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Editing training data for multi-label classification with the k -nearest neighbors rule

Sawsan Kanj^{a,b}, Fahed Abdallah^a, Thierry Dencœux^a,
Kifah Tout^b

^a*Heudiasyc, UMR CNRS 7253, Université de Technologie de Compiègne,
Rue Roger Couttolenc,
CS 60319,
60203 COMPIEGNE CEDEX,
FRANCE,
Tel : (33) 3 44 23 52 15 fax : (33) 3 44 23 44 77
firstname.lastname@hds.utc.fr*

^b*AZM center for biotechnology research, EDST, Lebanese University,
Rue miten, face malaab baladi,
Tripoli, Lebanon,
ktout@ul.edu.lb*

Abstract

Multi-label classification allows instances to belong to several classes at once. It has received significant attention in machine learning and has found many real world applications in recent years, such as text categorization, automatic video annotation and functional genomics, resulting in the development of many multi-label classification methods. Based on labelled examples in the training dataset, a multi-labelled method extracts inherent information in order to output a function that predicts the labels of unlabelled data. Due to several problems, like errors in the input vectors or in their labels, this information may be wrong and might lead the multi-label algorithm to fail. In this paper, we propose a simple algorithm for overcoming these problems by editing the existing training dataset, and adapting this edited set with different multi-label classification methods. Evaluation on benchmark datasets demonstrates the usefulness and effectiveness of our approach.

Key words: Classification; multi-label; k -nearest neighbors rule; prototype selection; edition.

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1 Introduction

Multi-label classification is the supervised classification task where each instance can be associated with multiple classes simultaneously from a set of disjoint classes; the classes are then no longer mutually exclusive. Contrary to single-label classification, the multi-label problem is influenced by intrinsic latent correlations between labels, in the sense that the membership of an instance to a class can be helpful to predict its set of labels [44]. For example, a patient with a high blood pressure is more likely to develop heart disease than an other person, but less likely to develop a muscular dystrophy.

Multi-label classification methods have been applied with modern applications like text categorization, where each document can be associated with a set of predefined topics [30]. In bioinformatics, each protein may be labelled with multiple functional labels such as metabolism, energy and cellular biogenesis [17]. In video annotation, a film might be annotated with several labels or tags [25].

Multi-label methods learn usually a classifier function from the training dataset with known class labels. However, real world data often suffer from noisy or erroneous instances due to several problems, like errors in the input vectors or in their labels. To cope with this problem in the framework of single-label learning, several methods based on data reduction have been introduced. These techniques are usually based on prototype selection [4,13,27,39].

Prototype selection methods are usually applied to remove erroneous or redundant instances from the training dataset [13,20,24]. These methods are widely used with the traditional nearest neighbor rule due to their simplicity and effectiveness. In addition to improving classification accuracy for unseen instances, using prototypes dramatically decreases storage and classification-time costs.

However, despite extensive work in multi-label learning [5,21,26,37,42,44], there is a lack of methods for improving the quality of multi-labelled training instances. This fact motivated us to study this problem in the framework of multi-label learning. In this paper, we develop an original method based on a prototype selection using the nearest neighbor rule and a local evaluation criterion, in order to purify training dataset and improve the performance of multi-label classification algorithms. The evaluation criterion used in this paper is the very well known Hamming loss metric. Nevertheless, the proposed method may be straightforwardly adapted to any other criterion. Given one training instance with known set of labels, we consider the editing rule which, based on the Hamming Loss calculated by estimating to this instance a set of predicted labels from the neighborhood, either delete or remain the instance

unchanged. After applying this edited rule on all observations of the training dataset and eliminating the less relevant in the sense of the chosen criterion, a learning algorithm on the edited training set may be applied efficiently.

To show the effectiveness of this method, we apply existing multi-label classification methods, which are the evidential multi-label k -nearest neighbor (EML k NN) [10] and the Rank-SVM [12] methods, on the edited dataset. The proposed algorithm is applied to several multi-labelled data from different domains using several multi-label classification measures. Even if the Hamming loss is used as a criterion to edit the data, the performances are evaluated using several multi-label classification measures. Note that, more than increasing classification performance, the new method has the advantage of needing less of storage requirements and decreasing the running time of the initial classification algorithms.

Note that a short paper on the purification (or edition) of multi-labelled datasets was presented at the conference Fusion [18]. In this paper, the edition method is more thoroughly interpreted and discussed. Furthermore, we add the effect of editing on the SVM techniques and we provide an illustrative example on a simulated dataset. In addition, extensive comparisons on several real world datasets are presented, and the effectiveness of the method compared to that before editing is shown using statistical tests (t-test and Friedman test).

This paper is structured as follows. Background notions on the nearest neighbor rule in the classical single-label framework and some related techniques for prototype selection will first be recalled in Section 2. Section 3 will introduce the principle of multi-label classification and review the EML k NN and Rank-SVM methods. Our approach will then be exposed in Section 4. Section 5 will report the experimental evaluation of the presented methods on synthetic and real-world datasets. Finally, our contribution will be summarized in Section 6.

2 Related work on prototype selection for single-labelled data

The problem of noise handling has received considerable attention in the literature on machine learning. Seeking to start with something relatively simple, scientists have focused on the nearest neighbor classifier considered as one of the most well-known technique in machine learning and data mining due to its simplicity and effectiveness. Given a training set of single-labelled data, the idea is to select an optimal set of training instances, known as prototypes, in order to maximize the performances of the Nearest Neighbor (NN) classifier and/or to minimize the computing time of this classifier [8]. Later, the idea of selecting "good" instances has also been applied to other types of classi-

78 fiers [4]. In this section, we will rapidly review the nearest neighbor rule, and
79 give a definition and summary of work related to prototype selection methods
80 for the NN rule.

81 2.1 Nearest Neighbor classification

82 The Nearest Neighbor rule [7] is a well-known and non-parametric decision
83 procedure for machine learning and data mining tasks. It has been considered
84 as one of the most effective algorithms in machine learning, and one of the top
85 ten methods in data mining [13,41]. In traditional supervised learning, this
86 rule assigns to an unseen sample $\mathbf{x}$, the class of the nearest training instance
87 according to some distance metric. The voting k -nearest neighbor rule (k -NN),
88 with $k > 1$, is a generalization of the NN approach where the predicted class of
89 $\mathbf{x}$ is set as equal to the class represented a majority of its k nearest neighbors
90 in the training set.

91 However, the k -NN rule suffers from several problems such as large storage re-
92 quirements, high computational complexity in the operational phase, and low
93 tolerance to noise due to considering all instances as relevant while the train-
94 ing set may contain noisy or mislabelled examples. Different techniques have
95 been proposed in the literature to alleviate these problems. One technique,
96 known as prototype selection, consists of selecting an appropriate subset of
97 the training data that yields a similar or even higher classification accuracy.
98 Prototype selection methods can be categorized into three different families.
99 First, *edition methods* eliminate noisy instances from the original training
100 set in order to improve classification accuracy. Second, *condensation meth-*
101 *ods* select a sufficiently small subset of training instances which lead to the
102 same performance of the single nearest neighbor rule (1-NN), by removing
103 instances that will not affect classification accuracy. Finally, *hybrid methods*
104 select a small subset of training instances that incorporates the goals of these
105 two previous methods [13,3]. In the following, we consider only the editing
106 methods.

107 2.2 Editing methods

108 Editing methods process the training data by removing border and noisy in-
109 stances or making other necessary cleaning, with the aim of improving classi-
110 fication accuracy of learning algorithms on test data. Below we review some
111 algorithms related to the editing approach for the nearest neighbor rule.

112 Wilson proposed the first editing rule [40], called Edited Nearest Neighbor
113 (ENN), to improve the performance of the 1-NN rule. This method can be

described in the following manner. Each instance in the training set is classified using the k -NN rule, and it is marked for deletion if its predicted class does not agree with the true class. Edition is achieved by deleting all misclassified instances at once. After, any input sample is classified using the 1-NN rule with the remaining instances. Experiments with the editing rule were reported by Tomek who proposed two variants of the ENN rule: RENN and All k -NN [34]. The Repeated Edited Nearest Neighbor (RENN) rule repeats the ENN algorithm until a stable set is obtained where no more samples are edited out. The All k -NN applies iteratively the ENN algorithm with the i -NN rule where i is going from 1 to k .

In [19], the generalized editing procedure based on the kk' -NN rule was introduced. The purpose of this procedure was two-fold: improving the level of performance of the ENN algorithm and reducing the proportion of deleted samples. Based on the class of a majority of k' instances from a group of k nearest samples to an instance $\mathbf{x}$, the group of k samples is either deleted or relabelled as belonging to the majority class. The 1-NN is then used on the edited set to classify an input instance. In [11], the authors proposed the well-known Multiedit algorithm, which randomly breaks the initial training set into different subsets. In each subset, every instance is classified using the 1-NN rule with the instances in the next subset. Misclassified instances are discarded. The remaining instances constitute a new set and the algorithm is iteratively repeated until no more instances are edited out.

