REVIEW ARTICLE

Binary relevance for multi-label learning: an overview

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Abstract Multi-label learning deals with problems where each example is represented by a single instance while being associated with multiple class labels simultaneously. Binary relevance is arguably the most intuitive solution for learning from multi-label examples. It works by decomposing the multi-label learning task into a number of independent binary learning tasks (one per class label). In view of its potential weakness in ignoring correlations between labels, many correlation-enabling extensions to binary relevance have been proposed in the past decade. In this paper, we aim to review the state of the art of binary relevance from three perspectives. First, basic settings for multi-label learning and binary relevance solutions are briefly summarized. Second, representative strategies to provide binary relevance with label correlation exploitation abilities are discussed. Third, some of our recent studies on binary relevance aimed at issues other than label correlation exploitation are introduced. As a conclusion, we provide suggestions on future research directions.

Keywords machine learning, multi-label learning, binary relevance, label correlation, class-imbalance, relative labeling-importance

1 Introduction

Multi-label learning is a popular learning framework

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for modeling real-world objects with multiple semantic

meanings [1,2]. For instance, in text categorization, a news document on government reform can cover multiple topics, such as politics, economics, and society [3]; in image classification, a natural scene image can depict multiple types of scenery, such as sky, sand, sea, and yacht [4]. Multi-label objects exist in many real-world applications, including information retrieval [5], bioinformatics [6], multimedia content annotation [7], and Web mining [8].

The goal of multi-label learning is to induce a multi-label predictor that can assign a set of relevant labels for the unseen instance. In order to achieve this, the most intuitive solution is to learn one binary classifier for each class label, where the relevance of each class label for the unseen instance is determined by the prediction yielded by the corresponding binary classifier [9]. Specifically, the binary relevance procedure works in an independent manner, where the binary classifier for each class label is learned by ignoring the existence of other class labels. Due to its conceptual simplicity, binary relevance has attracted considerable attention in multi-label learning research. 1)

However, a consensus assumption for multi-label learning is that the correlations between labels should be exploited in order to build multi-label prediction models with strong generalization ability [1,2,10,11]. The decomposition nature of binary relevance leads to its inability to exploit label correlations. Therefore, many correlation-enabling extensions to binary relevance have been proposed in the past decade [12– 29]. Generally, representative strategies to provide binary relevance with label correlation exploitation abilities include the chaining structure assuming random label correlations, the

¹⁾ According to Google Scholar (June 2017), the seminal work on binary relevance [9] has received more than 1,100 citations

stacking structure assuming full-order label correlations, and the *controlling* structure assuming pruned label correlations.

Although label correlation plays an essential role in inducing effective multi-label learning models, recent studies have shown that some inherent properties of multi-label learning should also be investigated in order to achieve good generalization performance. On one hand, class labels in the label space typically have *imbalanced distributions*, meaning the number of positive instances w.r.t. each class label is far less than its negative counterpart [30–39]. On the other hand, class labels in the label space typically have different labelingimportance, meaning the importance degrees of each class label for characterizing the semantics of a multi-label example are relative to each other [40–45]. Therefore, in order to enhance the generalization performance of binary relevance models, it is beneficial to consider these inherent properties in addition to label correlation exploitation during the learning procedure.

In this paper, we aim to provide an overview of the state of the art of binary relevance for multi-label learning. In Section 2, formal definitions for multi-label learning, as well as the canonical binary relevance solution are briefly summarized. In Section 3, representative strategies to provide label correlation exploitation abilities to binary relevance are discussed. In Section 4, some of our recent studies on related issues regarding binary relevance are introduced. Finally, Section 5 provides suggestions for several future research directions regarding binary relevance.

2 Binary relevance

Let $X = \mathbb{R}^d$ denote the d-dimensional instance space and let $\mathcal{Y} = \{\lambda_1, \lambda_2, \dots, \lambda_q\}$ denote the label space, consisting of q class labels. The goal of multi-label learning is to induce a multi-label predictor $f: X \mapsto 2^{\mathcal{Y}}$ from the multi-label training set $\mathcal{D} = \{(\boldsymbol{x}^i, \boldsymbol{y}^i) \mid 1 \leq i \leq m\}$. Here, for each multi-label training example $(\boldsymbol{x}^i, \boldsymbol{y}^i), \ \boldsymbol{x}^i \in X$ is a d-dimensional feature vector $[x_1^i, x_2^i, \dots, x_d^i]^{\top}$ and $\boldsymbol{y}^i \in \{-1, +1\}^q$ is a q-bit binary vector $[y_1^i, y_2^i, \dots, y_q^i]^{\top}$, with $y_j^i = +1$ (-1) indicating that y_j^i is a relevant (or irrelevant) label for \boldsymbol{x}^i . Equivalently, the set of relevant labels $Y^i \subseteq \mathcal{Y}$ for \boldsymbol{x}^i corresponds to $Y^i = \{\lambda_j \mid y_j^i = +1, \ 1 \leq j \leq q\}$. Given an unseen instance $\boldsymbol{x}^* \in X$, its relevant label set Y^* is predicted as $Y^* = f(\boldsymbol{x}^*) \subseteq \mathcal{Y}$.

Binary relevance is arguably the most intuitive solution for

learning from multi-label training examples [1,2]. It decomposes the multi-label learning problem into q independent binary learning problems. Each binary classification problem corresponds to one class label in the label space \mathcal{Y} [9]. Specifically, for each class label λ_j , binary relevance derives a binary training set \mathcal{D}_j from the original multi-label training set \mathcal{D} in the following manner:

$$\mathcal{D}_j = \{ (\boldsymbol{x}^i, y_j^i) \mid 1 \leqslant i \leqslant m \}. \tag{1}$$

In other words, each multi-label training example (x^i, y^i) is transformed into a binary training example based on its *relevancy* to λ_i .

