for the fact that RA*k*EL$_d$'s performance is not always degrading with respect to k. Nevertheless, values of k that are close to M perform worst and approximate the performance of LP.

Concerning the performance of RA*k*EL$_d$ with respect to the number of labels (M), we notice that the greatest improvement is achieved in datasets with large number of labels such as *reuters* (101 labels), *bibtex* (159 labels) and *enron* (53 labels), where the performance of LP is poor (micro F_1: 0.0979, 0.2897, 0.3953 respectively). An exception to this rule is *mediamill* (101 labels), where the improvement is similar to datasets with small M. This can be explained firstly by the higher performance of LP in this dataset (micro F_1: 0.4539). Secondly, even the smallest k value in the graph ($\lceil M/10 \rceil$) is quite large for *mediamill* (equal to 10). If we select smaller values for k we will observe greater improvement over LP. For example $k = 2$ leads to an 11.23% improvement and $k = 3$ leads to an 8.9% improvement.

In conclusion, we could state that setting k to small values is expected to lead to substantial better results compared to LP, especially in datasets with large number of labels.

5.1.2 Evaluation of RA*k*EL$_o$

Figure 7 presents the percentage of improvement of RA*k*EL$_o$ over LP in terms of micro F_1 measure with respect to the size of the labelset (k) in all datasets. Based on the conclusions of the previous section we use small values for k (from 2 to 10). The number of models (m) is set to $2M$, so that each label appears in the output of RA*k*EL$_o$'s models approximately $2k$ times irrespectively of the number of labels in the dataset. Note that the *scene* plot can not be extended more than $k = 4$ because the small number of labels (6) limits the number of different labelsets that can be created.

We first observe that RA*k*EL$_o$ outperforms LP for all values of k in all datasets. As k increases, the performance of RA*k*EL$_o$ exhibits an increasing trend in most of the datasets, in contrast to what we have seen for RA*k*EL$_d$ in the previous section. The reason is that in this experiment, bigger values of k lead to more votes for each label, as the number of models is constant ($2M$). In turn, more votes lead to more accurate estimates of the true value of each label. Finally, as in RA*k*EL$_d$, the
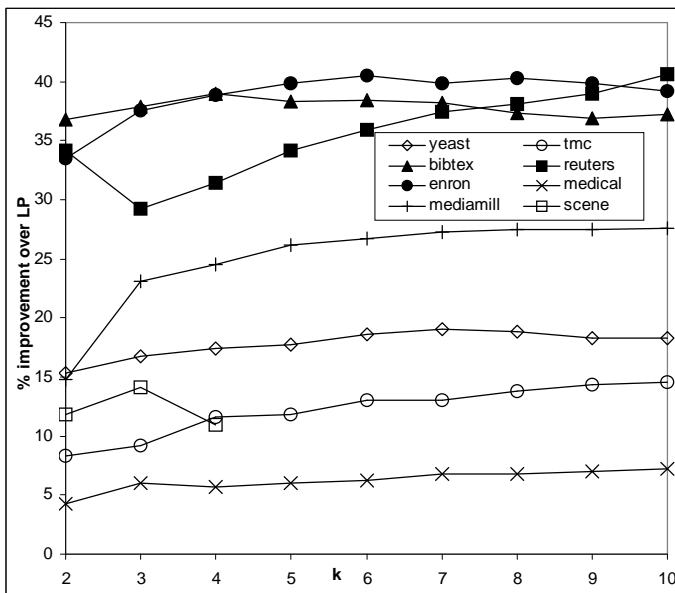
Fig. 7. Percentage of micro F_1 improvement of RAkEL$_o$ ($m = 2M$) over LP with respect to k.

Fig. 8. Percentage of micro F_1 measure improvement for RAkEL ($k = 3$) over LP with respect to m

improvement in performance is in general greater in data sets with larger number of labels.

