Multi-label Ranking: Mining Multi-label and Label Ranking Data

Lihi Dery

Abstract We survey multi-label ranking tasks, specifically multi-label classification and label ranking classification. We highlight the unique challenges, and re-categorize the methods, as they no longer fit into the traditional categories of transformation and adaptation. We survey developments in the last demi-decade, with a special focus on state-of-the-art methods in deep learning multi-label mining, extreme multi-label classification and label ranking. We conclude by offering a few future research directions.

1 Introduction

Multi-label ranking (MLR) is the problem of predicting and ranking multiple labels for a single instance. The predicted labels are known as the instance’s labelset. MLR can be typically reduced to two sub-problems: The first is multi-label classification, where the task is to bipartite the data into relevant labels (the labelset) and irrelevant labels. The second is label ranking classification, where the task is to rank labels for each instance. A label ranking may contain ties; in the extreme case relevant labels hold a tie on first place, and irrelevant labels hold a tie on second place, thus turning the label ranking classification into a multi-label one.

The first studies of MLR originated from text categorization problems, where each document was labeled with several predefined topics [69, 87, 113]. The labels were sometimes ranked in order of importance [68]. While multi-label for text categorization continues to be an active field [90, 92], multi-label ranking has spread to many more domains. In bioinformatics, a gene can belong to multiple functional families [33]. In music, a tune can spark many emotions [124]. In medical diagnosis, an x-ray image can have multiple labels [8]. In social networks, people may belong to
several interest groups [135] and in visual object recognition, objects can be ordered according to their relevance to the picture [18, 151].

There are six common challenges in MLR that either do not exist in single-label classification or are intensified in MLR settings.

- **High dimensionality in the output space.** High dimensionality in the input space (i.e., data with millions of instances) or in the feature space (i.e., data with thousands or millions of features) is also common in single-label classification, though in MLR it might be harder to solve. However, high dimensionality in the output space is unique to MLR. The number of possible labelsets (i.e. label combinations) grows exponentially with the number of labels. This often leads to sparseness of available data and to class imbalance, as some labelsets may appear often, while others may be rare or may not appear in the training set at all. See an example in figure 1.

- **Label correlation.** This aspect is fundamental in MLR. If there are no relations between the labels, the problem can be split into multiple binary classification problems without loss of information. However, in MLR, the relation between the labels is complex. For example, if two labels have a high concurrence, the model is supposed to somehow boost the prediction of one label, if the other is predicted. If two labels have a parallel relation, i.e., they do not concur, the model is expected to handle that as well. See an example of label concurrence in figure 2.

- **Label imbalance.** The label distribution is highly skewed, most labels have only a handful of positive training instances and a few labels dominate with many training instances. See an example in figure 3.

- **Labelset size imbalance.** The labelset size of each instance is highly skewed [110]. Few instances have much more labels than average, while most instances have very few labels. See an example in figure 4.

- **Label importance.** Not all labels are equally important to the characterization of the instance. The label importance is explicitly known if the target class input labelset is ranked (i.e, if a ranked labels are provided as input in the training data). Otherwise, the label importance remains to be inferred.

- **Zero-shot labels and labelsets.** Some labels and labelsets never appear in the training set.

Figures 1 - 4, were created using the mlrGUI [22] with the Genebase dataset [39] as an example. The dataset contains the classification of proteins into families with similar function. Each instance is a protein, the attributes are the protein’s motifs. The labels are the families the protein belongs to. This is a multi-label setting since each protein can belong to more than one family. In it’s current online version [128], the dataset contains 662 instances (the proteins) with 1213 attributes each. There are 27 possible labels (families) and 32 possible labelsets.

Previous literature reviews on multi-label methods [47, 48, 61, 161] and label ranking methods [131, 166], while excellent, are slightly outdated. Our contributions in this survey are three-fold. First, we refresh the definition of MLR [17] and define it’s two sub-tasks: multi-label classification and label ranking classification. Second,
we suggest to re-categorize MLR methods, as they no longer fit into the traditional categories of transformation or adaptation. We thus suggest new categories such as deep learning multi-label methods, extreme multi-label methods and label ranking methods. Third, we focus on the last demi-decade which has not yet been surveyed.