Next, a binary classifier $g_j: X \mapsto \mathbb{R}$ can be induced from \mathcal{D}_j by applying a binary learning algorithm \mathcal{B} , i.e., $g_j \leftrightarrow \mathcal{B}(\mathcal{D}_j)$. Therefore, the multi-label training example (x^i, y^i) will contribute to the learning process for all binary classifiers g_j $(1 \le j \le q)$, where x^i is utilized as a positive (or negative) training example for inducing g_j based on its relevancy (or irrelevancy) to λ_j .³⁾

Given an unseen instance x^* , its relevant label set Y^* is determined by querying the outputs of each binary classifier:

$$Y^* = \{ \lambda_i \mid g_i(\mathbf{x}^*) > 0, \ 1 \le j \le q \}. \tag{2}$$

As shown in Eq. (2), the predicted label set Y^* will be empty when all binary classifiers yield negative outputs for x^* . In this case, one might choose the so-called *T-Criterion* method [9] to predict the class label with the *greatest* (least negative) output. Other criteria for aggregating the outputs of binary classifiers can be found in [9].

Algorithm 1 summarizes the pseudo-code for binary relevance. As shown in Algorithm 1, there are several properties that are noteworthy for binary relevance:

- First, the most prominent property of binary relevance lies in its conceptual simplicity. Specifically, binary relevance is a *first-order* approach that builds a classification model in a label-by-label manner and ignores the existence of other class labels. The modeling complexity of binary relevance is linear to the number of class labels *q* in the label space;
- Second, binary relevance falls into the category of *problem transformation* approaches, which solve multilabel learning problems by transforming them into other well-established learning scenarios (binary classification in this case) [1,2]. Therefore, binary relevance is not restricted to a particular learning technique and can

 $^{^{2)}}$ Without loss of generality, binary assignment of each class label is represented by +1 and -1 (rather than 1 and 0) in this paper

³⁾ In the seminal literature on binary relevance [9], this training procedure is also referred to as cross-training

be instantiated with various binary learning algorithms with diverse characteristics:

- Third, binary relevance optimizes macro-averaged *label-based* multi-label evaluation metrics, which evaluate the learning system's performance on each class label separately, and then return the mean value across all class labels. Therefore, the actual multi-label metric being optimized depends on the binary loss, which is minimized by the binary learning algorithm \$\mathcal{B}\$ [46,47];
- Finally, binary relevance can be easily adapted to learn from multi-label examples with missing labels, where the labeling information for training examples is incomplete due to various factors, such as high labeling cost, carelessness of human labelers, etc. [48–50]. In order to accommodate this situation, binary relevance can derive the binary training set in Eq. (1) by simply excluding examples whose labeling information y_j^i is not available.

Algorithm 1 Pseudo-code for binary relevance [9]

Inputs:

- \mathcal{D} : Multi-label training set $\{(x^i, y^i) \mid 1 \le i \le m\}$ $(x^i \in \mathcal{X}, y^i \in \{-1, +1\}^q, \mathcal{X} = \mathbb{R}^d, \mathcal{Y} = \{\lambda_1, \lambda_2, \dots, \lambda_q\})$
- B: Binary learning algorithm
- x^* : Unseen instance $(x^* \in \mathcal{X})$

Outputs:

 Y^* : Predicted label set for x^* ($Y^* \subseteq \mathcal{Y}$)

Process:

- 1: **for** j = 1 **to** q **do**
- 2: Derive the binary training set \mathcal{D}_i according to Eq. (1);
- 3: Induce the binary classifier $g_i : \leftarrow \mathcal{B}(\mathcal{D}_i)$;
- 4: end for
- 5: **return** $Y^* = \{\lambda_j \mid g_j(x^*) > 0, \ 1 \le j \le q\}$

3 Correlation-enabling extensions

As discussed in Section 2, binary relevance has been used widely for multi-label modeling due to its simplicity and other attractive properties. However, one potential weakness of binary relevance lies in its inability to exploit label correlations to improve the learning system's generalization ability [1,2]. Therefore, a natural consideration is to attempt to provide binary relevance with label correlation exploitation abilities while retaining its linear modeling complexity w.r.t. the number of class labels.

In light of the above consideration, many correlationenabling extensions have been proposed following the seminal work on binary relevance. In the following sections, three representative extension strategies are discussed: the chaining structure assuming *random* label correlations [12–18], the stacking structure assuming *full-order* label correlations [19–23], and the controlling structure assuming *pruned* label correlations [24–29].

3.1 Binary relevance with the chaining structure

In the chaining structure, a total of q binary classifiers are induced based on a chaining order specified over the class labels. Specifically, one binary classifier is built for each class label based on the predictions of the preceding classifiers in the chain [12,14].

Given the label space $\mathcal{Y} = \{\lambda_1, \lambda_2, \dots, \lambda_q\}$, let π : $\{1, 2, \dots, q\} \mapsto \{1, 2, \dots, q\}$ be the permutation used to specify a chaining order over all class labels, i.e., $\lambda_{\pi(1)} > \lambda_{\pi(2)} > \dots > \lambda_{\pi(q)}$. Thereafter, for the jth class label $\lambda_{\pi(j)}$ in the ordered list, the *classifier chain* approach [12,14] works by deriving a corresponding binary training set $\mathcal{D}_{\pi(j)}$ from \mathcal{D} in the following manner:

$$\mathcal{D}_{\pi(j)} = \left\{ \left(\left[x^{i}, y_{\pi(1)}^{i}, \dots, y_{\pi(j-1)}^{i} \right], y_{\pi(j)}^{i} \right) \mid 1 \leqslant i \leqslant m \right\}.$$
 (3)

Here, the binary assignments of preceding class labels in the chain, i.e., $[y^i_{\pi(1)}, \ldots, y^i_{\pi(j-1)}]$, are treated as additional features to append to the original instance x^i .

Next, a binary classifier $g_{\pi(j)}: \mathcal{X} \times \{-1, +1\}^{j-1} \mapsto \mathbb{R}$ can be induced from $\mathcal{D}_{\pi(j)}$ by applying a binary learning algorithm \mathcal{B} , i.e., $g_{\pi(j)} \leftrightarrow \mathcal{B}(\mathcal{D}_{\pi(j)})$. In other words, $g_{\pi(j)}$ determines the relevancy of $\lambda_{\pi(j)}$ by exploiting its correlations with the preceding labels $\lambda_{\pi(1)}, \ldots, \lambda_{\pi(j-1)}$ in the chain.