In [16], a Modified Edited k -NN rule (MEKNN) was proposed. According to this rule, a sample $\mathbf{x}$ is deleted from the initial set if its class does agree with the class of its k nearest neighbors and their tying instances (tying instances are those in the training set that are at the same distance to $\mathbf{x}$ as its furthest neighbor). In addition, this method introduces a fixed number of pairs (k, k') . k is the number of neighbors to make the edition process and k' is employed to classify any new instance in the obtained edited set. The goal was to obtain the optimal pairs of k and k' to employ the final editing reference set.

Another method for nearest neighbor editing was proposed in [15]. This method uses the concept of semi-supervised learning and edits the training instances by using the whole dataset including: labelled and unlabelled instances. The proposed method, called NNEAUD (Nearest Neighbor Editing Aided by Unlabelled Data), consists of two steps: labels are first predicted for unlabelled instances, and the augmented dataset is then used in data editing. The NNEAUD method uses ENN, RENN, and All k NN algorithms with unlabelled data to edit the training instances.

152 3 Multi-label learning

153 3.1 Problem

154 Let $\mathbb{X}$ denote an instance space, and let $\mathcal{Y} = \{\omega_1, \dots, \omega_Q\}$ be a finite set of
155 labels. Let $\mathcal{D} = \{(\mathbf{x}_1, Y_1), \dots, (\mathbf{x}_n, Y_n)\}$ denote a dataset composed of n multi-
156 labeled objects $(\mathbf{x}_i, Y_i)$, $\mathbf{x}_i \in \mathbb{X}$ and $Y_i \subseteq \mathcal{Y}$, where each instance is independent
157 and identically distributed (i.i.d.) drawn from an unknown distribution. The
158 goal of multi-label learning is to build a multi-label classifier $\mathcal{H}$ that maps
159 an instance $\mathbf{x}$ to its associated set of labels Y and optimizes some evaluation
160 metrics. Here, the set of all subsets of $\mathcal{Y}$ is the power set of $\mathcal{Y}$ denoted by $2^{\mathcal{Y}}$.

161 Numerous methods have been proposed in the literature to deal with multi-
162 label learning problems. Existing algorithms can be grouped into three cate-
163 gories as proposed in [21]: problem transformation approaches, problem adap-
164 tation algorithms and ensemble methods. The first category divides the multi-
165 label problem into one or more conventional single-label problems. Binary
166 Relevance and Label Powerset are two examples of such type of approaches.
167 The second category generalizes single-label algorithms to cope with multi-
168 labeled data directly. Examples include boosting [29], decision tree [2] and the
169 Multi-label k -nearest neighbors methods [44,47]. Finally, the third category
170 incorporates the merits of these two previous approaches. Several ensemble
171 methods have been proposed, among them: ensemble of classifier chains [26],
172 random k -label sets [38] and ensemble of multi-label classifiers [32].

173 3.2 Performance evaluation in multi-label learning

174 In the traditional single-label classification task, predictive performance is
175 determined under the traditional *accuracy* measure, where each test instance
176 can either be correctly or incorrectly classified, and performance is given by the
177 proportion of correctly classified test instances. In the multi-label classification
178 task, predictive performance is more complex than that of single-label systems,
179 where the classification of each test instance can be fully correct, partially
180 correct or fully wrong. Given a set $\mathcal{S} = \{(\mathbf{x}_1, Y_1), \dots, (\mathbf{x}_m, Y_m)\}$ of m test
181 examples, evaluation metrics can be divided into two groups: *prediction-based*
182 and *ranking-based* metrics [37]. *Prediction-based* metrics are calculated based
183 on the comparison between the predicted and the ground truth sets of labels,
184 while *ranking-based* metrics evaluate the label ranking quality depending on a
185 scoring function $f(.,.)$, ($f : \mathbb{X} \times \mathcal{Y} \rightarrow \mathbb{R}$, where $\mathbb{X}$ is the domain of instances
186 and $\mathcal{Y}$ is the set of Q target classes) that attributes a score to each class in
187 $\mathcal{Y}$ [44]. More details on evaluation metrics are given in appendix A.

188 We will focus in this paper on the Hamming loss and the Ranking loss metrics.
 189 The Hamming loss is a prediction-based metric regarded as an average of the
 190 error rate of the classifier on the Q binary problems where the decision is
 191 performed separately [28]. It is defined by:

$$\mathcal{H}Loss = \frac{1}{m} \sum_{i=1}^m \frac{|Y_i \Delta \hat{Y}_i|}{Q}, \quad (1)$$

192 where Y_i is the ground truth label set for the pattern $\mathbf{x}_i$, $\hat{Y}_i$ is the predicted
 193 label set for $\mathbf{x}_i$ and Δ denotes the symmetric difference between two sets.
 194 In other words, the Hamming loss is based on counting prediction errors (an
 195 incorrect label is predicted) and missing errors (a true label is not predicted).
 196 The Ranking loss is a ranking-based metric which evaluates the average frac-
 197 tion of crucial pairs of labels that are misordered for an instance [29]. The
 198 *Ranking Loss* is:

$$\mathcal{R}Loss = \frac{1}{m} \sum_{i=1}^m \frac{1}{|Y_i| |\bar{Y}_i|} |R(\mathbf{x}_i)|, \quad (2)$$

199 where $R(\mathbf{x}_i) = \{(\omega_q, \omega_r) \in Y_i \times \bar{Y}_i \mid f(\mathbf{x}_i, \omega_q) \leq f(\mathbf{x}_i, \omega_r)\}$, $\bar{Y}_i$ denotes the
 200 complement of Y_i in $\mathcal{Y}$. Smaller values of these metrics correspond to higher
 201 classification quality. Note that the value of these evaluation criteria is in the
 202 interval $[0, 1]$. We will present briefly in next sections the two multi-label
 203 algorithms that will be used in this paper and which are the Evidential multi-
 204 label k -NN and the Rank-SVM methods.

205 3.3 Evidential multi-label k -NN classification

206 The evidential k -NN (EML k NN) method introduced in [10] answers the multi-
 207 label classification problems under the belief functions framework and can
 208 be summarized as follows. Let $\mathcal{D} = \{(\mathbf{x}_1, A_1, B_1), \dots, (\mathbf{x}_n, A_n, B_n)\}$ be the
 209 learning set, where $A_i \subseteq \mathcal{Y} = \{\omega_1, \dots, \omega_Q\}$ denotes a set of classes that surely
 210 apply to the instance $\mathbf{x}_i$, and B_i is the complement of A_i in $\mathcal{Y}$, ($\mathcal{Y}$ is known
 211 as the *frame of discernment* of the problem).

212 To classify an unlabelled instance $\mathbf{x}$, we identify its k -nearest neighbors, de-
 213 noted as $\mathcal{N}_{\mathbf{x}}$, by computing the distance of $\mathbf{x}$ to the labelled objects in $\mathcal{D}$ based
 214 on a certain distance function. Each element $\mathbf{x}_i$ in $\mathcal{N}_{\mathbf{x}}$ constitutes an item of
 215 evidence regarding the label set of $\mathbf{x}$. This item of evidence can be described
 216 by the following simple two-valued mass function:

$$\begin{aligned} m_i(A_i, B_i) &= \alpha \exp(-\gamma d(\mathbf{x}, \mathbf{x}_i)), \\ m_i(\emptyset, \emptyset) &= 1 - \alpha \exp(-\gamma d(\mathbf{x}, \mathbf{x}_i)), \end{aligned} \quad (3)$$

217 where $d(\mathbf{x}, \mathbf{x}_i)$ is the distance between $\mathbf{x}$ and $\mathbf{x}_i$, α and γ are two parameters,
 218 such that $0 < \alpha < 1$ and $\gamma > 0$. Parameter α is usually fixed to a value close
 219 to 1 such as 0.95 [9], whereas γ can be optimized or fixed heuristically [48].
 220 If the number of neighbors of the $\mathbf{x}$ is k , the resulting k mass functions are
 221 combined using the conjunctive rule:

$$m = \bigodot_{i: \mathbf{x}_i \in \mathcal{N}_{\mathbf{x}}} m_i \quad (4)$$

222 where the $\bigodot$ symbol denotes the unnormalized Dempster's rule of combi-
 223 nation [10]. This rule strongly emphasizes the agreement between multiple
 224 sources, where no elementary item of evidence should be counted twice. The
 225 predicted multi-label set for $\mathbf{x}$ is then determined by computing separately for
 226 each label $\omega \in \Omega$ two quantities: the degree of belief $bel(\{\omega\}, \emptyset)$ that the true
 227 label set Y contains ω , and the degree of belief $bel(\emptyset, \{\omega\})$ that it does not
 228 contain ω . The multi-label classifier $\mathcal{H}$ is defined finally as:

$$\mathcal{H}(\mathbf{x}) = \{\omega \in \mathcal{Y} | bel(\{\omega\}, \emptyset) \geq bel(\emptyset, \{\omega\})\}, \quad (5)$$

229 where $\emptyset$ denotes the empty set of $\mathcal{Y}$.