The rest of this survey is organized as follows: we first define MLR and place it in context with other tasks (section 2). Next, we survey recent developments in multi-label methods, with a special focus on deep learning methods and the emerging field of extreme multi-label classification (section 3). We then move on to discuss label ranking (section 4). We present up to date information about evaluation (section 5) and conclude by offering a few research directions on open problems (section 6).

![Fig. 1](image.png)  
Fig. 1 High dimensionality in the output space. The number of instances (y-axis) with a given labelset (x-axis) in the Genebase dataset.

2 Definition and context

We begin with a definition of MLR. Next we place MLR in context by detailing which problems can be seen as sub cases of MLR, and what MLR is a sub problem of.

**Definition 1. Multi-label ranking (MLR).** An MLR task is characterized by $\mathbf{x} \in \mathcal{X}$ instances and $l \in L$ labels with the following properties:

1. $\mathcal{X}$ is finite and contains $n$ instances.
Fig. 2  Label correlation: a chord diagram [54] showing the concurrence of 13 labels in the Genebase dataset. The arcs represent label concurrence. For example, the protein to the right of 12 o’clock (PDO-0196) co-occurs with only one other protein (PDO-0199) and that happens less frequently than other concurrences.

Fig. 3  Label imbalance. The number of instances (y-axis) with a given label (x-axis) in the Genebase dataset.
2. $L$ is finite and contains $m$ labels.

3. An ordered labelset $Y = \{l_1, ..., l_q\}$ with $q \leq |L|$ labels, contains a subset of the $L$ possible labels. $l_1$ is the label with the highest rank and $l_q$ is the label with the lowest rank.

4. The labelset size is exponential to the amount of labels: $Y \subseteq \mathcal{P}(L)$.

5. Ties in the labelset ranking are allowed, and in some cases all of the labels are tied in first place. A threshold $t \in 1, 2, ..., q$ indicates the partitioning of $Y$ into relevant and irrelevant labels. When $t = 1$ only the first label in $Y$ is relevant. When $t = q$, or when the threshold is not mentioned, all labels in $Y$ are relevant. When $1 \leq t \leq q$ the labelset is bipartite according to $t$.

6. The training dataset $D$ consists of a triplets $\{x_i, Y_i, t_i\}$

7. The goal is to find a mapping function: $h : X \rightarrow Y$ for a given $t$.

In multi-label ranking problems the labelset is bipartite, i.e., the instance belongs to a ranked subset of the labels, and doesn’t belong to the rest of the set. For example, this image contains mainly oranges, apples and bananas in this order, but no pears. Several problems are special cases of multi-label ranking: binary classification, multi-class classification, multi-label classification and label ranking. In binary classification, an instance can belong to one of two possible classes, e.g., this image contains either an apple or an orange. In multi-class problems, an instance can belong to one out of multiple possible classes, e.g., this image contains either an
apple, an orange or a banana. In **multi-label** problems, an instance can belong to many classes (labels), e.g. this image contains an apple and an orange but not a banana. In **label ranking** problems, an instance belongs to a ranked set of classes (labels), e.g. this image contains oranges, apples and bananas, in this order.

Multi-label ranking tasks, as defined in definition 1, refer to any problem whose **target class output** is a ranked list of labels and a threshold. Algorithms for solving these tasks are often divided into two sub-groups according to their **target class input**. When the input is a ranked set of labels, it is a label ranking task. When the input is just a set of labels, it is a multi-label task. Formally:

**Definition 2.** A **multi-label (ML)** task is an MLR with $1 \leq t \leq q$. The labelset is bipartite according to $t$, with labels $1 \leq t$ tied in first place and considered as relevant.