Given an unseen instance x^* , its relevant label set Y^* is determined by iteratively querying the outputs of each binary classifier along the chaining order. Let $\eta_{\pi(j)}^{x^*} \in \{-1, +1\}$ denote the predicted binary assignment of $\lambda_{\pi(j)}$ on x^* , which is recursively determined as follows:

$$\eta_{\pi(1)}^{\mathbf{x}^*} = \operatorname{sign} \left[g_{\pi(1)}(\mathbf{x}^*) \right],
\eta_{\pi(j)}^{\mathbf{x}^*} = \operatorname{sign} \left[g_{\pi(j)} \left(\left[\mathbf{x}^*, \eta_{\pi(1)}^{\mathbf{x}^*}, \dots, \eta_{\pi(j-1)}^{\mathbf{x}^*} \right] \right) \right].$$
(4)

Here, $sign[\cdot]$ represents the signed function. Therefore, the relevant label set Y^* is derived as:

$$Y^* = \left\{ \lambda_{\pi(j)} \mid \eta_{\pi(j)}^{x^*} = +1, \ 1 \le j \le q \right\}. \tag{5}$$

Algorithm 2 presents the pseudo-code of the classifier chain. As shown in Algorithm 2, the classifier chain is a *high-order* approach that considers correlations between labels in a random manner specified by the permutation π . In order to account for the randomness introduced by the permutation

ordering, one effective choice is to build an *ensemble* of classifier chains with n random permutations $\{\pi^r \mid 1 \le r \le n\}$. One classifier chain can be learned based on each random permutation, and then the outputs from all classifier chains are aggregated to yield the final prediction [12,14,16].

Algorithm 2 Pseudo-code of the classifier chain [12,14]

Inputs:

- \mathcal{D} : Multi-label training set $\{(x^i, y^i) \mid 1 \le i \le m\}$ $(x^i \in \mathcal{X}, y^i \in \{-1, +1\}^q, \mathcal{X} = \mathbb{R}^d, \mathcal{Y} = \{\lambda_1, \lambda_2, \dots, \lambda_q\})$
- π : Permutation used to specify chaining order
- B: Binary learning algorithm
- x^* : Unseen instance $(x^* \in X)$

Outputs:

 Y^* : Predicted label set for x^* ($Y^* \subseteq \mathcal{Y}$)

Process:

- 1: **for** j = 1 **to** q **do**
- 2: Derive the binary training set $\mathcal{D}_{\pi(j)}$ using Eq. (3);
- 3: Induce the binary classifier $g_{\pi(j)}$: $\leftarrow \mathcal{B}(\mathcal{D}_{\pi(j)})$;
- 4. end for
- 5: Determine the binary assignments $\eta_{\pi(j)}^{x^*}$ $(1 \le j \le q)$ using Eq. (4);
- 6: **return** $Y^* = \{\lambda_{\pi(j)} \mid \eta_{\pi(j)}^{x^*} = +1, \ 1 \le j \le q \}$ w.r.t. Eq. (4)

It is also worth noting that predictive errors incurred in preceding classifiers will be propagated to subsequent classifiers along the chain. These undesirable influences become more pronounced if error-prone class labels happen to be placed at early chaining positions [12,14,28,51]. Furthermore, during the training phase, the additional features appended to the input space X correspond to the ground-truth labeling assignments (Eq. (3)). However, during the testing phase, the additional features appended to X correspond to predicted labeling assignments (Eq. (4)). One way to rectify this discrepancy is to replace the extra features $\left[y_{\pi(1)}^i,\ldots,y_{\pi(j-1)}^i\right]$ in Eq. (3) with $\left[\eta_{\pi(1)}^{x^i},\ldots,\eta_{\pi(j-1)}^{x^i}\right]$ such that the predicted labeling assignments are appended to X in both the training and testing phases [17,51].

From a statistical point of view, the task of multi-label learning is equivalent to learning the conditional distribution $p(y \mid x)$ with $x \in X$ and $y \in \{-1, +1\}^q$. Therefore, $p(y \mid x)$ can be factorized w.r.t. the chaining order specified by π as follows:

$$p(\mathbf{y} \mid \mathbf{x}) = \prod_{j=1}^{q} p\left(y_{\pi(j)} \mid \mathbf{x}, y_{\pi(1)}, \dots, y_{\pi(j-1)}\right).$$
 (6)

Here, each term on the RHS of Eq. (6) represents the conditional probability of observing $y_{\pi(j)}$ given x and its preceding labels in the chain. Specifically, this term can be estimated by utilizing a binary learning algorithm \mathcal{B} , which is

capable of yielding probabilistic outputs (e.g., Naive Bayes). Thereafter, the relevant label set for the unseen instance is predicted by performing exact inference [13] or approximate inference (when q is large) over the probabilistic classifier chain [15,18].

3.2 Binary relevance with the stacking structure

In the stacking structure, a total of 2q binary classifiers are induced by stacking a set of q meta-level binary relevance models over another set of q base-level binary relevance models. Specifically, each meta-level binary classifier is built upon the predictions of all base-level binary classifiers [19].

Following the notations in Section 2, let g_j $(1 \le j \le q)$ denote the set of base-level classifiers learned by invoking the standard binary relevance procedure on the multi-label training set, i.e., $g_j \leftarrow \mathcal{B}(\mathcal{D}_j)$. Thereafter, for each class label λ_j , the *stacking aggregation* approach [1,19] derives a meta-level binary training set \mathcal{D}_j^M in the following manner:

$$\mathcal{D}_{j}^{M} = \left\{ \left(\left[\mathbf{x}^{i}, \operatorname{sign}[g_{1}(\mathbf{x}^{i})], \dots, \operatorname{sign}[g_{q}(\mathbf{x}^{i})] \right], y_{j}^{i} \right) | 1 \leq i \leq m \right\}. (7)$$

Here, the signed predictions of base-level classifiers, i.e., $\left[\text{sign}[g_1(\mathbf{x}^i)], \dots, \text{sign}[g_q(\mathbf{x}^i)]\right]$, are treated as additional features to append to the original instance \mathbf{x}^i in the meta-level.