Figure 8 presents the percentage of micro F_1 improvement of RAkEL$_o$ over LP using $k = 3$ with respect to various values of m in all datasets. In order to improve the legibility of the figure, the values of m correspond to different fractions of the total number of labels (from $\lceil M/5 \rceil$ to $2M$). What we observe is that as the number of classifiers increases, so does the performance of the ensemble. As before, this is due to the fact that bigger values of m lead to more votes for each label. An important finding that holds for all datasets is that after a certain number of models, the performance of RAkEL$_o$ does not exhibit substantial improvement. In most cases M is a good approximation of this number.

In conclusion, increasing either m or k leads RAkEL$_o$ to improved performance. The main reason for this behavior is that the number of votes received for each label is proportional to km. Since the complexity of RAkEL grows exponentially with respect to k, but only linearly with respect to m, it is more efficient to increase the value of m instead of k. As a guideline, we suggest using a small value for k (e.g. $k = 3$), and a value that is between M and $2M$ for m.

One thing to note, however, is that the process of selecting the labels is random, and as such, it could lead to the case, where none of the labelsets include one or more from the original set of labels. In this case, the algorithm will not be able to make a rational decision about the value of this (or these) particular label(s). In this respect, increasing m further, reduces the probability of a label receiving no votes from the models
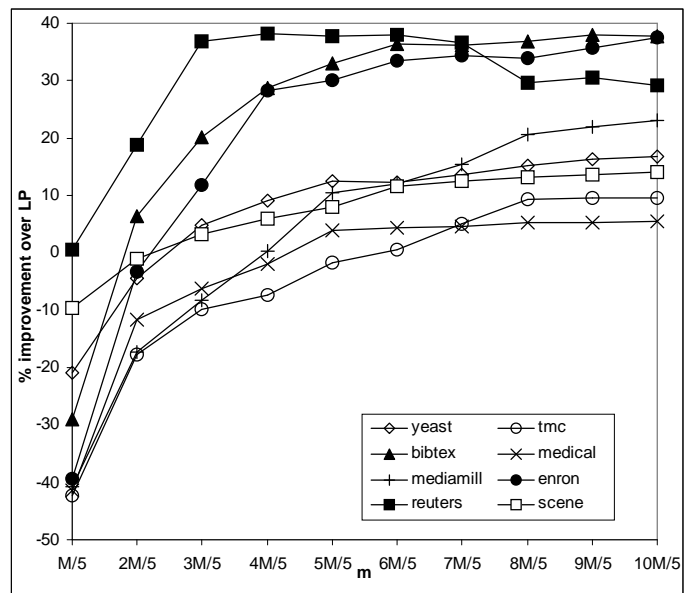
5.1.3 Disjoint vs. Overlapping Labelsets

Table 3 presents the micro F_1 value of LP, RAkEL$_d$ ($k = 3$), and RAkEL$_o$ ($k = 3$, $m = 2M$). For RAkEL$_d$ and RAkEL$_o$ the percentage of improvement in micro F_1 over LP is also presented.

We observe that RAkEL$_o$ provides a higher improvement over LP than RAkEL$_d$. This fact confirms the assumption that ensemble voting will further enhance the overall performance. An exception to this observation is the *medical* dataset, where RAkEL$_o$ provides a slightly smaller improvement. However, in this dataset there is a very small number of distinct labelsets (94), despite the relatively large number of labels (45). This explains both the good performance of LP and the minor improvements of RAkEL$_o$ due to the small diversity of its ensemble of LP classifiers.

In Table 3 the number of classes resulting from the transformation process of the three methods is presented. For RAkEL$_d$ and RAkEL$_o$ the classes of all LP models are summed. The number of classes can be considered as an estimator of computational requirements. We observe that RAkEL$_d$ presents less classes than LP in all datasets. Note the substantial reduction in number of classes in datasets *tmc*, *enron*, *mediamill*, *reuters* and *bibtex*. RAkEL$_o$, as expected, presents greater number of classes compared to RAkEL$_d$ due to the additional classifiers. However, in datasets *bibtex*, *enron* and *tmc* it presents lower number of classes than LP.