230 3.4 Rank-SVM

231 Rank-SVM is a multi-label ranking approach introduced by Elisseff and We-
 232 ston in [12]. The ultimate goal was to minimize a criterion measure for multi-
 233 label learning, called Ranking loss, and to maximize the margin. The authors
 234 introduce a special multi-label margin defined on $(\mathbf{x}, Y)$ as the signed distance
 235 between the instance $\mathbf{x}$ and the decision boundary. Note that the boundary of
 236 class q is a grouping of several boundaries separating the class q and the other
 237 classes. For Rank SVM method, which ranks the values of $r_q(x) = \langle w_q, \mathbf{x} \rangle + b_q$,
 238 the decision boundaries for $\mathbf{x}$ are defined by the hyperplanes whose equations
 239 are $\langle w_q - w_l, \mathbf{x} \rangle + b_q - b_l = 0$. Thus, the margin with respect to class q is equal
 240 to:

$$\min_{(q,l) \mid (\omega_q, \omega_l) \in (Y \times \bar{Y})} y_q \frac{\langle w_q - w_l, \mathbf{x} \rangle + b_q - b_l}{\|w_q - w_l\|}$$

241 where w_q, w_l and b_q, b_l denote the weight vectors and bias terms, and y_q is a
 242 binary element equal to +1 if label q is in Y , -1 otherwise. According to [12],
 243 q denotes a relevant label, and l the irrelevant one. For training instances, it is
 244 desirable that any relevant label should be ranked higher than any irrelevant
 245 one.

246 The Rank-SVM model is built from two different sub-systems. The first one,
 247 named ranking system, orders the labels via a quadratic optimization problem,
 248 according to their outputs, $r_q(x) = \langle w_q, \mathbf{x} \rangle + b_q$ for $q = 1, \dots, Q$. The other
 249 goal of this method is to predict a threshold $t(\mathbf{x})$ and all integer q such that

250 $r_q(\mathbf{x}) > t(\mathbf{x})$ are considered to belong to the label set Y of $\mathbf{x}$. It is well-known
 251 that such an algorithm can be generalized to non-linear separating boundaries
 252 by just replacing the dot products $\langle \mathbf{x}_i, \mathbf{x}_j \rangle$ by kernels $k(\mathbf{x}_i, \mathbf{x}_j)$.

253 4 Editing multi-labelled data using the k -NN rule

254 4.1 Motivation

255 In multi-label learning, the goal is to generate a multi-label classifier that will
 256 generalize from a set of multi-labelled training instances in such a way that
 257 classification performances for labelling new data are optimized. However, er-
 258 rors in multi-labelled training datasets can occur for several reasons. One cause
 259 is the subjectivity, when the boundaries of each class are based on individ-
 260 ual perspectives. For example, in genre classification of musical signals, each
 261 musical genre may have its boundaries shifted from person to person [1]. A sec-
 262 ond cause of anomalies or noisy instances is ambiguity during data-entry. For
 263 example, in clinical text for multi-label classification (medical multi-labelled
 264 data collected from Cincinnati children’s hospital medical center), abbrevia-
 265 tions and acronyms used to anonymization of patients may lead to ambiguity
 266 when processing such data by taking more than one sense and having multi-
 267 purposes (in a clinical setting, *FT* can be an abbreviation for *full-term*, *foot*
 268 *test*, *field test*, *full-time* or *family therapy*) [23]. Other errors can arise from
 269 missing information and data transformation or storage. Furthermore, many
 270 examples may have an erroneous set of labels due to an experimental assign-
 271 ment problem or even a human annotation error. To the best of our knowledge,
 272 no algorithm addressing these problems under the multi-label framework has
 273 been proposed so far.

274 In the following, we propose an original method to edit multi-labelled data
 275 by identifying and eliminating erroneous or anomalous samples. The purpose
 276 of this method is three-fold: first, to increase the quality of training instances
 277 assumed to become more reliable; second, to improve the performances of
 278 the classifier built from the resulting training data; and third to increase the
 279 response time of the learning algorithm. This method is based on the k -nearest
 280 neighbor rule for multi-label classification, and on an evaluation criterion used
 281 locally in the set $\mathcal{N}_{\mathbf{x}}$ of k -nearest neighbors of $\mathbf{x}$ to evaluate the quality of
 282 an instance $\mathbf{x}$. Based on this evaluation criterion, we can delete the most
 283 irrelevant, or the *worst* samples from the initial training dataset. We will
 284 present hereafter a simple method using this metric conjointly with a k -NN
 285 rule for multi-label classification in order to edit the training dataset.

287 Let $\mathbf{x}$ be an unseen instance for which we wish to estimate the set of labels.
 288 In the following steps, we describe the proposed method to edit the training
 289 dataset:

- 290 (1) For each training instance $\mathbf{x}_i$ in $\mathcal{D}$, search for $\mathcal{N}_{\mathbf{x}_i}$, the set of its k nearest
 291 neighbors;
- 292 (2) Apply a k -NN based multi-label classifier and calculate a predicted set
 293 of labels $\hat{Y}_i$ for $\mathbf{x}_i$;
- 294 (3) For each training instance in $\mathcal{D}$, calculate the associated Hamming loss
 295 given by:

$$\mathcal{H}Loss_i = \frac{|Y_i \triangle \hat{Y}_i|}{Q}; \quad (6)$$

- 296 (4) Estimate the Hamming loss $\mathcal{H}Loss$, which is the mean of the associated
 297 Hamming loss for all instances in $\mathcal{D}$:
  - 298 • if $\mathcal{H}Loss$ is less than a predefined threshold t , then stop the algorithm;
  - 299 • else,
    - 300 (a) Rank the training instances in $\mathcal{D}$ with respect to their $\mathcal{H}Loss_i$ and
 301 select a subset $\mathcal{E}^l$ containing l instances with the higher Hamming
 302 loss $\mathcal{H}Loss_i$;
    - 303 (b) Update the training set by deleting those in $\mathcal{E}^l$: $\mathcal{D} \leftarrow \mathcal{D} \setminus \mathcal{E}^l$;
    - 304 (c) Return to step 1.

305 Note that any k -NN based multi-label classifier [44,10,46] can be applied in
 306 Step 2. In this paper, we chose the EML k NN method introduced in Section 3.3.
 307 According to this method, each element in $\mathcal{N}_{\mathbf{x}_i}$ represents a piece of knowledge
 308 about the labelling of $\mathbf{x}_i$. A two-valued mass function is then associated to each
 309 of the k neighbors in $\mathcal{N}_{\mathbf{x}_i}$ according to Equation 3. These items of evidence
 310 are combined to produce a global mass function, using the conjunctive rule
 311 of Equation 4. In order to estimate the label set for $\mathbf{x}_i$ denoted by $\hat{Y}_i$, the
 312 global mass function is used according to Equation 5. Intuitively, k should
 313 be set to a small value because if k is high, undesirable instances elimination
 314 will occur on the boundary between different classes. If k is equal to 1, the
 315 EML k NN algorithm boils down to the 1-NN algorithm, and the set of labels
 316 to be assigned to an example is the same as that of his neighbor. In Step 3,
 317 one can use other stopping criteria than the general $\mathcal{H}Loss$. For example, we
 318 can stop editing if the Hamming loss associated to each instance is less than
 319 a predefined threshold t . We can also substitute the Hamming loss by another
 320 multi-label metric evaluation. In Steps 4a and 4b, we delete instances with
 321 high value of $\mathcal{H}Loss_i$, which means deleting the *worst* instances with respect
 322 to a local EML k NN rule. One can add a condition to keep instances belonging
 323 to classes with low occurrence.

324 5 Experimental Evaluation

325 In this section, we present experiment results with synthetic and real-world
 326 datasets from different domains to demonstrate the effect of edition on the
 327 performances of the two multi-label classification methods described below.

328 5.1 Experiments with Synthetic Data

329 In this section, we will illustrate the behavior of our editing algorithm on
 330 synthetic datasets using the two methods of classification discussed above.
 331 The goal of these experiments is to study the effects of edition on multi-label
 332 learning algorithms.

333 A dataset with three-overlapping classes in two-dimension was first considered.
 334 The dataset contains 600 instances belonging to three possible labels $\Omega =$
 335 $\{\omega_1, \omega_2, \omega_3\}$. These instances were drawn from seven Gaussian distributions
 336 with means $(-5, -5)$, $(5, -5)$, $(0, 5)$, $(0, -5)$, $(-3, 1)$, $(3, 1)$, and $(0, 0)$. The
 337 standard deviations was equal two for the first three distributions and one for
 338 the others. We assigned the following classes, respectively, for samples drawn
 339 from each of these distributions: $\{\omega_1\}$, $\{\omega_2\}$, $\{\omega_3\}$, $\{\omega_1, \omega_2\}$, $\{\omega_1, \omega_3\}$, $\{\omega_2, \omega_3\}$,
 340 $\{\omega_1, \omega_2, \omega_3\}$. This dataset was randomly divided into training and test datasets
 341 with size 400 and 200, respectively. Table 1 gives the distribution of instances
 342 over the different labels.

Table 1

Description of the synthetic data without the erroneous instances.