Next, a meta-level classifier $g_j^M: \mathcal{X} \times \{-1, +1\}^q \mapsto \mathbb{R}$ can be induced from \mathcal{D}_j^M by applying a binary learning algorithm \mathcal{B} , i.e., $g_j^M \leftarrow \mathcal{B}(\mathcal{D}_j^M)$. In other words, g_j^M determines the relevancy of λ_j by exploiting its correlations with all the class labels.

Given an unseen instance x^* , its relevant label set Y^* is determined by using the outputs of the base-level classifiers as extra inputs for the meta-level classifiers:

$$Y^* = \left\{ \lambda_j \mid g_j^M(\tau^{x^*}) > 0, \ 1 \le j \le q \right\},$$
 where $\tau^{x^*} = \left[x^*, \text{sign}[g_1(x^*)], \dots, \text{sign}[g_q(x^*)] \right].$ (8)

Algorithm 3 presents the pseudo-code for stacking aggregation. As shown in Algorithm 3, stacking aggregation is a *full-order* approach that assumes that each class label has correlations with all other class labels. It is worth noting that stacking aggregation employs ensemble learning [52] to combine two sets of binary relevance models with deterministic label correlation exploitation. Ensemble learning can also be applied to the classifier chain to compensate for its randomness of label correlation exploitation.

Rather than using the outputs of the base-level classifiers $\left[\text{sign}[g_1(\mathbf{x}^i)], \dots, \text{sign}[g_q(\mathbf{x}^i)]\right]$ by appending them to the inputs of the meta-level classifiers, it is also feasible to use the

ground-truth labeling assignments $[y_1^i, \ldots, y_q^i]$ to instantiate the meta-level binary training set (i.e., Eq. (21)) [21]. However, similar to the standard classifier chain approach, this practice would also lead to the discrepancy issue regarding the additional features appended to the input space X in the training and testing phases.

Algorithm 3 Pseudo-code of stacking aggregation [19]

Inputs:

- \mathcal{D} : Multi-label training set $\{(x^i, y^i) \mid 1 \le i \le m\}$ $(x^i \in \mathcal{X}, y^i \in \{-1, +1\}^q, \mathcal{X} = \mathbb{R}^d, \mathcal{Y} = \{\lambda_1, \lambda_2, \dots, \lambda_q\})$
- \mathcal{B} : Binary learning algorithm
- x^* : Unseen instance $(x^* \in X)$

Outputs:

 Y^* : Predicted label set for x^* ($Y^* \subseteq \mathcal{Y}$)

Process:

- 1: **for** i = 1 **to** q **do**
- 2: Derive the binary training set \mathcal{D}_i using Eq. (1);
- 3: Induce the base-level binary classifier $g_i : \leftarrow \mathcal{B}(\mathcal{D}_i)$;
- 4: end for
- 5: **for** j = 1 **to** q **do**
- 6: Derive the binary training set \mathcal{D}_{i}^{M} using Eq. (7);
- 7: Induce the meta-level binary classifier $g_i^M : \leftarrow \mathcal{B}(\mathcal{D}_i^M)$;
- 8. end for
- 9: **return** $Y^* = \left\{ \lambda_j \mid g_j^M(\tau^{x^*}) > 0, \ 1 \le j \le q \right\}$ w.r.t Eq. (8)

There are other ways to make use of the stacking strategy to induce a multi-label prediction model. Given the base-level classifiers g_j ($1 \le j \le q$) and the meta-level classifiers g_j^M ($1 \le j \le q$), rather than relying only on the meta-level classifiers to yield final predictions (i.e., Eq. (8)), one can also aggregate the outputs of both the base-level and meta-level classifiers to accomplish this task [20]. Furthermore, rather than using the binary labeling assignments as additional features for stacking, one can also adapt specific techniques to generate tailored features for stacking, such as discriminant analysis [22] or rule learning [23].

3.3 Binary relevance with the controlling structure

In the controlling structure, a total of 2q binary classifiers are induced based on a dependency structure specified over the class labels. Specifically, one binary classifier is built for each class label by exploiting the pruned predictions of q binary relevance models [25].

A Bayesian network (or *directed acyclic graph*, DAG) is a convenient tool to explicitly characterize correlations between class labels in a compact manner [25–27]. As mentioned in Subsection 3.1, a statistical equivalence for multilabel learning corresponds to modeling the conditional dis-

tribution $p(y \mid x)$ with $x \in X$ and $y = \{-1, +1\}^q$. Given the Bayesian network structure \mathcal{G} specified over (x, y), the conditional distribution $p(y \mid x)$ can be factorized based on \mathcal{G} as follows:

$$p(\mathbf{y} \mid \mathbf{x}) = \prod_{j=1}^{q} p(y_j \mid \mathbf{pa}_j, \mathbf{x}).$$
 (9)

Here, x serves as the common parent for each y_j ($1 \le j \le q$) because all class labels inherently depend on the feature space X. Additionally, \mathbf{pa}_j represents the set of parent class labels of y_j implied by \mathcal{G} . Figure 1 illustrates two examples of how the conditional distribution $p(y \mid x)$ can be factorized based on the given Bayesian network structure.

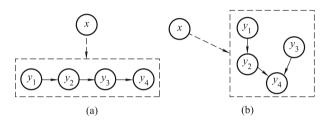


Fig. 1 Examples of two Bayesian network (DAG) structures with x serving as the common parent. The conditional distribution $p(y \mid x)$ factorizes based on each structure as: (a) $p(y \mid x) = p(y_1 \mid x) \cdot p(y_2 \mid y_1, x) \cdot p(y_3 \mid y_2, x) \cdot p(y_4 \mid y_3, x)$; (b) $p(y \mid x) = p(y_1 \mid x) \cdot p(y_2 \mid y_1, x) \cdot p(y_3 \mid x) \cdot p(y_4 \mid y_2, y_3, x)$

Learning a Bayesian network structure \mathcal{G} from a multilabel training set $\mathcal{D} = \{(x^i, y^i) \mid 1 \le i \le m\}$ is difficult. Existing Bayesian network learning techniques [53] are not directly applicable for two major reasons. First, variables in the Bayesian network have mixed types with y (class labels) being discrete and x (feature vector) being continuous. Second, computational complexity is prohibitively high when input dimensionality (i.e., number of features) is too large.