5.2 Comparison with Other Methods

In this section, the evaluation is based on both the micro F_1 and the macro F_1 measures, estimated via 10 repeated holdout experiments, each using a random 66% of each dataset for training and the rest for evaluation. So, in this

TABLE 3
Comparison of RAkEL$_d$ and RAkEL$_o$

	LP		RAkEL$_d$ ($k = 3$)			RAkEL$_o$ ($k = 3, m = 2M$)		
	micro F_1	classes	micro F_1	Imp. over LP	classes	micro F_1	Imp. over LP	classes
scene	58.75%	14	58.76±0.49%	0.02%	10.8	67.02±0.69%	14.08%	66.3
yeast	52.65%	164	54.11±0.63%	2.78%	33.7	61.50±0.62%	16.81%	207.3
tmc2007	78.79%	1172	83.03±0.37%	5.38%	53.6	85.76±2.53%	8.84%	317.4
medical	74.54%	77	78.81±0.53%	5.72%	58.3	78.69±1.04%	5.56%	351.8
enron	39.53%	545	49.94±1.29%	26.33%	91.8	54.39±0.62%	37.59%	554.7
mediamill	45.39%	4913	49.43±0.25%	8.90%	176.7	55.80±0.39%	22.94%	1054.7
reuters	9.79%	523	12.40±0.16%	26.64%	151.4	12.71±0.18%	29.80%	922.9
bibtex	28.97%	2058	39.07±0.33%	34.85%	255.8	39.95±0.27%	37.89%	1542.8

case RAkEL$_d$ and RAkEL$_o$ are run a total of 100 times each, as 10 different seeds are used for each different holdout experiment. To calculate the performance of RAkEL for a specific holdout experiment we average the values obtained from these 10 additional internal executions.

RAkEL is compared against the simple baseline methods BR and LP, as well as against three high performing multi-label methods that have been found to perform better than a number of other multi-label methods in a variety of datasets. The first one is a multi-label version of the k nearest neighbors algorithm, called MLkNN [2]. The second one is a multi-label version of the back propagation algorithm for training multi-layer perceptrons, called BPMLL [25]. The last one is the pairwise comparison method, called calibrated label ranking (CLR) [17].

The C4.5 decision tree learning algorithm was used as the base-level single-label classification algorithm of BR, LP, the LP classifiers of RAkEL and the binary classifiers of CLR. For RAkEL$_d$ we set k to 3 and for RAkEL$_o$ we set k to 3 and m to $2M$ in all data sets. Note that these are generic settings based on the conclusions of the previous section, and definitely not the optimal ones as also shown in the previous section. For MLkNN, the number of neighbors is set to 10 and the smoothing factor is set to 1 as recommended in [2]. For BPMLL, the learning rate is set to 0.05, the number of epochs is set to 100 and the number of hidden units is set to 20% of the input units, as recommended in [25]. We used the implementation of C4.5 within Weka [40] and our implementations of BR, LP, RAkEL, CLR, MLkNN and BPMLL within Mulan [13] for unified experiments and evaluation.

Tables 4 and 6 present the average and standard deviation of the micro F_1 and macro F_1 measure respectively, for all method-dataset pairs. Tables 5 and 7 present the rank of each method in terms of micro F_1 and macro F_1 respectively in each dataset, along with the average rank of each method. Following the suggestions in [41], we compare the different methods according to their average rank.

We observe that RAkEL$_o$ exhibits the highest average rank both in the micro F_1 and the macro F_1 measures. RAkEL$_d$ presents the second worst average rank in terms

of micro-F_1 (outperforming only LP) but the third best average rank in terms of macro F_1 outperforming LP, MLkNN, BPMLL and CLR. It is interesting to notice that the baseline BR presents the second best average rank in both metrics.