Label set	Training instances	Testing instances
$\{\omega_1\}$	85	41
$\{\omega_2\}$	84	41
$\{\omega_3\}$	82	46
$\{\omega_1, \omega_2\}$	30	20
$\{\omega_1, \omega_3\}$	42	18
$\{\omega_2, \omega_3\}$	46	23
$\{\omega_1, \omega_2, \omega_3\}$	31	11

343 To test our editing algorithm, 40 instances drawn in the region allocated to
 344 classes $\{\omega_1\}$, $\{\omega_2\}$ and $\{\omega_1, \omega_2\}$ were wrongly assigned to class $\{\omega_3\}$. These
 345 noisy samples are generated randomly from two normal distributions with
 346 means $(-4, -6)$ and $(4, -6)$, respectively, and a standard deviation equal to
 347 2. Figure 1 shows the dataset (initial + noisy instances) with their class as-

signments.

Fig. 1. Training instances of synthetic data

348

349 Figures 2(a) and 2(b) show the decision boundaries for our synthetic data with
 350 a support vector domain using a Gaussian kernel. The boundary region for
 351 each class label was drawn using the Rank-SVM method, with the Gaussian
 352 kernel: $k(\mathbf{x}, \mathbf{x}') = \exp(-\gamma_r \|\mathbf{x} - \mathbf{x}'\|^2)$, $\gamma_r = 5$. We used the same parameters
 353 values for the Rank-SVM method with the training data before and after editing.
 354 Figure 2(a) shows the decision boundaries for the initial training dataset.
 355 As we can see, these decision boundaries are significantly influenced by noisy
 356 instances and there is no clear separation between classes. In the area of class
 357 $\{\omega_2\}$ (on the right of this figure), we can see several zones belonging to classes
 358 $\{\omega_1, \omega_2, \omega_3\}$. Also, in the area of class $\{\omega_1\}$, the erroneous instances create
 359 many zones with instances belonging to class $\{\omega_3\}$.

360 In Figure 2(b), we can see the decision boundaries for the same dataset after
 361 editing. In this figure, we can see that, with editing, noisy instances have been
 362 removed, and, smoother decision boundaries are produced. The area is now
 363 divided into seven zones. Instances belonging to class $\{\omega_1\}$ are on the left of
 364 Figure 2(b), instances assigned by label $\{\omega_2\}$ are on the right, and instances
 365 labelled with $\{\omega_3\}$ are at the top. Using a geometrical interpretation, we can
 366 easily distinguish the area belonging to each combination of these classes.
 367 Instances annotated by three classes are in the middle of this figure. Note
 368 that the number of training instances was reduced to 382 (initial number of
 369 training data was 440), and the number of support vectors was decreased
 370 from 409 to 352. Table 2 reports the experimental results on three evaluation

(a)

(b)

Fig. 2. The Rank-SVM decision boundaries between classes with the training instances, a) before editing, b) after editing.

371 criteria: Hamming loss, accuracy and the F1-measure.

Table 2

Some evaluation measures for the Rank-SVM method before and after the edition of the synthetic dataset.

	Before Editing	After Editing
Hamming loss ⁻	0.1667	0.1017
Accuracy ⁺	0.7283	0.8358
F1 ⁺	0.7422	0.8423

+(-): the higher (smaller) the value, the better the performance.

372 From these two figures, we can observe that training the Rank-SVM method
 373 with a purified dataset leads to smoother separating boundaries, creates ho-
 374 mogeneous clusters and reduces the number of support vectors.

375 Figure 3 shows the performance of our editing approach on the synthetic data
 376 using the EML k NN method. We used from the library of multi-label measures
 377 three evaluation criteria: Hamming loss, accuracy and the F1-measure. The
 378 values of these metrics are shown as a function of the number of neighbors k .
 379 From this figure, we can observe that when k takes small values, the EML k NN
 380 algorithm tested on the edited dataset performs better than EML k NN tested
 381 on noisy dataset. As k increases, the EML k NN method tends to have the same
 382 performance on these two datasets . This can be explained by the fact that,
 383 when increasing the number of neighbors, the effect of randomly erroneous
 384 instances decreases giving that we use more information (coming from more
 385 instances), and also the applied method (EML k NN) is based on an evidential
 386 distance-weighted k -nearest neighbor rule.

387 5.2 Experiments on Real-World Data

388 In this section, we apply the two multi-label classification methods discussed
 389 above (EML k NN and Rank-SVM) to our datasets and we evaluate their per-
 390 formances before and after editing. In the following, we will report the bench-
 391 mark datasets, the evaluation metrics used in our experiments and parameter
 392 settings for edition. Finally, we will provide a discussion of experimental re-
 393 sults.

Fig. 3. Some evaluation measures for the EMLkNN method before and after the edition of the synthetic dataset.

5.2.1 Datasets

The datasets¹ that were included in our experiments cover different application domains: multimedia classification (Emotions), bioinformatics (Yeast) and text categorization (Medical, Enron and Webpage).

- *Emotions dataset*. This dataset consists of 593 songs labeled by experts according to the emotions they generated. Each piece of music is described by 8 rhythmic features and 64 timbre features, and can be annotated with the following emotions: *amazed-surprised*, *happy-pleased*, *relaxed-calm*, *quiet-still*, *sad-lonely* and *angry-fearful*. The average number of labels for each song is 1.869, and the number of distinct label sets is equal to 27 [35].
- *Yeast dataset*. The *yeast Saccharomyces cerevisiae* is one of the best studied organisms. Each gene is described by the concatenation of micro-array expression data and phylogenetic profile and it is associated with a subset of 14 functional classes from the Comprehensive Yeast Genome Database

¹ Datasets available at <http://mulan.sourceforge.net/datasets.html>, and <http://cse.seu.edu.cn/people/zhangml/>.

of the Munich Information Center for Protein Sequences². This dataset contains 2417 genes and 14 possible labels [22].

- *Medical dataset*. This dataset contains 978 documents for patient symptom histories collected from the *Computational Medicine Center* concerning a challenge task on the automated processing of clinical free text. Each document is represented by a vector of 1449 features [23].
- *Enron dataset*. The *Enron email*³ dataset was made public by the Federal Energy Regulatory Commission during its investigation. It contains around 517.431 emails (without attachments) from 151 users distributed in 3500 folders. Each message includes the senders and the receiver email address, date and time, subject, body, text and some other email specific technical details. After preprocessing and careful selection of these documents, 53 different labels are obtained with 753 combinations of distinct label sets [31].
- *Webpage categorization dataset*. This dataset were collected from the "yahoo.com" domain [33]. Eleven different webpage categorization subproblems are considered, corresponding to 11 independent multi-label categories: *Arts and Humanities, Business and Economy, Computers and Internet, Education, Entertainment, Health, Recreation and Sports, Reference, Science, Social and Science, and Society and Culture*. Each subproblem consists of 5000 documents (2000 as training dataset and 3000 as testing dataset). Each webpage was represented as a bag of words and normalized to the unit length.

Tables 3 and 4 provide an overview of the different characteristics of all experimental datasets. These characteristics are explained in the appendix B at the end of the article.

Table 3

Characteristics of the Emotions, Yeast, Medical and Enron datasets.

	Domain	Number of instances	Feature vector dimension	Number of labels	Label cardinality	Label density	Distinct label sets
Emotions	music	593	72	6	1.868	0.311	27
Yeast	biology	2417	103	14	4.237	0.303	198
Medical	text	978	1449	45	1.245	0.028	94
Enron	text	1702	1001	53	3.378	0.064	753

5.3 Parameter Tuning

In this section, we comment how to tune different parameters to apply the different algorithms described in this paper. We call *editing* parameters those applied on the initial dataset with the editing algorithm in order to obtain an edited training dataset. We call *testing* parameters those used in a multi-label

² <http://mips.gsf.de/genre/proj/yeast/>

³ <http://enrondata.org/content/research/>

Table 4
Characteristics of the Webpage categorization dataset.

	Number of instances	Feature vector dimension	Number of labels	Label cardinality	Label density	Distinct label sets
Arts and Humanities	5000	462	26	1.627	0.063	462
Business and Economy	5000	438	30	1.590	0.053	161
Computers and Internet	5000	681	33	1.487	0.046	253
Education	5000	550	33	1.465	0.044	308
Entertainment	5000	640	21	1.426	0.068	232
Health	5000	612	32	1.667	0.052	257
Recreation and Sports	5000	606	22	1.414	0.065	322
Reference	5000	793	33	1.159	0.035	217
Science	5000	743	40	1.489	0.036	398
Social and Science	5000	1047	39	1.274	0.033	226
Society and Culture	5000	636	27	1.705	0.063	582

classification algorithm learnt from initial or edited learning dataset. Note that the number k of neighbors to be used is not necessarily the same as that used in the editing algorithm. To avoid confusion, the number of neighbors used in the editing algorithm will be noted by k' . Hereafter, we will show the influence of these parameters by using the *Emotions* dataset.

5.3.1 Editing parameters

For the editing algorithm presented in Section 4.2, there are three tunable parameters:

- γ : Parameter used in Equation 3 to scale the distance to each neighbor. It was fixed at the best value obtained by cross validation using the EML k NN method on the initial training dataset.
- k' : Number of neighbors used in the editing algorithm.
- t : Threshold used to determine the number l of instances to delete. We use in the simulation a Hamming loss calculated on each instance as in Equation (6). This Hamming loss calculated on only one instance will have a value equals q/Q , where $q \in \{0, \dots, Q\}$. Note that the value of the parameter t to be taken should depend on the global Hamming loss calculated on the training dataset.