These two issues are brought about by the involvement of the feature vector x when learning the Bayesian network structure. In light of this information, the *LEAD* approach [25] chooses to eliminate the effects of features in order to simplify the Bayesian network generation procedure. Following the notations in Section 2, let g_j $(1 \le j \le q)$ denote the binary classifiers induced by the standard binary relevance procedure, i.e., $g_j \leftarrow \mathcal{B}(\mathcal{D}_j)$. Accordingly, a set of *error* random variables are derived to decouple the influences of x from all class labels:

$$e_i = y_i - \text{sign}(g_i(x)) \ (1 \le j \le q).$$
 (10)

Thereafter, the Bayesian network structure \mathcal{G} for all class labels (conditioned on x) can be learned from e_j ($1 \le j \le q$) using off-the-shelf packages [54–56].

Based on the DAG structure implied by \mathcal{G} , for each class label λ_j , the LEAD approach derives a binary training set $\mathcal{D}_j^{\mathcal{G}}$

from \mathcal{D} in the following manner:

$$\mathcal{D}_{j}^{\mathcal{G}} = \left\{ \left(\left[\mathbf{x}^{i}, \mathbf{p} \mathbf{a}_{j}^{i} \right], y_{j}^{i} \right) \middle| 1 \leqslant i \leqslant m \right\}. \tag{11}$$

Here, the binary assignments of parent class labels, i.e., \mathbf{pa}_{j}^{i} , are treated as additional features to append to the original instance \mathbf{x}^{i} .

Next, a binary classifier $g_j^{\mathcal{G}}: \mathcal{X} \times \{-1,+1\}^{|\mathbf{pa}_j|} \mapsto \mathbb{R}$ can be induced from $\mathcal{D}_j^{\mathcal{G}}$ by applying a binary learning algorithm \mathcal{B} , i.e., $g_j^{\mathcal{G}} \leftrightarrow \mathcal{B}(\mathcal{D}_j^{\mathcal{G}})$. In other words, $g_j^{\mathcal{G}}$ determines the relevancy of λ_j by exploiting its correlations with the parent class labels \mathbf{pa}_j implied by \mathcal{G} .

Given an unseen instance x^* , its relevant label set Y^* is determined by iteratively querying the outputs of each binary classifier w.r.t. the Bayesian network structure. Let $\pi^{\mathcal{G}}$: $\{1,2,\ldots,q\}\mapsto\{1,2,\ldots,q\}$ be the causal order implied by \mathcal{G} over all class labels, i.e., $\lambda_{\pi^{\mathcal{G}}(1)}>\lambda_{\pi^{\mathcal{G}}(2)}>\cdots\lambda_{\pi^{\mathcal{G}}(q)}$. Furthermore, let $\eta^{x^*}_{\pi^{\mathcal{G}}(j)}\in\{-1,+1\}$ denote the predicted binary assignment of $\lambda_{\pi^{\mathcal{G}}(j)}$ on x^* , which is recursively determined as follows:

$$\eta_{\pi^{\mathcal{G}}(1)}^{\mathbf{x}^{*}} = \operatorname{sign}\left[g_{\pi^{\mathcal{G}}(1)}^{\mathcal{G}}(\mathbf{x}^{*})\right],
\eta_{\pi^{\mathcal{G}}(j)}^{\mathbf{x}^{*}} = \operatorname{sign}\left[g_{\pi^{\mathcal{G}}(j)}^{\mathcal{G}}\left(\left[\mathbf{x}^{*}, \langle \eta_{a}^{\mathbf{x}^{*}} \rangle_{y_{a} \in \mathbf{pa}_{\pi^{\mathcal{G}}(j)}}\right]\right)\right].$$
(12)

Accordingly, the relevant label set Y^* becomes:

$$Y^* = \left\{ \lambda_{\pi^{\mathcal{G}}(j)} \mid \eta_{\pi^{\mathcal{G}}(j)}^{x^*} = +1, \ 1 \le j \le q \right\}. \tag{13}$$

Algorithm 4 Pseudo-code of LEAD [25]

Inputs:

- \mathcal{D} : Multi-label training set $\{(x^i, y^i) \mid 1 \le i \le m\}$ $(x^i \in \mathcal{X}, y^i \in \{-1, +1\}^q, \mathcal{X} = \mathbb{R}^d, \mathcal{Y} = \{\lambda_1, \lambda_2, \dots, \lambda_q\})$
- \mathcal{B} : Binary learning algorithm
- L: Bayesian network structure learning algorithm
- x^* : Unseen instance $(x^* \in \mathcal{X})$

Outputs:

 Y^* : Predicted label set for x^* ($Y^* \subseteq \mathcal{Y}$)

Process:

- 1: **for** j = 1 **to** q **do**
- 2: Derive the binary training set \mathcal{D}_j using Eq. (1);
- 3: Induce the binary classifier g_j : $\leftarrow \mathcal{B}(\mathcal{D}_j)$;
- 4: end for
- 5: Derive the *error* random variables e_j $(1 \le j \le q)$ using Eq. (10);
- 6: Learn the Bayesian network structure $\mathcal{G} \leftarrow \mathcal{L}(e_1, e_2, \dots, e_q)$;
- 7: **for** j = 1 **to** q **do**
- 8: Derive the binary training set $\mathcal{D}_{i}^{\mathcal{G}}$ using Eq. (11);
- 9: Induce the binary classifier $g_i^{\mathcal{G}}$: $\prec \mathcal{B}(\mathcal{D}_i^{\mathcal{G}})$;
- 10: **end for**
- 11: Specify the causal order $\pi^{\mathcal{G}}$ over all class labels w.r.t. \mathcal{G} ;
- 12: **return** $Y^* = \left\{ \lambda_{\pi^{\mathcal{G}}(j)} \mid \eta_{\pi^{\mathcal{G}}(j)}^{\mathbf{x}^*} = +1, \ 1 \leq j \leq q \right\}$ w.r.t. Eq. (12)

Algorithm 4 presents the pseudo-code of LEAD. As shown in Algorithm 4, LEAD is a *high-order* approach that controls the order of correlations using the number of parents of each class label implied by \mathcal{G} . Similar to stacking aggregation, LEAD also employs ensemble learning to combine two sets of binary classifiers g_j $(1 \le j \le q)$ and $g_j^{\mathcal{G}}$ $(1 \le j \le q)$ to yield the multi-label prediction model. Specifically, predictions of the q binary classifiers g_j are pruned w.r.t. the parents for label correlation exploitation.