**Definition 3.** A **label ranking (LR)** task is an MLR with $t = q$ and no ties in $Y$.

Table 1 summarizes the differences between MLR and it’s sub-tasks according to a few parameters:

- Is $m > 2$? - There may be many labels available for each instance, or just two.
- Is $q > 1$? - It may be possible to assign many labels for each instance, or just one.
- Are there ties in $Y$? - Is the labelset completely ordered, or can ties between labels exist?
- Does $t = q$? - Are all labels in $Y$ relevant, or does the threshold $t$ partitions the labels into relevant and irrelevant labels?

| Table 1 Table of sub-cases of multi-label ranking | $m > 2$ | $q > 1$ | ties in $Y$ | $t = q$ |
|---------------------------------------------|--------|--------|-------------|--------|
| Multi-label Ranking (MLR)                   | yes    | yes    | yes         | yes    |
| Label ranking (LR)                          | yes    | yes    | yes         | no     |
| Multi-label (ML)                            | yes    | yes    | no          | yes    |
| Multi-class (MC)                            | yes    | no     | no          | yes    |
| Binary classification                       | no     | no     | no          | no     |

A recent survey categorizes multi-label mining as a sub-problem in multi-target learning [133]. Related problems in the multi-target domain, that are not covered in this survey, include:

- **Multi variate regression** [12] and **dyadic prediction** where the goal is to predict a score for the fit between the instance and the label.
- **Hierarchical multi-label** [20] where there is explicit side information about the dependencies between the labels.
- **Multi-instance** [62] and **multi-instance multi-label** [168, 65] where the training data is composed of a bag of instances that are all assigned the same label or labels.
- **Multi-view** [165] is similar to multi-instance but the instances may have different feature spaces.
3 Multi-label algorithms

To date, surveys classify multi-label algorithms as either problem transformation techniques or algorithm adaptation techniques [21, 48, 161]. In the first, the problem is transformed into a simpler single label classification task. In the second, an algorithm used for single label classification is adapted to perform multi-label tasks. Sometimes ensembles techniques are added as a third class of problems and other times they are listed by their underlying base classifier’s category (transformation or adaptation).

However, in the last decade algorithms that are especially designed for multi-label tasks have emerged. These algorithms either: try to maximize a specific evaluation measure (e.g. [98, 99, 143]), focus on a certain sub-task (e.g., feature selection [97, 118, 162]), or attempt to address specific multi-label challenges such as high dimensionality output space, label correlation (e.g.[53, 66]), imbalance or zero-shot (e.g. [108]).

Moreover, deep learning algorithms designed specifically for multi-label tasks have been rapidly developing, exhibiting promising results. Indeed, a minority of these algorithms can be classified as algorithm transformation techniques (see e.g. the method suggested in [151]), but more often, the algorithm is not adapted but rather specially tailored for the problem at hand.

As transformation and adaptation techniques have been exquisitely covered [9, 21, 48, 61, 158, 161] and as there is only a minor increase in research on them in comparison with other aspects of MLR, we lightly scan these foundations (sections 3.1 and 3.2), and then direct our focus on methods from the last demi-decade, specifically on deep learning (section 3.3) and extreme multi-label methods (section 3.4).

3.1 Problem adaptation and problem transformation

Problem adaptation techniques were originally suggested for text categorization. However the adaptations soon expanded beyond the text domain and into other scenarios as well. Some of the most noticed adaptations include: Expectation maximization (EM) [87], SVM [42, 69, 147, 145], k-NN [19, 31, 64, 117, 160], decision trees [4, 33], association rules [122] and genetic algorithms [50].

Problem transformation techniques [9] focus on transforming the problem into simpler sub-tasks. One classifier is created for each label or pair of labels. The classifiers are then trained separately, and their output is combined. The possible transformations are:

• **Binary Relevance.** The transformation into a binary classification task is known as binary relevance (BR) [158]. The first BR solutions [13, 49] did not consider label correlation. However, many correlation-enabling extensions to binary relevance have been proposed in the past decade. These correlations are classified into
three sub-classes: first order correlation, pairwise correlation, or full correlation [161].