Figure 4 shows the box plot for the Hamming loss metric obtained by the EML k NN method on the initial dataset before editing the data for different values of γ , where k was varied from 1 to 12 (thus each box plot corresponds to 12 values of the Hamming loss obtained for a given γ). Figure ?? shows the Hamming loss measure obtained as a function of t , where k' was varied from 1 to 12, γ was fixed to 0.1, and k was fixed to 3 (we can get the same results for any value of k , for that we chose for it a small value). The box plot in Figure

Fig. 4. Hamming loss measure for EML k NN on the initial Emotions training set for different values of γ .

Fig. 5. Hamming loss measure for EML k NN after editing the Emotions training set as a function of t .

463 6 shows the Hamming loss criterion with respect to the number of neighbors
 464 k' . k was varied from 1 to 12, and γ was fixed to 0.1.

465 5.3.2 Testing parameters

466 In the testing phase, the EML k NN and the Rank-SVM methods are tested
 467 with the edited data. EML k NN has two parameters: the number of neighbors
 468 k , and the discounting parameter γ . These parameters were determined using
 469 grid search and by focusing on the Hamming loss measure: k was varied from

Fig. 6. Hamming loss measure for EMLkNN on the edited Emotions training set as a function of k' .

1 to 12, and γ from 0 to 1 with 0.01 steps. Note that the algorithm presented in Section 4.2 was repeated only once by taking the best value of t ; i.e., the one that eliminates an important number of erroneous instances at once.

For the Rank-SVM method, we used the Gaussian kernel with three tunable parameters: kernel scale parameter γ_r , penalty constant C , and maximal iterations M . By focusing on the Hamming loss measure, cross-validation via grid search was applied for parameter tuning as explained in [43]. The γ_R and C parameters took values from $2^7, 2^6, \dots$, to 2^{-7} respectively. M was set to 50, 100, 150 and 200.

5.4 Results and Discussion

In this section, we evaluate the performance of the editing algorithm by comparing the results achieved by the EMLkNN and Rank-SVM methods before and after editing. Using the optimal parameter values obtained on the training datasets, we studied the performance using independent test datasets. The experimental results on datasets are given in Tables 5-8. For the webpage dataset, the average performance out of the 11 different categorization problems is reported in Table 9. The rank of each method is given, and the best value on each evaluation criterion is highlighted in bold letters. These results can be summarized as follows:

- From the results in Tables 5-9, we can observe that EMLkNN applied on edited data improves the performance of the same method on the initial dataset for all prediction-based metrics except the Hamming loss measure.

492 The Hamming loss criterion is similar before and after edition.
 493 • Regarding the Rank-SVM method, results on editing datasets are better
 494 than those on initial datasets for all measures (prediction-based and ranking-
 495 based metrics).
 496 • The Rank-SVM applied on editing datasets gives the best performance ac-
 497 cording to the majority of evaluation measures for the Yeast, Medical, En-
 498 ron, and Webpage datasets. For the Emotions dataset, the best performance
 499 on the ranking-based measures was obtained by the Rank-SVM method
 500 applied to the edited dataset, while the best results according to predicted-
 501 based measures were obtained by the EMLkNN algorithm applied to the
 502 edited dataset.

503 In order to show the effect of edition on data storage, Table 10 reports infor-
 504 mation about the used datasets: the number of instances of full and edited
 505 training datasets, and the time necessary to editing each of these datasets.
 506 The results indicate that the edited datasets require less storage space than
 507 do the initial datasets.

508 In order to study the impact of edition on classification time, we compared
 509 the time used by each method (programmed in Matlab) applied to the ini-
 510 tial and edited datasets. Table 11 presents the total running time (learning +
 511 testing time) using the initial training and edited datasets. We can see that
 512 the running time of the two classifiers (EMLkNN and Rank-SVM) are signif-
 513 icantly reduced in our experiments, except for the Enron dataset. In general,
 514 EMLkNN is faster than Rank-SVM, due to the space complexity of the Rank-
 515 SVM method which is proportional to $n * Q^2$. The machine used was Intel(R)
 516 Xeon(R) CPU at 2.67 GHz, 12 GB RAM with Matlab2012a.

517 To statistically measure the significance of performance difference between
 518 results on initial datasets and those on edited datasets, two statistical in-
 519 dicators are carried out using ten-fold cross validation: the *pairwise t-tests*
 520 and the *Friedman test* [14]. The average results of different evaluation crite-
 521 ria using ten-fold cross validation are reported in Tables 12-16 in which we
 522 use the *pairwise t-test*. The significance is usually determined under a signif-
 523 icance level of $\alpha = 0.05$. To be able to see *the power* of our conclusions, the
 524 *p-values* of *Friedman test* and *t-test* on the different datasets are indicated in
 525 Tables 17-21. Note that small values for the *p-values* indicate strong presump-
 526 tion against null hypothesis, which is the hypothesis saying that the results
 527 of the two methods are not different. For the chosen significance level, we can
 528 consider that the results of the two methods (before and after editing) are
 529 different if *p-value* < 0.05 . We can see also from the tables that the results
 530 of the *pairwise t-test* and the *Friedman test* are correlated leading almost to
 531 similar conclusion about the significance of the difference between methods.

532 The results presented in this section show the advantage of editing multi-label
533 datasets to improve the performance of multi-label classifiers. By comparing
534 the performance of multi-label classifiers (EML k NN and Rank-SVM) before
535 and after edition, we can conclude that editing initial multi-label datasets
536 improve the performance evaluation of some classifiers. Furthermore, we may
537 reduce the complexity of classifiers since we need to train less instances, which
538 are distributed into more homogeneous clusters. We might deduce also that
539 editing training datasets is a way to reduce the running time complexity of
540 some multi-label classification methods. Even if we use the Hamming loss
541 criterion to edit the training datasets, we can get better performance on other
542 metrics.

543 Note that we tested the use of the edited data set on other multi-label clas-
544 sifiers, namely the C4.5 based on decision trees [6], and the *MLMLP* based
545 on neural network [45]. The results we obtained show better performances of
546 these methods on all the datasets, which follows the behavior of the previ-
547 ous presented methods (EML k NN and Rank-SVM). We are not showing the
548 numerical results for a better readability of the paper.

549 6 Conclusion

550 In this paper, we have addressed the problem of prototype selection in the
551 framework of multi-label learning. Although the extensive work in multi-label
552 classification, to the best of our knowledge, the topic of prototype selection has
553 not received any attention so far. The goal is not only to optimize performance
554 of some classifiers, but also the size of the training dataset must be reduced
555 as well as the computational time of learning algorithms.

556 Edited Nearest Neighbor for Multi-Labelled data is an efficient editing method.
557 The idea is, first, to classify all training instances using a k -NN rule, and, sec-
558 ond, to eliminate erroneous instances based on a local criterion induced from
559 the Hamming loss measure. The reduced set of instances is then used to classify
560 unseen instances. We have demonstrated the effect of editing dataset on two
561 learning algorithms: the EML k NN and the Rank-SVM. This was illustrated
562 through an example on synthetic data.

563 We applied our algorithm of editing to five real-world datasets from different
564 domains of application: multimedia classification, bioinformatics and text cat-
565 egorization. Experimenting with these datasets, we observed that the learning
566 algorithms (EML k NN and Rank-SVM) with the editing datasets significantly
567 outperformed the same algorithms on the initial datasets in terms of classi-
568 fication performance and computational costs. The explanation is that the
569 editing datasets are distributed in more homogeneous clusters by reducing the

number of irrelevant instances. Learning from these new instances is faster with better generalization ability.

Note that the scalability of the presented approach depends on that of the k -NN algorithm. Several approaches exist to adapt the use of the k -NN on large datasets. For example, a simple approach is to use the idea of clustering in order to not to compute distances of a testing instance with respect to all training instances. It is clear that if the training data is *very noisy*, our method of edition may be a solution to reduce the number of training data by using only clean instances with a relatively small number with respect to the initial dataset.

Future research should consider applying the existing algorithm to other application domains, e.g., audio, video and images and showing extensive results on several classifiers, including for example decision trees [6], neural networks [45] and classifier chains [26], to investigate better the merit of editing in these settings. A very interesting idea will be to apply the edition on the training set using another method than the k -NN based one. Surely, this idea will not be straightforward. For example, if we decide to use the Rank SVM, we have to edit instances that are misclassified (since these instances increase the Hamming Loss), but it is well known that these instances (with non zero Lagrange multipliers) are involved in the construction of decision boundaries.

Table 5
Experimental results on the Emotions dataset.

	EML k NN		Rank-SVM	
	Before Editing	After Editing	Before Editing	After Editing
Hamming loss ⁻	0.209(4)	0.204(2)	0.206(3)	0.194(1)
One-Error ⁻	0.287(2)	0.297(3)	0.302(4)	0.277(1)
Coverage ⁻	1.881(2)	2.010(4)	1.896(3)	1.847(1)
Ranking loss ⁻	0.168(3)	0.220(4)	0.166(2)	0.158(1)
Average Precision ⁺	0.7994(2)	0.7959(4)	0.7993(3)	0.8080(1)
Accuracy ⁺	0.519(4)	0.569(1)	0.546(3)	0.561(2)
Precision ⁺	0.656(3)	0.705(1)	0.651(4)	0.690(2)
Recall ⁺	0.592(3)	0.657(1)	0.642(2)	0.642(2)
F1 ⁺	0.596(4)	0.648(1)	0.621(3)	0.637(2)

+(-): the higher (smaller) the value, the better the performance.