There are also other ways to consider pruned label correlations with specific controlling structures. First, a tree-based Bayesian network can be utilized as a simplified DAG structure where second-order label correlations are considered by pruning each class label with (up to) one parent [26,27]. Second, the stacking structure can be adapted to fulfill controlled label correlation exploitation by pruning the uncorrelated outputs of base-level classifiers for stacking meta-level classifiers [24,29]. Third, class labels with error-prone predictions can be filtered out of the pool of class labels for correlation exploitation [28].

4 Related issues

As discussed in Section 3, in order to enhance binary relevance, it is necessary to enable label correlation exploitation during the learning process. However, it is also noteworthy that some inherent properties of multi-label learning should be investigated in order to further enhance the generalization ability of binary relevance. Specifically, recent studies on the issue of *class-imbalance*, i.e., the number of positive instances and negative instances w.r.t. each class label are imbalanced [30–39], and the issue of *relative labeling-importance*, i.e., each class label has different labeling-importance [40–45], are introduced.

4.1 Class-imbalance

The issue of class-imbalance exists in many multi-label learning tasks, especially those where the label space consists of a significant number of class labels. For each class label $\lambda_j \in \mathcal{Y}$, let $\mathcal{D}_j^+ = \{(x^i, +1) \mid y_j^i = +1, 1 \leq i \leq m\}$ and $\mathcal{D}_j^- = \{(x^i, -1) \mid y_j^i = -1, 1 \leq i \leq m\}$ denote the set of *positive* and *negative* training examples w.r.t. λ_j . The level of class-imbalance can then be characterized by the imbalance ratio:

$$ImR_{j} = \frac{\max\left(|\mathcal{D}_{j}^{+}|, |\mathcal{D}_{j}^{-}|\right)}{\min\left(|\mathcal{D}_{j}^{+}|, |\mathcal{D}_{j}^{-}|\right)}.$$
 (14)

Here, $|\cdot|$ returns the cardinality of a set and, in most cases,

 $|\mathcal{D}_{j}^{+}| < |\mathcal{D}_{j}^{-}|$ holds. Generally, the imbalance ratio is high for most benchmark multi-label data sets [1,57]. For instance, among the 42 class labels of the rcv1 benchmark data set, the average imbalance ratio (i.e., $\frac{1}{q}\sum_{j=1}^{q}ImR_{j}$) is greater than 15 and the maximum imbalance ratio (i.e., $\max_{1 \le j \le q}ImR_{j}$) is greater than 50 [38].

In order to handle the issue of class-imbalance in multilabel learning, existing approaches employ binary relevance as an intermediate step in the learning procedure. Specifically, by decomposing the multi-label learning task into q independent binary learning tasks, each of them can be addressed using prevalent binary imbalance learning techniques, such as over-/under-sampling [32,36,37], thresholding the decision boundary [31,33,34], or optimizing imbalance-specific metrics [30,35,39]. Because standard binary relevance is applied prior to subsequent modeling, existing approaches handle class-imbalance in multi-label learning at the expense of ignoring the exploitation of label correlations.

Therefore, a favorable solution to class-imbalance in multilabel learning is to consider the exploitation of label correlations and the exploration of class-imbalance simultaneously. In light of this information, the COCOA approach was proposed based on a specific strategy called *cross-coupling aggregation* [38]. For each class label λ_j , a binary classifier g_j^I is induced from \mathcal{D}_j (i.e., Eq. (1)) by applying a binary imbalance learning algorithm \mathcal{B}^I [58], i.e., $g_j^I \leftrightarrow \mathcal{B}^I(\mathcal{D}_j)$. Additionally, a random subset of K class labels $J_K \subset \mathcal{Y} \setminus \{\lambda_j\}$ is extracted for pairwise cross-coupling with λ_j . For each coupling label $\lambda_k \in J_K$, COCOA derives a tri-class training set \mathcal{D}_{jk}^{tri} for the label pair (λ_j, λ_k) from \mathcal{D} in the following manner:

$$\mathcal{D}_{jk}^{\text{tri}} = \{ (\mathbf{x}^{i}, \psi^{\text{tri}}(\mathbf{y}^{i}, \lambda_{j}, \lambda_{k})) \mid 1 \leq i \leq m \},$$
where $\psi^{\text{tri}}(\mathbf{y}^{i}, \lambda_{j}, \lambda_{k}) = \begin{cases} 0, & \text{if } y_{j}^{i} = -1 \text{ and } y_{k}^{i} = -1; \\ +1, & \text{if } y_{j}^{i} = -1 \text{ and } y_{k}^{i} = +1; \\ +2, & \text{if } y_{j}^{i} = +1. \end{cases}$

Among the three derived class labels, the first two labels (i.e., 0 and +1) exploit label correlations by considering the joint labeling assignments of λ_j and λ_k w.r.t. y^i , and the third class label (i.e., +2) corresponds to the case of λ_j being a relevant label.

Next, a tri-class classifier $g_{jk}^{I}: X \times \{0, +1, +2\} \mapsto \mathbb{R}$ can be induced from $\mathcal{D}_{jk}^{\text{tri}}$ by applying a multi-class imbalance learning algorithm \mathcal{M}^{I} [59–61], i.e., $g_{jk}^{I} \leftrightarrow \mathcal{M}^{I}(\mathcal{D}_{jk}^{\text{tri}})$. In other words, a total of K+1 classifiers, including g_{j}^{I} and g_{jk}^{I} ($\lambda_{k} \in J_{K}$), are induced for the class label λ_{j} .

Given an unseen instance x^* , its relevant label set Y^* is determined by aggregating the predictions of the classifiers induced by the binary and multi-class imbalanced learning algorithms:

$$Y^* = \{\lambda_j \mid f_j(\mathbf{x}^*) > t_j, \ 1 \le j \le q\}$$
 where $f_j(\mathbf{x}^*) = g_j^I(\mathbf{x}^*) + \sum_{\lambda_k \in J_K} g_{jk}^I(\mathbf{x}^*, +2).$ (16)

Here, t_j is a bipartition threshold, which is set by optimizing an empirical metric (e.g., F-measure) over \mathcal{D}_i .