In addition, the Wilcoxon signed-rank test (a=0.05) was applied in order to examine if RAkEL$_o$ (or even RAkEL$_d$) have a statistical significant advantage over the rest of the methods. Over all datasets, RAkEL$_o$ proved to outperform significantly BR, LP, RAkEL$_d$ and CLR in terms of micro F_1. On the other hand, RAkEL$_d$, proved significantly better than LP only. In terms of macro F_1, RAkEL$_o$ proved to be significantly better than LP, RAkEL$_d$, MLkNN and CLR. RAkEL$_d$ significantly outperformed LP only, as for micro F_1.

5.3 The Effect of the Classification Algorithm

This section studies the effect of the single-label classification algorithm that is used to train the LP models of RAkEL$_o$ on the performance of RAkEL$_o$. We compare the performance of RAkEL$_o$ with $k = 3$ and $m = 2M$ using three different base-level learning algorithms: a) the C4.5 algorithm that was used in the experiments so far, b) a naive Bayes (NB) algorithm and c) a support vector machine (SVM) learning algorithm (one-vs-rest). We used the implementations of these algorithms that are available within Weka [40] (The Weka port of Lib-SVM [42] was used for the SVM). The SVM was set with polynomial kernel. We tuned the regularization (C) and degree (d) parameters of the SVM by searching the space defined by the values $d = \{1, 2, 3\}$ and $C = \{1, 10, 100\}$. As in Section 5.1, the evaluation here is also based on the micro F_1 measure, estimated via the holdout method using the original train and test subsets provided with the releases of the 8 datasets.

Table 8 presents the results of the experiments. The best performance at each dataset is indicated with bold typeface. In general, C4.5 and SVM perform better than NB in almost all datasets. C4.5 and SVM achieve the best performance in 4 datasets each. This phenomenon can be explained by considering that SVMs are more accurate classifiers but, on the other handed, decision trees are well suited for training ensembles of classifiers as RAkEL$_o$ does.

TABLE 4
Comparative results in terms of micro F_1.

	BR	LP	RAkEL$_d$	RAkEL$_o$	MLkNN	BPMLL	CLR
scene	62.36±1.01%	60.05±1.14%	59.87±0.82%	69.58±1.53%	72.29±1.08%	48.18±5.19%	62.82±0.92%
yeast	57.67±1.89%	53.04±1.03%	54.26±0.58%	61.89±0.74%	63.93±1.06%	63.11±1.47%	61.69±1.29%
tmc2007	68.80±0.28%	61.87±0.30%	67.78±0.32%	71.78±0.22%	63.21±0.52%	71.23±0.23%	70.73±0.32%
medical	79.34±1.02%	74.37±1.87%	79.21±0.89%	79.34±1.22%	66.23±1.77%	60.40±5.81%	78.67±1.14%
enron	51.93±1.93%	41.33±1.00%	50.69±0.48%	55.35±0.94%	44.42±3.00%	56.01±1.15%	54.65±1.24%
mediamill	55.35±0.22%	49.21±0.27%	54.28±0.14%	60.81±0.16%	58.15±0.27%	49.30±0.58%	58.51±0.24%
reuters	37.12±0.47%	29.88±0.71%	36.31±0.38%	38.21±0.13%	20.10±1.55%	05.99±0.33%	32.74±0.81%
bibtex	39.58±0.74%	29.32±0.69%	39.13±0.67%	40.36±0.71%	20.56±0.94%	45.81±0.45%	32.54±0.70%

TABLE 5
Ranking of methods according to their micro F_1 performance (see Table 4)

	BR	LP	RAkEL$_d$	RAkEL$_o$	MLkNN	BPMLL	CLR
scene	4	5	6	2	1	7	3
yeast	5	7	6	3	1	2	4
tmc	4	7	5	1	6	2	3
medical	1	5	3	2	6	7	4
enron	4	7	5	2	6	1	3
mediamill	4	7	5	1	3	6	2
reuters	2	5	3	1	6	7	4
bibtex	3	6	4	2	7	1	5
average rank	3.38	6.13	4.63	1.75	4.50	4.13	3.50

TABLE 6
Comparative results in terms of macro F_1.