Table 6
Experimental results on the Yeast dataset.

	EMLkNN		Rank-SVM	
	Before Editing	After Editing	Before Editing	After Editing
Hamming loss ⁻	0.205(4)	0.202(3)	0.197(2)	0.193 (1)
One-Error ⁻	0.261(4)	0.249(3)	0.221 (1)	0.238(2)
Coverage ⁻	6.494(3)	6.577(4)	6.424(2)	6.269 (1)
Ranking loss ⁻	0.188(3)	0.201(4)	0.167(2)	0.165 (1)
Average precision ⁺	0.751(3)	0.751(4)	0.767(2)	0.768 (1)
Accuracy ⁺	0.515(4)	0.529(2)	0.522(3)	0.539 (1)
Precision ⁺	0.685(4)	0.689(3)	0.697(2)	0.703 (1)
Recall ⁺	0.599(4)	0.618(3)	0.625(3)	0.635 (1)
F1 ⁺	0.613(4)	0.627(3)	0.628(3)	0.641 (1)

+(-): the higher (smaller) the value, the better the performance.

Table 7
Experimental results on the Medical dataset.

	EMLkNN		Rank-SVM	
	Before Editing	After Editing	Before Editing	After Editing
Hamming loss ⁻	0.018(3)	0.018(4)	0.012(2)	0.011 (1)
One-Error ⁻	0.285(2)	0.291(3)	0.141 (1)	0.141 (1)
Coverage ⁻	3.541(3)	3.661(4)	1.135 (1)	1.255(2)
Ranking loss ⁻	0.124(3)	0.126(4)	0.015 (1)	0.018(2)
Average precision ⁺	0.779(3)	0.776(4)	0.897(2)	0.898 (1)
Accuracy ⁺	0.559(4)	0.585(3)	0.688(2)	0.726 (1)
Precision ⁺	0.617(4)	0.647(3)	0.744(2)	0.781 (1)
Recall ⁺	0.569(4)	0.594(3)	0.718(2)	0.754 (1)
F1 ⁺	0.581(4)	0.608(3)	0.716(2)	0.754 (1)

+(-): the higher (smaller) the value, the better the performance.

A Evaluation measures

As discussed in Section 3.2, Performance evaluation for multi-label learning systems differs from that of single-label classification. Let $\mathcal{H} : \mathbb{X} \rightarrow 2^{\mathcal{Y}}$ be a multi-label classifier that assigns a predicted label subset of $\mathcal{Y} = \{\omega_1, \dots, \omega_Q\}$ to each instance $\mathbf{x} \in \mathbb{X}$, and let $f : \mathbb{X} \times \mathcal{Y} \rightarrow [0, 1]$ be the corresponding scoring function which gives a score for each label ω_q which in turn is interpreted as

Table 8
Experimental results on the Enron dataset.

	EMLkNN		Rank-SVM	
	Before Editing	After Editing	Before Editing	After Editing
Hamming loss ⁻	0.057(3)	0.059(4)	0.055(2)	0.053(1)
One-Error ⁻	0.437(3)	0.478(4)	0.287(2)	0.275(1)
Coverage ⁻	21.959(3)	26.226(4)	13.758(2)	12.772(1)
Ranking loss ⁻	0.261(3)	0.395(4)	0.099(2)	0.090(1)
Average precision ⁺	0.568(3)	0.509(4)	0.619(2)	0.647(1)
Accuracy ⁺	0.303(4)	0.318(3)	0.398(2)	0.436(1)
Precision ⁺	0.473(4)	0.484(3)	0.574(2)	0.587(1)
Recall ⁺	0.340(4)	0.359(3)	0.495(2)	0.556(1)
F1 ⁺	0.372(4)	0.390(3)	0.511(2)	0.550(1)

+(-): the higher (smaller) the value, the better the performance.

Table 9
Experimental results on the Webpage dataset.

	EMLkNN		Rank-SVM	
	Before Editing	After Editing	Before Editing	After Editing
Hamming loss ⁻	0.065(4)	0.058(3)	0.043(2)	0.042(1)
One-Error ⁻	0.589(4)	0.558(3)	0.417(2)	0.402(1)
Coverage ⁻	12.164(3)	12.906(4)	5.080(2)	4.169(1)
Ranking loss ⁻	0.506(3)	0.545(4)	0.128(2)	0.1000(1)
Average precision ⁺	0.471(3)	0.470(4)	0.651(2)	0.673(1)
Accuracy ⁺	0.338(4)	0.364(3)	0.402(2)	0.437(1)
Precision ⁺	0.393(4)	0.426(3)	0.465(2)	0.508(1)
Recall ⁺	0.387(4)	0.391(3)	0.435(2)	0.467(1)
F1 ⁺	0.371(4)	0.392(3)	0.432(2)	0.469(1)

+(-): the higher (smaller) the value, the better the performance.

the probability that ω_q is relevant. The function $f(.,.)$ can be transformed to a ranking function $rank_f(.,.)$ which maps the outputs of $f(\mathbf{x}, \omega)$ for any $\omega \in \mathcal{Y}$ to $\{\omega_1, \omega_2, \dots, \omega_Q\}$ so that $f(\mathbf{x}_i, \omega_q) > f(\mathbf{x}_i, \omega_r)$ implies that $rank_f(\mathbf{x}_i, \omega_q) < rank_f(\mathbf{x}_i, \omega_r)$.

Given a set $\mathcal{S} = \{(\mathbf{x}_1, Y_1), \dots, (\mathbf{x}_m, Y_m)\}$ of m test examples, the evaluation metrics of multi-label learning systems are divided into two groups: *prediction-based* and *ranking-based* metrics. *Prediction-based* measures are calculated

Table 10

Information about the used datasets.

	Number of instances in initial training data	Number of instances in edited training data	Editing Time (seconds)
Emotions	391	113	2.4
Yeast	1500	832	30.8
Medical	645	624	6.2
Enron	1123	861	9.2
Webpage	22000	13693	435.3

Table 11

Running Time (in Seconds) for learning and testing for the two methods.

	EMLkNN		Rank-SVM	
	Before Editing	After Editing	Before Editing	After Editing
Emotions	1.4	0.4	162.9	9.9
Yeast	12.4	10.1	$1.1 * 10^4$	$0.2 * 10^4$
Medical	7.3	3.7	$1.6 * 10^4$	$1.4 * 10^4$
Enron	18.8	8.2	$1.0 * 10^4$	$1.6 * 10^4$
Webpage	61.7	47.7	$2.1 * 10^4$ s $\simeq$ 14 h	$8.6 * 10^3$ s $\simeq$ 5.9 h

Table 12

Experimental results (mean $\pm$ std) on the Emotions dataset.

	EMLkNN		Rank-SVM	
	Before Editing	After Editing	Before Editing	After Editing
Hamming loss ⁻	0.191 $\pm$ 0.019●	0.146 $\pm$ 0.064	0.192 $\pm$ 0.022●	0.148 $\pm$ 0.0474
One-Error ⁻	0.266 $\pm$ 0.044●	0.188 $\pm$ 0.100	0.256 $\pm$ 0.081●	0.158 $\pm$ 0.0691
Coverage ⁻	1.816 $\pm$ 0.198○	1.524 $\pm$ 0.402	1.702 $\pm$ 0.293○	1.505 $\pm$ 0.4016
Ranking loss ⁻	0.173 $\pm$ 0.028○	0.131 $\pm$ 0.061	0.156 $\pm$ 0.039●	0.100 $\pm$ 0.0495
Average precision ⁺	0.799 $\pm$ 0.030●	0.864 $\pm$ 0.054	0.807 $\pm$ 0.044●	0.874 $\pm$ 0.0477
Accuracy ⁺	0.558 $\pm$ 0.045●	0.681 $\pm$ 0.119	0.541 $\pm$ 0.049●	0.658 $\pm$ 0.0946
Precision ⁺	0.688 $\pm$ 0.052●	0.774 $\pm$ 0.095	0.663 $\pm$ 0.065●	0.757 $\pm$ 0.0805
Recall ⁺	0.641 $\pm$ 0.051●	0.772 $\pm$ 0.086	0.654 $\pm$ 0.062●	0.768 $\pm$ 0.1017
F1 ⁺	0.635 $\pm$ 0.045●	0.748 $\pm$ 0.095	0.626 $\pm$ 0.052●	0.735 $\pm$ 0.0850

●(○): statistically significant (non-significant) difference of performance of the classification algorithm applied on the initial and the edited dataset, based on two-tailed paired t-test at 5% significance.

603 based on the average difference of the actual and the predicted set of la-
604 bels over all test examples. *Ranking-based* metrics evaluate the label ranking
605 quality depending on the scoring function $f(.,.)$.

Table 13

Experimental results (mean $\pm$ std) on the Yeast dataset.