- **Multi-class.** The most known multi-class transformations are the Label Powerset methods that reduce the problem to a multi-class one by treating each individual labelset as an independent class label [13]. In both BR and multi-class transformations, there is a computational complexity problem, as the solutions do not scale well as the number of labels increase. Thus solutions that reduce the number of classifiers were suggested [86, 88].

- **Pairwise label comparisons.** Calibrated Label Ranking [46] transform the dataset into pairs of labels and thus train $k(k-1)/2$ binary classifiers. The output of the classifiers are combined into a ranking of the output labels, with the highest ranked labels considered as relevant. A fictional label can be used to automatically create a bi-partition of the labels into relevant and irrelevant ones [17].

### 3.2 Multi-label ensembles

The 2BR method [125] uses BR twice and employs stacking. It first learns a BR model, and then builds a second, meta-model that takes the output of the first model and includes a explicit coefficient for correlated labels. The PruDent method focuses on unnecessary label dependencies and error-propagation showing improved results over 2BR [5].

In Classifier chains (CC) [104], the first classifier is trained on the input attributes. The classifier’s output is then added as a new input attribute, and a second classifier is trained, and so on. In this way the classifiers are chained, taking into account the possible label dependencies. In ensembles of classifier chains (ECC) [104], a set of CCs with different orders are trained and the outputs are aggregated.

Hierarchy Of Multi-label classifications (HOMER) [126] creates a tree of BR methods, were each leaf contains one label. To classify a new instance, HOMER begin at the root classifier and passes the instance to each child only if the parent predicted any of its labels. The union of the predicted labels by the leaves generates output for the given instance.

AdaBoost.MH [113] is the multi-label variation of the well known AdaBoost algorithm [45]. AdaBoost.MH weights the labels as well as the instances. Training instances and their corresponding labels that are hard to predict, get incrementally higher weights in following classifiers while instances and labels that are easy to classify get lower weights. This algorithm is designed to minimize the hamming loss. ADTBoost.MH [35] which uses ADT Trees is an extension of AdaBoost.MH.

Random k-Labelsets (RAkEL) [129] selects a number of random k-labelsets and learns a Label Powerset classifier for each of them. These are then aggregated. Enhancements over RAkEL include RAkEL++ [109] and RAkELLd [127].

An experimental study on most of the above multi-label ensembles suggests that ECC, followed by RAkEL, exhibit the best overall performance for all of the examined metrics [91].
A few notable ensemble methods were published in the last three years. ML-FOREST [141] builds on Random Forest and ML-TSVM [27] on SVM. PRAkEL, a cost-sensitive extension of RAkEL that considers the evaluation criteria and is sensitive to the cost of misclassifying an instance [143]. fRAkEL speeds up RAkEL by shrinking the samples with irrelevant labels [146]. The TSEN ensemble [164] is based on three-way-decisions [154]. The MULE ensemble [95] relies on a heterogeneous ensemble that is composed of different base models. The assumption is that different labels can be approximated better by different types of models. MULE incorporates a statistical test to combine the base models. Most of these methods compare their performance to earlier methods, mainly to variations of 2BR, ECC, AdaBoost.MH and RAkEL. However an evaluation of these methods in comparison to one another is still missing.

3.3 Deep learning methods

Deep learning uses multiple layers to represent the abstractions of data and to automatically discover useful features [79, 114]. Deep learning can cope with large amounts of input features, eliminating the need for feature selection methods. The learnt feature representations are often accurate for other unseen data as well. While this quality, known as transfer learning [94] is not unique to deep learning, in the case of multiple labels it can provide a solution to the label and labelset imbalance problems. This also means that parameters for a new model (such as number of layers and number of nodes) can be learnt from previous successful models instead of by trial and error. Deep learning models are devised using different architectures [100]. Convolutional Neural Network (CNN) models [34, 80] are often used for image processing. Recurrent neural network (RNN) models [78] and their variant Long Short-Term Memory (LSTM) [43, 119] are often used with text and speech. Generative adversarial networks (GANs) [52] and Restricted Boltzmann Machine (RBM) [1, 121] have been used for unsupervised multi-label learning tasks but we herein focus on a supervised MLR setting as defined in definition 1.

