Learning to Calibrate and Rerank Multi-label Predictions

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Abstract. A multi-label classifier assigns a set of labels to each data object. A natural requirement in many end-use applications is that the classifier also provides a well-calibrated confidence (probability) to indicate the likelihood of the predicted set being correct; for example, an application may automate high-confidence predictions while manually verifying low-confidence predictions. The simplest multi-label classifier, called Binary Relevance (BR), applies one binary classifier to each label independently and takes the product of the individual label probabilities as the overall label-set probability (confidence). Despite its many known drawbacks, such as generating suboptimal predictions and poorly calibrated confidence scores, BR is widely used in practice due to its speed and simplicity. We seek in this work to improve both BR's confidence estimation and prediction through a post calibration and reranking procedure. We take the BR predicted set of labels and its product score as features, extract more features from the prediction itself to capture label constraints, and apply Gradient Boosted Trees (GB) as a calibrator to map these features into a calibrated confidence score. GB not only produces well-calibrated scores (*aligned with accuracy* and *sharp*), but also models label interactions, correcting a critical flaw in BR. We further show that reranking label sets by the new calibrated confidence makes accurate set predictions on par with state-of-the-art multi-label classifiers—yet calibrated, simpler, and faster.

Keywords: Multi-label classification · Confidence score calibration · Reranking

1 Introduction

Multi-label classification is an important machine learning task wherein one predicts a subset of labels to associate with a given object. For example, an article can belong to multiple categories; an image can be associated with several tags; in medical billing, a patient report is annotated with multiple diagnosis codes. Formally, in a multi-label classification problem, we are given a set of label candidates $\mathcal{Y} = \{1, 2, ..., L\}$. Every data point $x \in \mathbb{R}^D$ matches a subset of labels $\mathbf{y} \subseteq \mathcal{Y}$, which is typically written in the form of a binary vector $\mathbf{y} \in \{0, 1\}^L$, with each bit y_ℓ indicating the presence or absence of the corresponding label. The

goal of learning is to build a classifier $h : \mathbb{R}^D \to \{0,1\}^L$ which maps an instance to a subset of labels. The predicted label subset can be of arbitrary size.

The simplest approach to multi-label classification is to apply one binary classifier (e.g., binary logistic regression or support vector machine) to predict each label separately. This approach is called binary relevance (BR) [35] and is widely used due to its simplicity and speed. BR's training time grows linearly with the number of labels, which is considerably lower than many methods that seek to model label dependencies, and this makes BR run reasonably fast on commonly used datasets. (Admittedly, BR may still fail to scale to datasets with extremely large number of labels, in which case specially designed multi-label classifiers with sub-linear time complexity should be employed instead. But in this paper, we shall not consider such *extreme* multi-label classification problem.)

BR has two well-known drawbacks. First, BR neglects label dependencies and this often leads to prediction errors: some BR predictions are incomplete, such as tagging `cat` but not `animal` for an image, and some are conflicting, such as predicting both the code `Pain in left knee` and the code `Pain in unspecified knee` for a medical note. Second, the confidence score or probability (we shall use "confidence score" and "probability" interchangeably) BR associates to its overall set prediction $\mathbf{y}$ is often misleading, or uncalibrated. BR computes the overall set prediction confidence score as the product of the individual label confidence scores, i.e., $p(\mathbf{y}|x) = \prod_{l=1}^{L} p(y_l|x)$. This overall confidence score often does not reflect reality: among all the set predictions on which BR claims to have roughly 80% confidence, maybe only 60% of them are actually correct (a predicted set is considered "correct" if it matches the ground truth set exactly). Having such uncalibrated prediction confidence makes it hard to integrate BR directly into a decision making pipeline where not only the predictions but also the confidence scores are used in downstream tasks.

In this work, we seek to address these two issues associated with BR. We first improve the BR set prediction confidence scores though a feature-based post calibration procedure to make confidence scores indicative of the true set accuracy (described in Section 2). The features considered in calibration capture label dependencies that have otherwise been missing in standard BR. Next we improve BR's set prediction accuracy by reranking BR's prediction candidates using the new calibrated confidence scores (described in Section 3). There exist multi-label methods that avoid the label independence assumption from the beginning and perform joint probability estimations [30, 7, 22, 13, 9, 23]; such methods often require more complex training and inference procedures. In this paper we show that BR base model together with our proposed post calibration/reranking makes accurate set predictions on par with (or better than) these state-of-the-art multi-label methods —yet *calibrated*, *simpler*, and *faster*.