	BR	LP	RAkEL$_d$	RAkEL$_o$	MLkNN	BPMLL	CLR
scene	63.41±0.91%	61.04±1.16%	60.90±0.88%	70.26±1.64%	72.63±1.37	51.29±5.26%	64.23±0.89%
yeast	38.29±0.59%	37.36±1.09%	38.84±0.50%	40.66±0.77%	36.34±0.79	42.85±1.02%	38.52±0.96%
tmc2007	57.82±0.52%	50.37±0.47%	57.04±0.54%	59.90±0.41%	41.61±1.08	61.88±0.69%	58.59±0.67%
medical	35.67±2.27%	33.38±1.94%	35.62±2.07%	36.98±1.81%	20.26±1.36	22.83±3.04%	34.63±1.65%
enron	14.21±0.74%	13.66±1.43%	14.45±0.55%	14.65±0.63%	7.43±1.18	17.04±1.18%	13.10±0.70%
mediamill	18.64±0.61%	17.90±0.33%	19.78±0.38%	21.26±0.50%	14.18±0.23	9.86±0.24%	11.81±0.33%
reuters	21.81±0.79%	16.81±0.87%	21.12±0.60%	21.25±0.45%	8.40±0.68	5.22±0.08%	11.77±0.57%
bibtex	27.12±0.66%	20.39±0.79%	26.40±0.59%	26.77±0.58%	6.42±0.41	31.73±0.32%	16.68±0.53%

TABLE 7
Ranking of methods according to their macro F_1 performance (see Table 6)

	BR	LP	RAkEL$_d$	RAkEL$_o$	MLkNN	BPMLL	CLR
scene	4	5	6	2	1	7	3
yeast	5	6	3	2	7	1	4
tmc	4	6	5	2	7	1	3
medical	2	5	3	1	7	6	4
enron	4	5	3	2	7	1	6
mediamill	3	4	2	1	5	7	6
reuters	1	4	3	2	6	7	5
bibtex	2	5	4	3	7	1	6
average rank	3.13	5.00	3.63	1.88	5.88	3.88	4.63

6 CONCLUSIONS

This paper has presented a new multi-label classification method, called RAkEL, that learns an ensemble of LP classifiers, each one targeting a different small random subset of the set of labels. The motivation was the computational efficiency and predictive performance problems of the simple and effective standard LP method, when faced with domains with large number of labels and training examples.

We examined both disjoint and overlapping subsets and found that both lead to improved results over the standard LP method, especially in domains with many labels. We also found that overlapping subsets lead to better results compared to disjoint ones, due to the classifier fusion process that takes place for each label. The results of comparing the predictive performance of the proposed approach with three high-performing algorithm adaptation methods were in favor of the proposed approach (using overlapping subsets).

RAkEL could be more generally thought of as a new approach for creating an ensemble of multi-label classifiers by manipulating the label space using randomization. In this sense, RAkEL could be independent of the underlying method for multi-label learning, which in this paper is LP. However, we should note that only multi-label learning methods that strongly depend on

TABLE 8
Micro F_1 of RAkEL$_o$ using three different single-label classification algorithms

dataset	NB	C4.5	SVM
scene	62.96±0.38%	67.02±0.69%	**72.59**±0.21%
yeast	57.00±0.65%	61.50±0.62%	**64.88**±0.37%
tmc2007	60.42±1.86%	**85.76**±2.53%	71.74±0.35%
medical	46.54±0.43%	**78.69**±1.04%	78.05±0.52%
enron	33.02±0.72%	54.39±0.62%	**55.81**±0.32%
mediamill	17.42±0.34%	**55.80**±0.39%	47.37±0.13%
reuters	8.88±0.60%	**12.71**±0.18%	3.39±0.03%
bibtex	22.31±0.10%	39.95±0.27%	**41.66**±0.11%

the specific set of labels used to annotate each example, such as LP and PPT [43] (an extension of LP), are good candidates for this generalized version of RAkEL. BR for example wouldn't benefit at all, while MLkNN would only slightly be affected, as it is heavily based on the feature space (the nearest neighbors will always be the same for all different labelsets).

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