Deep learning for multi-label tasks is a growing field, with new papers appearing frequently. We survey some of the recent developments in two main multi-label tasks, which belong to the media domain: image annotation and text annotation.

3.3.1 Image annotation

The growing interest in deep learning for multi-label image annotation is partly driven by new publicly accessible large-scale datasets with quality labels. A few of the most notable ones include:

- **The Visual Genome dataset [74]**. Contains over 108K images with an average of 35 labelled objects, 26 attributes, and 21 pairwise relationships between objects.
• **The ChestX-ray14 dataset [136].** Contains over 112k chest X-rays from over 30k patients, labeled with up to 14 pathologies or “No Finding”.

• **The MS COCO dataset [83].** Contains 328k images with 2.5 million labelled objects, out of a set of 91 labels.

• **The NUS-WIDE dataset [32].** Contains almost 270k Flickr images and their associated labels, with a total of 5,018 unique labels.

Recent reviews of deep learning for medical images highlight the vast amount of emerging research in this field [44, 70, 112]. On the chest X-rays dataset, various CNN based methods have been suggested. One approach is to transform the problem into multiple single-label classification problems, to which a CNN architecture is applied [51]. Another suggestion is Hypotheses-CNNPooling (HCP), where a number of object (i.e., image) segment hypotheses are taken as the inputs, then a shared CNN is connected with each hypothesis, and finally the CNN output results from different hypotheses are aggregated with max pooling to produce the multi-label predictions [138]. The CNN-RNN model uses an underlying RNN model [89] to capture the high order label dependencies. Then, CNN and RNN are combined into one framework to exploit the label dependencies at the global level [134]. Other models exist (e.g. [40, 55, 56, 57, 103, 116]), as well as a cascade ensemble [76]. Though multi-instance methods are out of our scope, we note that a multi-instance method, that integrates the images with other information about the patients has recently been reported to enhance performance [8].

Various studies have been conducted on non-medical images as well. For a recent review see Voulodimos et al. [132]. Some of these models focus on learning the label correlations. A model that learns image-dependent conditional structures [82] has been proposed. A Spatial Regularization Network (SRN) that captures the spatial correlation between labels as well as the semantic correlation has been suggested [169]. A feature attention network (FAN) focuses on more important features and learn the correlations among convolutional features [150]. The Regional Latent Semantic Dependencies (RLSD) model [157] specializes in predicting small objects (alongside prediction of large objects) by first extracting convolutional features, which are further sent to an RPN-like (Regional Proposal Network) localization layer. The layer is designed to localize the regions in an image that may contain multiple semantically dependent labels. These regions are encoded with a fully-connected neural network and further sent to an RNN, which captures the latent semantic dependencies at the regional level. The RNN unit sequentially outputs a multi-class prediction, based on the outputs of the localization layer and the outputs of previous recurrent neurons. Finally, a max-pooling operation is carried out to fuse all the regional outputs as the final prediction. Once again, multi-instance methods can enhance performance [85].

Comparisons of cutting-edge image annotation methods are still lacking. A precedent study compared the performance of ten foreground deep learning multi-label APIs on the Visual Genome dataset [75]. The APIs were evaluated using various metrics. In addition, a semantic similarity metric was used allowing for words with similar meaning to be classified as correct predictions. For example, “bicycle” and “bike” were both classified as correct for an image of a pedal driven two-wheeler. The
3.3.2 Text Annotation

One of the earliest models to employ deep learning for text classification was BP-MLL [159]. It formulated multi-label classification problems as a neural network with multiple output nodes, one for each label. It was later suggested [93] to replace the pairwise ranking loss in the model with a cross-entropy loss instead. However, these models do not consider label dependencies. A CNN model that has a final hidden layer which considers label co-occurrence weights was suggested next [77]. The model was analyzed on a small dataset with 103 labels. In the CNN-RNN model [26], the RNN is set to deal with label co-occurrence. The C2AE algorithm employs a DNN-based label embedding framework and performs joint feature and label embedding [155].