2 Calibrate BR Multi-label Predictions

We first address BR's confidence mis-calibration issue. There are two types of confidence scores in BR: the confidence of an individual label prediction $p(y_l|x)$,

and the confidence of the entire predicted set $p(\mathbf{y}|x)$. In this work we take for granted that the individual label scores have already been calibrated, which can be easily done with established univariate calibration procedures such as isotonic regression [31] or Platt scaling [39, 28]. We are concerned here with the set confidence calibration; note that calibrating all individual label confidence scores does not automatically calibrate set prediction confidence scores.

2.1 Metrics for Calibration: Alignment Error, Sharpness and MSE

To describe our calibration method, we need the following formal definitions:
• $c(\mathbf{y}) \in [0, 1]$ is the confidence score associated with the set prediction $\mathbf{y}$;
• $v(\mathbf{y}) \in \{0, 1\}$ is the 0/1 correctness of set prediction $\mathbf{y}$;
• $e(\mathrm{c}) = p[v(\mathbf{y}) = 1|c(\mathbf{y}) = \mathrm{c}]$ is the average set accuracy among all predictions whose confidence is c. In practice, this is estimated by bucketing predictions based on confidence scores and computing the average accuracy for each bucket.

We use the following standard metrics for calibration [21]:
• Alignment error, defined as $\mathbb{E}_{\mathbf{y}}[e(c(\mathbf{y})) - c(\mathbf{y})]^2$, measures, on average over all predictions, the discrepancy between the claimed confidence and the actual accuracy. The smaller the better.
• Sharpness, defined as $\mathrm{Var}_{\mathbf{y}}[e(c(\mathbf{y}))]$, measures how widely spread the confidence scores are. The bigger the better.
• The mean squared error (MSE, also called Brier Score) defined as $\mathbb{E}_{\mathbf{y}}[(v(\mathbf{y}) - c(\mathbf{y}))^2]$, measures the difference between the confidence and the actual 0/1 correctness. It can be decomposed into alignment error, sharpness and an irreducible constant "uncertainty" due to only classification (not calibration) error [21]:

$$\underbrace{\mathbb{E}_{\mathbf{y}}[(v(\mathbf{y}) - c(\mathbf{y}))^2]}_{MSE} = \underbrace{\mathrm{Var}_{\mathbf{y}}[v(\mathbf{y})]}_{uncertainty} - \underbrace{\mathrm{Var}_{\mathbf{y}}[e(c(\mathbf{y}))]}_{sharpness} + \underbrace{\mathbb{E}_{\mathbf{y}}[(e(c(\mathbf{y})) - c(\mathbf{y}))^2]}_{alignment\ error} \quad (1)$$

Alignment error and sharpness capture two orthogonal aspects of confidence calibration. A small alignment error implies that the confidence score is well aligned with the actual accuracy. However, small alignment error, alone, is not meaningful: the calibration can trivially achieve zero alignment error while being completely uninformative by assigning to all predictions the same confidence score, which is the average accuracy among all predictions on the dataset. A useful calibrator should also separate good predictions from bad ones as much as possible by assigning very different confidence scores to them. In other words, a good calibrator should simultaneously minimize alignment error and maximize sharpness. This can be achieved by minimizing MSE, thus MSE makes a natural objective for calibrator training. Minimizing MSE leads to a standard regression task: one can simply train a regressor c that maps each prediction $\mathbf{y}$ to its binary correctness $v(\mathbf{y})$. Note that training a calibrator by optimizing MSE does not require estimation of $e(c(\mathbf{y}))$, but evaluating its sharpness and alignment error does. Estimating $e(c(\mathbf{y}))$ by bucketing predictions has some subtle issues, as we shall explain later when we present evaluation results in Section 2.4.

2.2 Features for Calibration

Besides the training objective, we also need to decide the parametric form of the calibrator and the features to be used. In order to explain the choices we make, we shall use the calibration on WISE dataset[1] as a running example.