	EMLkNN		Rank-SVM	
	Before Editing	After Editing	Before Editing	After Editing
Hamming loss ⁻	0.201 $\pm$ 0.010●	0.168 $\pm$ 0.041	0.195 $\pm$ 0.006●	0.157 $\pm$ 0.0384
One-Error ⁻	0.242 $\pm$ 0.027●	0.170 $\pm$ 0.074	0.216 $\pm$ 0.032○	0.165 $\pm$ 0.0724
Coverage ⁻	6.481 $\pm$ 0.263●	5.727 $\pm$ 0.800	6.336 $\pm$ 0.236●	5.496 $\pm$ 0.7416
Ranking loss ⁻	0.186 $\pm$ 0.015●	0.139 $\pm$ 0.053	0.165 $\pm$ 0.007●	0.116 $\pm$ 0.0451
Average precision ⁺	0.757 $\pm$ 0.018●	0.813 $\pm$ 0.059	0.773 $\pm$ 0.013●	0.829 $\pm$ 0.0587
Accuracy ⁺	0.524 $\pm$ 0.021●	0.604 $\pm$ 0.074	0.529 $\pm$ 0.016●	0.611 $\pm$ 0.0763
Precision ⁺	0.682 $\pm$ 0.024●	0.734 $\pm$ 0.060	0.695 $\pm$ 0.016●	0.755 $\pm$ 0.0571
Recall ⁺	0.614 $\pm$ 0.023●	0.705 $\pm$ 0.076	0.633 $\pm$ 0.022●	0.713 $\pm$ 0.0795
F1 ⁺	0.621 $\pm$ 0.021●	0.697 $\pm$ 0.068	0.634 $\pm$ 0.011●	0.707 $\pm$ 0.0692

●(○): statistically significant (non-significant) difference of performance of the classification algorithm applied on the initial and the edited dataset, based on two-tailed paired t-test at 5% significance.

Table 14

Experimental results (mean $\pm$ std) on the Medical dataset.

	EMLkNN		Rank-SVM	
	Before Editing	After Editing	Before Editing	After Editing
Hamming loss ⁻	0.017 $\pm$ 0.003○	0.015 $\pm$ 0.002	0.011 $\pm$ 0.002○	0.010 $\pm$ 0.001
One-Error ⁻	0.277 $\pm$ 0.068○	0.242 $\pm$ 0.028	0.137 $\pm$ 0.033○	0.118 $\pm$ 0.034
Coverage ⁻	3.356 $\pm$ 1.164○	4.129 $\pm$ 0.881	1.070 $\pm$ 0.370○	0.864 $\pm$ 0.284
Ranking loss ⁻	0.108 $\pm$ 0.034●	0.151 $\pm$ 0.027	0.014 $\pm$ 0.007○	0.011 $\pm$ 0.005
Average precision ⁺	0.784 $\pm$ 0.047○	0.796 $\pm$ 0.019	0.906 $\pm$ 0.022○	0.915 $\pm$ 0.021
Accuracy ⁺	0.592 $\pm$ 0.064●	0.642 $\pm$ 0.034	0.719 $\pm$ 0.042●	0.769 $\pm$ 0.030
Precision ⁺	0.654 $\pm$ 0.065●	0.705 $\pm$ 0.033	0.761 $\pm$ 0.049●	0.810 $\pm$ 0.034
Recall ⁺	0.611 $\pm$ 0.061●	0.668 $\pm$ 0.038	0.757 $\pm$ 0.041●	0.819 $\pm$ 0.032
F1 ⁺	0.619 $\pm$ 0.063●	0.672 $\pm$ 0.034	0.746 $\pm$ 0.044●	0.799 $\pm$ 0.030

●(○): statistically significant (non-significant) difference of performance of the classification algorithm applied on the initial and the edited dataset, based on two-tailed paired t-test at 5% significance.

606 A.1 Prediction-based measures

607 **Hamming loss:** The hamming loss metric for the set of labels is defined as
 608 the fraction of labels whose relevance is incorrectly predicted:

$$\mathcal{H}Loss(\mathcal{H}, \mathcal{S}) = \frac{1}{m} \sum_{i=1}^m \frac{|Y_i \triangle \hat{Y}_i|}{Q}, \quad (\text{A.1})$$

609 where $\triangle$ denotes the symmetric difference between two sets.

610 **Accuracy:** The accuracy metric gives an average degree of similarity between
 611 the predicted and the ground truth label sets:

$$\mathcal{A}ccuracy(\mathcal{H}, \mathcal{S}) = \frac{1}{m} \sum_{i=1}^m \frac{|Y_i \cap \hat{Y}_i|}{|Y_i \cup \hat{Y}_i|}. \quad (\text{A.2})$$

Table 15

Experimental results (mean $\pm$ std) on the Enron dataset.

	EMLkNN		Rank-SVM	
	Before Editing	After Editing	Before Editing	After Editing
Hamming loss ⁻	0.062 $\pm$ 0.010 $\circ$	0.057 $\pm$ 0.004	0.056 $\pm$ 0.014 $\circ$	0.049 $\pm$ 0.003
One-Error ⁻	0.571 $\pm$ 0.098 $\bullet$	0.390 $\pm$ 0.075	0.294 $\pm$ 0.111 $\circ$	0.215 $\pm$ 0.049
Coverage ⁻	25.645 $\pm$ 6.323 $\circ$	23.242 $\pm$ 2.423	13.937 $\pm$ 3.234 $\bullet$	11.476 $\pm$ 1.167
Ranking loss ⁻	0.334 $\pm$ 0.086 $\circ$	0.294 $\pm$ 0.058	0.098 $\pm$ 0.024 $\bullet$	0.072 $\pm$ 0.012
Average precision ⁺	0.467 $\pm$ 0.056 $\circ$	0.577 $\pm$ 0.052	0.614 $\pm$ 0.087 $\bullet$	0.702 $\pm$ 0.035
Accuracy ⁺	0.165 $\pm$ 0.058 $\bullet$	0.366 $\pm$ 0.048	0.380 $\pm$ 0.125 $\bullet$	0.486 $\pm$ 0.040
Precision ⁺	0.334 $\pm$ 0.106 $\bullet$	0.542 $\pm$ 0.059	0.575 $\pm$ 0.097 $\bullet$	0.660 $\pm$ 0.038
Recall ⁺	0.184 $\pm$ 0.066 $\bullet$	0.421 $\pm$ 0.054	0.466 $\pm$ 0.110 $\bullet$	0.599 $\pm$ 0.044
F1 ⁺	0.219 $\pm$ 0.075 $\bullet$	0.448 $\pm$ 0.054	0.494 $\pm$ 0.105 $\bullet$	0.602 $\pm$ 0.040

$\bullet(\circ)$: statistically significant (non-significant) difference of performance of the classification algorithm applied on the initial and the edited dataset, based on two-tailed paired t-test at 5% significance.

Table 16

Experimental results (mean $\pm$ std) on the Webpage dataset.

	EMLkNN		Rank-SVM	
	Before Editing	After Editing	Before Editing	After Editing
Hamming loss ⁻	0.063 $\pm$ 0.001 $\bullet$	0.050 $\pm$ 0.007	0.042 $\pm$ 0.005	0.041 $\pm$ 0.004$\circ$
One-Error ⁻	0.564 $\pm$ 0.007 $\bullet$	0.523 $\pm$ 0.059	0.399 $\pm$ 0.036	0.394 $\pm$ 0.035$\circ$
Coverage ⁻	12.124 $\pm$ 0.149 $\bullet$	10.313 $\pm$ 1.531	5.253 $\pm$ 0.397	4.321 $\pm$ 0.687$\bullet$
Ranking loss ⁻	0.494 $\pm$ 0.006 $\bullet$	0.415 $\pm$ 0.064	0.132 $\pm$ 0.009	0.108 $\pm$ 0.015$\bullet$
Average precision ⁺	0.485 $\pm$ 0.004 $\bullet$	0.532 $\pm$ 0.057	0.631 $\pm$ 0.031	0.678 $\pm$ 0.028$\bullet$
Accuracy ⁺	0.359 $\pm$ 0.004 $\circ$	0.372 $\pm$ 0.063	0.402 $\pm$ 0.028	0.440 $\pm$ 0.039$\bullet$
Precision ⁺	0.417 $\pm$ 0.004 $\circ$	0.425 $\pm$ 0.061	0.467 $\pm$ 0.032	0.500 $\pm$ 0.037$\bullet$
Recall ⁺	0.402 $\pm$ 0.006 $\circ$	0.396 $\pm$ 0.062	0.439 $\pm$ 0.030	0.486 $\pm$ 0.040$\bullet$
F1 ⁺	0.391 $\pm$ 0.005 $\circ$	0.397 $\pm$ 0.062	0.434 $\pm$ 0.030	0.474 $\pm$ 0.039$\bullet$

+(-): the higher (smaller) the value, the better the performance.

$\bullet(\circ)$: statistically significant (non-significant) difference of performance of the classification algorithm applied on the initial and the edited dataset, based on two-tailed paired t-test at 5% significance.