The Seq2seq model [152] uses an LSTM to generate labels sequentially, and predicts the next label based on its previously predicted labels. The LSTM² model [149] utilizes LSTM twice. The algorithm first builds a representation of the documents in the training set. This is done with an LSTM network that considers word sequences. For each document in the test set, the algorithm searches for the most similar documents in the training set and retrieves their labels. The labels are represented as a semantic tree that is trained with dependency parsing. This tree can capture the correlations between labels. Based on the document representation, another LSTM is utilized to rank the document labels.

Recently, text categorization has also been employed in the context of X-ray images. For example, it has been pointed out that China’s chest X-ray reports focus more on characterization than on labelling the possible diseases. A recent study uses LSTM to read the X-ray reports, and output labels of pathologies [148]. Another study combines the reports and the instances (a multi-instance model) for the same purpose [137].

3.4 Extreme multi-label classification

Extreme multi-label (XML) problems, also known as large-scale multi-label problems, refer to problems with an extremely large set of labels, usually in the millions. Due to the huge amount of labels, the zero-shot problem, as well as the label and labelset imbalance problems (see section 1), are intensified. Deep learning models work well here since they consider both the relatedness of the representations and the context information.

Currently, all of these problems focus on text classification or on traditional recommender system problems that have been reformulated as XML problems [120, 130]. The instances are of one of the following kinds:
• **Text.** Assigning categories (the labels) to a Wikipedia page out of the million categories (labels) available, recommending bid phrases (the labels) to an advertiser with a given ad landing page [2], assigning tags (the labels) to an image. In these cases, the instance, be it a web page or an image, is represented by a bag of words.

• **Item.** Assigning a number of categories (the labels) to an Amazon product item. The instance is represented by item features.

• **User.** Recommending YouTube videos (the labels) to a user [140]. The instance is represented by user features.

We note that these tasks often require a ranked output, and that a ranked input might be available. However, to the best of our knowledge, extreme label ranking which explicitly considers ranked inputs (as opposed to extreme multi-label) has not yet been explored.

PDSparse [156] and DiSMEC [7] tackle the sparseness (high dimensionality) by training one XML model per label. We thus consider them as XML problem transformation methods.

MLRF [2] designs a multi-label random forest. To cope with the high dimensionality problem, they assume label independence during the ensemble construction, but they do consider correlations during prediction. The FastXML model [102] provides a node partitioning formulation that improves MLRF results in settings with millions of labels. XML-CNN [84] uses a CNN model for the actual classification.

The SwiftXML model [101] learns label correlation using a word2vec embedding. This allows the discovery of similar labels as these labels are classified closely in the embedded vector. An example given by the authors is that although the labels of the Wikipedia pages of Einstein and Newton are very different, the SwiftXML label embedding will learn that the two are similar, and thus will be able to consider labels given to Einstein’s page, also for Newton’s page. Authors report to have outperformed SLEEC [10] which also employs label embedding and is considered state-of-the-art. A recent model [163] tackles both feature and label spaces using a non-linear embedding based on a graph structure.

### 4 Label ranking algorithms

Numerous label ranking algorithms were suggested in the literature. One approach is based on turning the problem into several binary classification problems and then combining them into output rankings [29, 38, 58, 60, 67]. Another common approach is based on modifying existing probabilistic algorithms to directly support label ranking. Some main examples are: naive Bayes models [3], k-nearest neighbor models [14] and decision tree models such as Label Ranking Trees (LRT) [30] and Entropy Based Ranking Trees (ERT) [36].