Algorithm 5 presents the pseudo-code of COCOA. As shown in Algorithm 5, COCOA is a *high-order* approach that considers correlations between labels in a random manner via the K coupling class labels in J_K . Specifically, during the training phase, label correlation exploitation is enabled by an ensemble of pairwise cross-couplings between class labels. During the testing phase, class-imbalance exploration is enabled by aggregating the classifiers induced from the classimbalance learning algorithms.

Algorithm 5 Pseudo-code of COCOA [38]

Inputs:

```
\mathcal{D}: Multi-label training set \{(x^i, y^i) \mid 1 \le i \le m\}
(x^i \in \mathcal{X}, y^i \in \{-1, +1\}^q, \mathcal{X} = \mathbb{R}^d, \mathcal{Y} = \{\lambda_1, \lambda_2, \dots, \lambda_q\})
```

 \mathcal{B}^I : Binary imbalance learning algorithm

MI: Bulti-class imbalance learning algorithm

K: Number of coupling class labels

 x^* : Unseen instance $(x^* \in \mathcal{X})$

Outputs:

 Y^* : Predicted label set for x^* ($Y^* \subseteq \mathcal{Y}$)

Process:

1: **for** j = 1 **to** q **do**

2: Derive the binary training set \mathcal{D}_j using Eq. (1);

3: Induce the binary classifier $g_i^I : \leftarrow \mathcal{B}^I(\mathcal{D}_i)$;

4: Extract a random subset $J_K \subset \mathcal{Y} \setminus \{\lambda_j\}$ with K coupling class labels;

5: **for** each $\lambda_k \in J_K$ **do**

6: Derive the tri-class training set \mathcal{D}_{ik}^{tri} using Eq. (15);

7: Induce the tri-class classifier g_{ik}^I : $\longleftrightarrow \mathcal{M}^I(\mathcal{D}_{ik}^{\mathbf{tri}});$

8: end for

9: end for

10: Return $Y^* = \{\lambda_j \mid f_j(\mathbf{x}^*) > t_j, \ 1 \le j \le q \}$ w.r.t. Eq. (16)

4.2 Relative labeling-importance

Existing approaches to multi-label learning, including binary relevance, make the common assumption of equal labeling-importance. Here, class labels associated with the training example are regarded to be relevant, while their relative importance in characterizing the example's semantics is not differentiated [1,2]. Nevertheless, the degree of labeling importance for each associated class label is generally different

and not directly accessible from multi-label training examples. Figure 2 shows an example multi-label natural scene image with descending relative labeling-importance: sky > water > cloud > building > pedestrian. Similar situations hold for other types of multi-label objects, such as multi-category documents with different topical importance and multi-functionality genes with different expression levels.

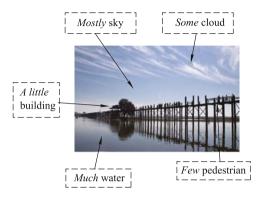


Fig. 2 An example natural scene image annotated with multiple class labels (The relative labeling-importance of each annotation is also illustrated in this figure, although it is not explicitly provided by the annotator [42])

It is worth noting that there have been studies on multilabel learning that have aimed to make use of *auxiliary* labeling-importance information. Different forms of auxiliary information exist, including *ordinal scale* over each class label [40], *full ranking* over relevant class labels [41], *importance distribution* over all class labels [43,44], and *oracle feedbacks* over queried labels of unlabeled examples [45]. However, in standard multi-label learning, this auxiliary information are not assumed to be available and the only accessible labeling information is the relevancy/irrelevancy of each class label.

By leveraging *implicit* relative labeling-importance information, further improvement in the generalization performance of the multi-label learning system can be expected. In light of this information, the RELIAB approach is proposed to incorporate relative labeling-importance information in the learning process [42]. Formally, for each instance \boldsymbol{x} and class label λ_j , the relative labeling-importance of λ_j in characterizing \boldsymbol{x} is denoted $\mu_{\boldsymbol{x}}^{\lambda_j}$. Specifically, the terms $\mu_{\boldsymbol{x}}^{\lambda_j}$ ($1 \le j \le q$) satisfy the non-negativity constraint $\mu_{\boldsymbol{x}}^{\lambda_j} \ge 0$ and the normalization constraint $\sum_{i=1}^q \mu_{\boldsymbol{x}}^{\lambda_j} = 1$.

In the first stage, RELIAB estimates the implicit relative labeling-importance information $\mathcal{U} = \{\mu_{x_i}^{\lambda_j} \mid 1 \leq i \leq m, \ 1 \leq j \leq q\}$ through iterative label propagation. Let G = (V, E) be a fully-connected graph constructed over all the training examples with $V = \{x^i \mid 1 \leq i \leq m\}$. Additionally, a similarity

matrix $\mathbf{W} = [w_{ik}]_{m \times m}$ is specified for G as follows:

$$\forall_{i,k=1}^{m}: w_{ik} = \begin{cases} \exp\left(-\frac{\|x^{i} - x^{k}\|_{2}^{2}}{2\sigma^{2}}\right), & \text{if } i \neq k; \\ 0, & \text{if } i = k. \end{cases}$$
 (17)

Here, $\sigma > 0$ is the width constant for similarity calculation. The corresponding label propagation matrix **P** is set as follows:

$$\mathbf{P} = \mathbf{D}^{-\frac{1}{2}} \mathbf{W} \mathbf{D}^{-\frac{1}{2}},$$
 where $\mathbf{D} = \text{diag}[d_1, d_2, \dots, d_m]$ with $d_i = \sum_{k=1}^m w_{ik}$. (18)

Additionally, the labeling-importance matrix $\mathbf{R} = [r_{ij}]_{m \times q}$ is initialized with $\mathbf{R}^{(0)} = \mathbf{\Phi} = [\phi_{ij}]_{m \times q}$ as follows:

$$\forall 1 \le i \le m, \ \forall 1 \le j \le q: \quad \phi_{ij} = \begin{cases} 1, & \text{if } y_j^i = +1; \\ 0, & \text{if } y_j^i = -1. \end{cases}$$
 (19)