Precision: The precision metric computes the proportion of true positive predictions:

$$\text{Precision}(\mathcal{H}, \mathcal{S}) = \frac{1}{m} \sum_{i=1}^m \frac{|Y_i \cap \hat{Y}_i|}{|\hat{Y}_i|}. \quad (\text{A.3})$$

Recall: This metric estimates the proportion of true labels that have been predicted as positives:

$$\text{Recall}(\mathcal{H}, \mathcal{S}) = \frac{1}{m} \sum_{i=1}^m \frac{|Y_i \cap \hat{Y}_i|}{|Y_i|}. \quad (\text{A.4})$$

F1-measure: F1 measure is defined as the harmonic mean of precision and

Table 17

P-values on the Emotions dataset.

	t-test		Friedman test	
	EMLkNN	Rank-SVM	EMLkNN	Rank-SVM
Hamming loss ⁻	0.048	0.016	0.058	0.206
One-Error ⁻	0.037	0.009	0.527	0.011
Coverage ⁻	0.054	0.225	0.206	1
Ranking loss ⁻	0.061	0.011	0.058	0.206
Average precision ⁺	0.004	0.004	0.011	0.011
Accuracy ⁺	0.007	0.003	0.011	0.058
Precision ⁺	0.021	0.010	0.011	0.011
Recall ⁺	0.001	0.007	0.011	0.206
F1 ⁺	0.003	0.003	0.011	0.058

+(-): the higher (smaller) the value, the better the performance.

Table 18

P-values on the Yeast dataset.

	t-test		Friedman test	
	EMLkNN	Rank-SVM	EMLkNN	Rank-SVM
Hamming loss ⁻	0.023	0.007	0.206	0.058
One-Error ⁻	0.011	0.059	0.206	0.058
Coverage ⁻	0.011	0.003	0.058	0.058
Ranking loss ⁻	0.015	0.003	0.058	0.051
Average precision ⁺	0.010	0.008	0.206	0.058
Accuracy ⁺	0.004	0.004	0.058	0.058
Precision ⁺	0.020	0.005	0.206	0.011
Recall ⁺	0.002	0.007	0.508	0.058
F1 ⁺	0.004	0.004	0.058	0.058

+(-): the higher (smaller) the value, the better the performance.

617 recall. It is calculated as:

$$\mathcal{F}1(\mathcal{H}, \mathcal{S}) = \frac{1}{m} \sum_{i=1}^m \frac{2|Y_i \cap \hat{Y}_i|}{|Y_i| + |\hat{Y}_i|}. \quad (\text{A.5})$$

618 Note that the smaller the value of the Hamming loss, the better the perfor-
619 mance. For the other metrics, higher values correspond to better classification
620 quality.

Table 19

P-values on the Medical dataset.

	t-test		Friedman test	
	EMLkNN	Rank-SVM	EMLkNN	Rank-SVM
Hamming loss ⁻	0.105	0.136	0.527	0.527
One-Error ⁻	0.144	0.224	0.058	1
Coverage ⁻	0.111	0.178	0.206	0.058
Ranking loss ⁻	0.006	0.325	0.058	0.058
Average precision ⁺	0.476	0.336	1	1
Accuracy ⁺	0.043	0.007	0.206	0.058
Precision ⁺	0.04	0.021	0.058	0.527
Recall ⁺	0.022	0.002	0.206	0.011
F1 ⁺	0.032	0.005	0.058	0.058

+(-): the higher (smaller) the value, the better the performance.

Table 20

P-values on the Enron dataset.

	t-test		Friedman test	
	EMLkNN	Rank-SVM	EMLkNN	Rank-SVM
Hamming loss ⁻	0.154	0.112	0.058	0.011
One-Error ⁻	0	0.054	0.011	0.058
Coverage ⁻	0.276	0.036	0.206	0.011
Ranking loss ⁻	0.232	0.007	0.206	0.011
Average precision ⁺	0	0.008	0.011	0.011
Accuracy ⁺	0	0.019	0.002	0.011
Precision ⁺	0	0.018	0.011	0.011
Recall ⁺	0	0.002	0.002	0.011
F1 ⁺	0	0.007	0.001	0.011

+(-): the higher (smaller) the value, the better the performance.

621 A.2 Ranking-based measures

622 **One-error:** This metric computes how many times the top-ranked label is
623 not in the true set of labels of the instance, and it ignores the relevancy of all
624 other labels.

$$OErr(f, \mathcal{S}) = \frac{1}{m} \sum_{i=1}^m \langle [\arg \max_{\omega \in Y} f(\mathbf{x}_i, \omega)] \notin Y_i \rangle, \quad (\text{A.6})$$

Table 21

P-values on the Web dataset.

	t-test		Friedman test	
	EMLkNN	Rank-SVM	EMLkNN	Rank-SVM
Hamming loss ⁻	0	0.537	0.002	0.206
One-Error ⁻	0.042	0.569	0.206	0.527
Coverage ⁻	0.002	0	0.058	0.002
Ranking loss ⁻	0.001	0	0.011	0.001
Average precision ⁺	0.018	0.028	0.206	0.058
Accuracy ⁺	0.500	0.117	0.058	0.058
Precision ⁺	0.675	0.281	0.206	0.206
Recall ⁺	0.744	0.054	0.011	0.058
F1 ⁺	0.757	0.117	0.058	0.058

+(-): the higher (smaller) the value, the better the performance.

where for any proposition H , $\langle H \rangle$ equals to 1 if H holds and 0 otherwise.
 Note that, for single-label classification problems, the One Error is identical
 to ordinary classification error.

Coverage: Coverage computes the average of how far we need to move down
 the ranked label list in order to cover all the labels assigned to a test instance.

$$Cov(f, \mathcal{S}) = \frac{1}{m} \sum_{i=1}^m \max_{\omega \in Y_i} rank_f(\mathbf{x}_i, \omega) - 1. \quad (\text{A.7})$$

Ranking loss: This metric computes the number of times that an incorrect
 label is ranked higher than a correct label.

$$\mathcal{RLoss}(f, \mathcal{S}) = \frac{1}{m} \sum_{i=1}^m \frac{1}{|Y_i| |\overline{Y}_i|} |(\omega_q, \omega_r) \in Y_i \times \overline{Y}_i \setminus f(\mathbf{x}_i, \omega_q) \leq f(\mathbf{x}_i, \omega_r)| \quad (\text{A.8})$$

where $\overline{Y}_i$ is the complementary set of Y_i in $\mathcal{Y}$.

Average precision: This metric evaluates the average fraction of labels
 ranked above a particular label $\omega \in Y_i$ which are actually in Y_i .

$$AvPrec(f, \mathcal{S}) = \frac{1}{m} \sum_{i=1}^m \frac{1}{|Y_i|} \sum_{\omega_q \in Y_i} \frac{|\{\omega_r \in Y_i \setminus rank_f(\mathbf{x}_i, \omega_r) \leq rank_f(\mathbf{x}_i, \omega_q)\}|}{rank_f(\mathbf{x}_i, \omega_q)}. \quad (\text{A.9})$$

635 Note that $AvPrec(f, \mathcal{S}) = 1$ means that the labels are perfectly ranked. For
 636 the other metrics, smaller values correspond to a better label ranking quality.

637 B Multi-labeled dataset statistics

638 Given a multi-labeled dataset $\mathcal{D} = \{(\mathbf{x}_i, Y_i), i = 1, \dots, n\}$ with $\mathbf{x}_i \in \mathbb{X}$ and
 639 $Y_i \subseteq \mathcal{Y}$, this dataset can be measured by the number of instances (n), the
 640 number of attributes in the input space, and the number of labels (Q). In the
 641 following, we review some statistics about the multi-labeled dataset $\mathcal{D}$ [36].

642 **Label Cardinality:** The Label Cardinality (LCard) of $\mathcal{D}$ is the average num-
 643 ber of labels per instance. Label cardinality is calculated as

$$LCard(\mathcal{D}) = \frac{1}{n} \sum_{i=1}^n |Y_i| \quad (\text{B.1})$$

644 **Label Density:** The Label Density (LDen) of $\mathcal{D}$ is defined as the average
 645 number of labels per instance divided by the total number of labels Q . Label
 646 density is calculated as:

$$LDen(\mathcal{D}) = \frac{1}{n} \sum_{i=1}^n \frac{|Y_i|}{Q} \quad (\text{B.2})$$

647 Both metrics indicate the number of alternative labels that characterize the
 648 examples of a multi-labeled dataset. Label cardinality is independent of the
 649 total number of labels in the classification problem, while label density takes
 650 into consideration the total number of labels. Two datasets with the same label
 651 cardinality but with different label densities may present different properties
 652 that influence the performance of the multi-label classification methods.

653 **Distinct Label sets:** The Distinct Label sets (DL) counts the number of
 654 label sets that are unique across the total number of examples. Distinct label
 655 sets is given by:

$$DL(\mathcal{D}) = |\{Y_i \subseteq \mathcal{Y} | \exists \mathbf{x}_i \in \mathbb{X} : (\mathbf{x}_i, Y_i) \in \mathcal{D}\}| \quad (\text{B.3})$$

656 This measure gives an idea of the regularity of the labeling scheme.

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³ http://www.wormbook.org/chapters/www_genomclassprot/genomclassprot.html

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