A few other stand-alone ideas are available as well. RPC (Ranking by Pairwise Comparison) [67] learns pairwise preferences from which a ranking is derived. Instance Based Logistic Regression (IBLR) combines instance-based learning and
logistic regression [30]. Under this approach, the label statistics of neighboring instances are regarded as features by the logistic regression classifier. A rule based approach learns a reduction technique and provides a mapping in the form of logical rules [59]. A recent work [72] adapts ideas from structured output prediction. They cast the label ranking problem into the structured prediction framework and propose embeddings dedicated to ranking representation. For each embedding they propose a solution to the pre-image problem. This latter suggestion is a harbinger for a bridge between label ranking and structured image prediction.

Surveys on label ranking algorithms [131, 166] capture some of the earlier methods.

### 4.1 Label ranking ensembles

To the best of our knowledge, only a few papers thus far have investigated the use of ensembles for label ranking [6, 111, 139, 167]. The ensembles proposed in these papers differ in: (1) the base label ranking algorithm used, (2) the method used to sample the data to train each of the simple models (if all models are trained with the exact same data they will output the exact same results, and then there is no need for an ensemble), and (3) the aggregation method used to combine the results of the simple models.

As the base label ranking algorithm [6] used Label Ranking Trees (LRT) [30], [111] used Ranking Trees (RT) and Entropy Ranking Trees (ERT) [36], [167] developed their own method named Top Label As Class (TLAC) and [139] used both LRT and Ranking by Pairwise Comparison (RPC) [67].

To select the training data for each simple classifier, [6] and [139] used a technique known as Bootstrap aggregation or Bagging [15]: they created \( b \) different bags by selecting a subset of the dataset’s instances with replacement. The other two papers [111, 167] suggested modifications to the well-known Random Forest ensemble model [16]. As for the aggregation method used, three studies used a voting rule (either Borda or Modal Ranking). The last study [139] presents VRS (Voting Rule Selector), a meta-model that automatically learns the best voting rule to be used. There four works are summarized in table 2.

|                   | Aledo et al. (2017) | Sa et al. (2017) | Zhou et al. (2018) | Werbin et al. (2019) |
|-------------------|---------------------|-----------------|-------------------|----------------------|
| Base algorithm    | LRT                 | ERT, RT         | TLAC              | LRT, RPC             |
| Data sampling     | Bagging             | Random Forest   | Random Forest     | Bagging              |
| Aggregation       | Modal ranking       | Borda           | Borda             | Voting Rule Selector |

Table 2 Label ranking ensemble frameworks

AdaBoost.MR is the label ranking variation of the well known AdaBoost algorithm [45]. The algorithm performs pairwise comparisons between labels. Training
instances and their corresponding label pairs that are hard to predict, get incrementally higher weights in following classifiers while instances and label pairs that are easy to classify get lower weights. The algorithm is designed to minimize the ranking loss. Another boosting-based approach suggests learning a linear utility function for each label, from which the ranking is deduced [37]. This approach is more general, as it allows the input to be any sort of preference graph over the labels. A ranking function assigns a utility score to each label. Then, relevant pairwise comparisons as deduced from the graph, are performed. Again, the label weights are updated and additional weight is given to each wrongly ranked pair. As these approaches rely on pairwise comparisons, they do not scale well in the case of many labels.

5 Evaluation

Evaluating the performance of multi-label algorithms is difficult. For example, it is maybe impossible to decide which mistake of the following two cases is more serious: one instance with three incorrect labels vs. three instances each with one incorrect label. Therefore, a number of performance measures focusing on different aspects have been proposed. Schapire and Singer [113] initially suggested five metrics: Hamming loss, ranking loss, one-error, average precision. The popular micro-F1 and macro-F1 were suggested by Tsoumakas et al. [127]. Instance-F1 and AUC measures were discussed by Koyejo et al. [73] A summary of the 11 most common measures is provided Wu et al. [142]. For label ranking, the most popular measure is Kendall-tau. The hamming distance is also often used when permutations represent matching of bipartite graphs.