Next, the label propagation procedure works by iteratively updating **R** as: $\mathbf{R}^{(t)} = \alpha \mathbf{P} \mathbf{R}^{(t-1)} + (1 - \alpha) \mathbf{\Phi}$. In practice, $\mathbf{R}^{(t)}$ will converge to \mathbf{R}^* as t grows to infinity [42,62,63]:

$$\mathbf{R}^* = (1 - \alpha)(\mathbf{I} - \alpha \mathbf{P})^{-1} \mathbf{\Phi}. \tag{20}$$

Here, $\alpha \in (0,1)$ is the trade-off parameter that balances the information flow from label propagation and initial labeling. Next, the implicit relative labeling-importance information \mathcal{U} is obtained by normalizing each row of \mathbf{R}^* as follows:

$$\forall 1 \le i \le m, \ \forall 1 \le j \le q: \ \mu_{x_i}^{\lambda_j} = \frac{r_{ij}^*}{\sum_{i=1}^q r_{ij}^*}.$$
 (21)

In the second stage, in order to make use of the information conveyed by \mathcal{U} , RELIAB chooses the maximum entropy model [64] to parametrize the multi-label predictor as follows:

$$f_j(\mathbf{x}) = \frac{1}{Z(\mathbf{x})} \exp\left(\boldsymbol{\theta}_j^{\mathsf{T}} \mathbf{x}\right) \quad (1 \leqslant j \leqslant q),$$
where $Z(\mathbf{x}) = \sum_{j=1}^q \exp\left(\boldsymbol{\theta}_j^{\mathsf{T}} \mathbf{x}\right)$. (22)

In order to induce the prediction model $\Theta = [\theta_1, \theta_2, \dots, \theta_q]$, RELIAB chooses to minimize the following objective function:

$$V(\mathbf{O}, \mathcal{U}, \mathcal{D}) = V_{dis}(\mathbf{O}, \mathcal{U}) + \beta \cdot V_{emp}(\mathbf{O}, \mathcal{D}). \tag{23}$$

Here, the first term $V_{dis}(\mathbf{\Theta}, \mathcal{U})$ evaluates how well the prediction model $\mathbf{\Theta}$ fits the estimated relative labeling-importance information \mathcal{U} (e.g., by Kullback-Leibler divergence) and the second term evaluates how well the prediction model $\mathbf{\Theta}$ classifies the training examples in \mathcal{D} (e.g., by empirical ranking

loss). Furthermore, β is the regularization parameter that balances the two terms of the objective function.

Given an unseen instance x^* , its relevant label set Y^* is determined by thresholding the parametrized prediction model as follows:

$$Y^* = \{ \lambda_i \mid f_i(\mathbf{x}^*) > t(\mathbf{x}^*), \ 1 \le j \le q \}. \tag{24}$$

Here, $t(x^*)$ is a thresholding function, which can be learned from the training examples [1,34,42].

Algorithm 6 presents the pseudo-code of RELIAB. As shown in Algorithm 6, RELIAB employs a two-stage procedure to learn from multi-label examples, where the relative labeling-importance information estimated in the first stage contributes to the model induction in the second stage. Furthermore, the order of label correlations considered by RELIAB depends on the empirical loss chosen to instantiate $V_{emp}(\mathbf{\Theta}, \mathcal{D})$.

Algorithm 6 Pseudo-code of RELIAB [42]

Inputs:

- \mathcal{D} : Multi-label training set $\{(\mathbf{x}^i, \mathbf{y}^i) \mid 1 \le i \le m\}$ $(\mathbf{x}^i \in \mathcal{X}, \mathbf{y}^i \in \{-1, +1\}^q, \mathcal{X} = \mathbb{R}^d, \mathcal{Y} = \{\lambda_1, \lambda_2, \dots, \lambda_q\})$
- α : Trade-off parameter in (0,1)
- β : Regularization parameter
- x^* : Unseen instance $(x^* \in X)$

Outputs:

 Y^* : Predicted label set for x^* ($Y^* \subseteq \mathcal{Y}$)

Process:

- 1: Construct the fully-connected graph G = (V, E) with $V = \{x^i \mid 1 \le i \le m\}$.
- 2: Specify the weight matrix W using Eq. (17);
- 3: Set the label propagation matrix **P** using Eq. (18);
- 4: Initialize the labeling-importance matrix **R** using Eq. (19), and then derive the converged solution **R*** using Eq. (20);
- 5: Obtain the relative labeling-importance information $\mathcal U$ using Eq. (21);
- Learn the parametrized prediction model Θ by minimizing the objective function specified in Eq. (23);
- 7: Return $Y^* = \{\lambda_j \mid f_j(\mathbf{x}^*) > t(\mathbf{x}^*), \ 1 \le j \le q \}$ w.r.t. Eq. (24)

5 Conclusion

In this paper, the state of the art of binary relevance, which is one of the most important solutions for multi-label learning, was reviewed. Specifically, the basic settings for binary relevance, a few representative correlation-enabling extensions, and related issues on class-imbalance and relative labeling-importance have been discussed. Code packages for the learning algorithms introduced in this paper are publicly-available at the MULAN toobox [57] (binary relevance [9], classifier chain [12,14], stacking aggregation [19]) and the

first author's homepage (LEAD [25], COCOA [38], RELIAB [42]).

For binary relevance, there are several research issues that require further investigation. First, the performance evaluation of multi-label learning is more complicated than singlelabel learning. A number of popular multi-label evaluation metrics have been proposed [1,2,10,11]. It is desirable to design correlation-enabling extensions for binary relevance that are tailored to optimize designated multi-label metrics, suitable for the multi-label learning task at hand. Second, in binary relevance, the same set of features is used to induce the classification models for all class labels. It is appropriate to develop binary relevance style learning algorithms that are capable of utilizing label-specific features to characterize distinct properties of each class label [65–67]. Third, the modeling complexities of binary relevance, as well as its extensions, are linear to the number of class labels in the label space. It is necessary to adapt binary relevance to accommodate extreme multi-label learning scenarios with huge (e.g., millions) numbers of class labels [68–72].

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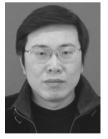
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