5.1 Dataset repositories

The Mulan repository [128] contains 27 multi-label datasets on various subjects. MEKA [105] contains datasets in arff format, suitable for Weka. An R package automates the use of these datasets [23]. The KDIS research group offers a repository of various datasets obtained from different sources. ¹

The Extreme Classification Repository stores 15 extreme multi-label text datasets, as well as code for various algorithms. ² LSHTC series challenge also stores extreme multi-label text datasets [96]. The SNAP library [81] contains social and information networks, some of which can (and were) utilized for extreme multi-label tasks (e.g. Amazon products). Lastly, it is possible to generate simulated data via a multi-label data generator [123].

¹ http://www.uco.es/kdis/mllresources/
² http://manikvarma.org/downloads/XC/XMLRepository.html#Prabhu14
As for datasets with a ranked target class as input, five real world label ranking datasets can be found in [106]. The 16 semi-syntetic label ranking datasets used in [28, 30] are stored on the webpage of one of the authors.  

5.2 Stratification of multi-label data

Estimating the accuracy of a model is traditionally done by splitting the data to training, test, and sometimes also validation subsets. Different techniques are available, such as cross validation, holdout and bootstrap [41, 107]. Random sampling works well when the labels have enough representation in the data. When this is not the case, a stratification approach assures that all subsets contain approximately the same proportions of labels as the original dataset. For single-label classification tasks, stratification has been shown to outperform cross-validation with random sampling [71].

For multi-label data, stratification is even more important, as some datasets may have very few patterns representing them and random sampling might place them all in either the training or the test data partitions.

Stratification for multi-label data can either consider the distinct labelsets available in the data, or consider each label separately. Since the number of labelsets grows exponentially to the number of labels, when the number of labels is large there might be only one instance for each example in the labelset, or even no examples at all. For this reason, a method that considers each label separately was suggested by [115]. Stratifying the data in this method is a slow procedure, but nonetheless, it improves the classifier performance.

6 Research directions and open problems

There are still many paths to explore for multi-label ranking. We outline a few of them here.

First, in many real-world scenarios, new labels emerge over time. For example, the label “valentine2030” will only emerge on year 2030. Multi-Label learning with emerging new labels has just begun to be considered, and we are aware of only one pioneering work on the subject [170]. We have seen herein that recommender system problems can be reformulated as multi-label ones. Perhaps it is time to reconsider the other direction as well [153]. The “cold-start” problem is fundamental in recommender systems. Perhaps their solutions can be adapted to multi-label ranking tasks. Moreover, evaluation measures need to be fine-tuned to this setting of emerging labels [108, 144].

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3 https://cs.uni-paderborn.de/?id=63912
Second, a recent study [11] compared recommender system and multi-label classification techniques concluding that AdaBoost with CC chains and BR with multi-label random forest outperform the best recommender system methods in a given cross-selling setting. However, state-of-the-art multi-label deep learning methods and extreme multi-label methods should be able to do even better but have not been considered in the above study. Moreover, it is interesting to reconsider other recommender and ranking scenarios and reformulate them as MLR tasks as well.

Third, for single-label problems, a set of complexity measures that calculate the overlap and separability of classes has been defined [63]. To the best of our knowledge, one characterization metric, called TCS (Theoretical Complexity Score) exists for multi-label tasks [24] but no complexity measures exist for label ranking, where the emphasis is on the correct order of labels. In a related context, SCUMBLE (Score of ConcUrrence among iMBalanced LabEls) is a new metrics that address label co-occurrence in multi-label datasets [25]. It can and should be used to gain better understanding of the available data.

Fourth, we have reviewed state-of-the-art deep learning algorithms for image annotation and separate algorithms for text classification. One cannot but wonder if these fields can inspire one another and furthermore, if a meta-method for both tasks can be developed.

Lastly, as explained in section 3.4, extreme label ranking problems where the target input space is ordered have yet to be explored.

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