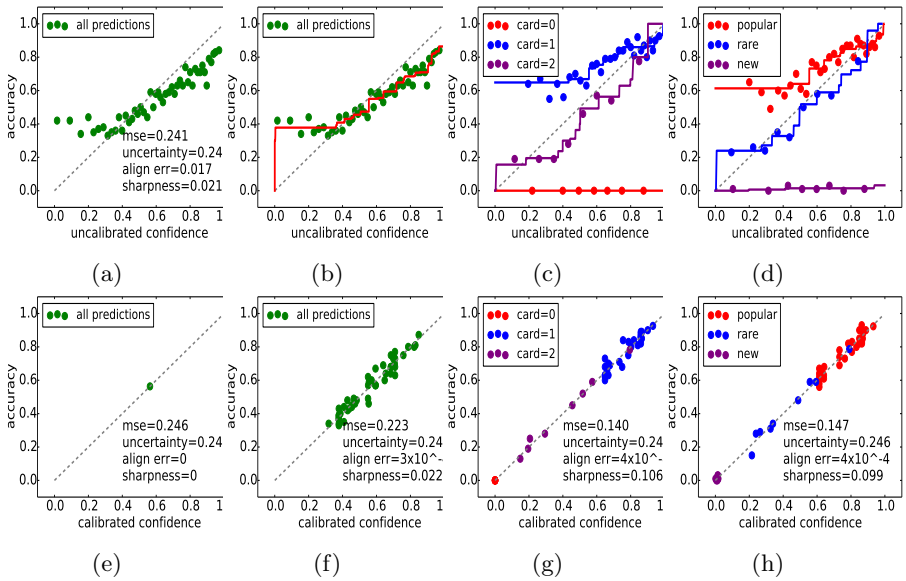


Fig. 1: Multi-label set prediction confidence vs. set prediction accuracy on the WISE dataset. In all sub-figures, each dot represents a group of 100 set predictions with similar confidence scores. The average confidence score in the group is used as x-coordinate, and the average prediction accuracy is used as y-coordinate. (a) BR predictions with the original BR confidence scores. (e) Trivial calibration that gives all predictions the same confidence score which is the overall set accuracy on the dataset. (b) Isotonic regression (the solid line) trained on all predictions. (f) Predictions with isotonic regression calibrated confidence. (c) Break down all predictions by the set cardinality and train a separate isotonic regression (the solid line) for each cardinality. (g) Predictions with confidence calibrated by cardinality-based isotonic regressions. (d) Group all predictions into 3 categories by the popularity of predicted label combination in the training data ground truth (*popular*=the predicted label combination appears at least 100 times; *rare*=the predicted label combination appears less than 100 times; *new*=the predicted label combination does not appear at all in training data), and train a separate isotonic regression (the solid line) for each category. (h) Predictions with confidence calibrated by popularity-based isotonic regressions. To simplify the presentation, all calibrators are trained and evaluated on the same data.

[1] `https://www.kaggle.com/c/wise-2014/data`

Let us start by visualizing BR's predictions together with its original set prediction confidence calculated as $p(\mathbf{y}|x) = \prod_{l=1}^{L} p(y_l|x)$, in which the individual label probabilities $p(y_l|x)$ have been well-calibrated by standard isotonic regression procedures. We group about every 100 predictions with similar confidence scores into a bucket, and plot those buckets as dots treating the average confidence in the group as the x-coordinate and treating the average prediction accuracy in the group as the y-coordinate[2]. Figure 1a shows that the set confidence scores computed this way are not calibrated even when the individual label confidence scores have been well-calibrated. Well calibrated set predictions should approximately lie on the diagonal line. In the figure, predictions above the diagonal are under-confident and those below the diagonal are over-confident.

The simplest way to improve the alignment is to fit another isotonic regression to these dots (see Figure 1b), and use the regression outputs as the new calibrated set prediction confidence scores (Figure 1f). This additional calibration makes the dots align with the diagonal much better. Quantitatively, the alignment error has been reduced to a small number. However, as mentioned earlier, having a small alignment error alone is not enough, as a trivial calibrator that outputs a constant would achieve zero alignment error (Figure 1e). One would also need to maximize the sharpness of the scores, by assigning very different scores to good predictions and bad predictions. Figure 1c and 1d show that there are features that can help the calibrator better separate good predictions from bad ones.

Figure 1c breaks down all predictions by the *cardinality* of the predicted set (i.e. the number of labels predicted). If we look at all predictions with uncalibrated confidence around 0.7, their average accuracy is around 0.58 (as shown in Figure 1b). However, Figure 1c shows that those singleton predictions have accuracy around 0.8; those predictions containing 2 labels only have accuracy about 0.54; and those empty set predictions have 0 accuracy (on this particular dataset, the ground truth set is always non-empty). Clearly, predictions with different cardinalities require different calibration mappings from the uncalibrated confidence to the actual accuracy. Fitting a separate isotonic regression for each cardinality results in Figure 1g, which is a clear improvement over the calibration without cardinality (Figure 1f); thus cardinality feature greatly increases sharpness and reduces MSE. Visually, more points have moved towards left and right ends.

Another useful feature is the *popularity* of predicted label set in the training data (i.e., prior probability). Between two predictions with the same uncalibrated BR confidence, the one that is more popular often has a higher chance of being correct, as shown in Figure 1d. One can quantize the prior probability into intervals and train separate isotonic regressions for different intervals. Figure 1h shows that this also performs better than having only one isotonic regression.

Both set cardinality and prior probability are features defined on the whole label set, rather than individual labels. Such features capture constraints and dependencies among labels, which were not originally considered by BR. Therefore

[2] This particular way of bucketing is only for visualization purpose; when we evaluate calibration quantitatively we follow the standard practice of using 10 equal-width buckets.

these features supplement BR's own prediction score and allow the calibrator to make better overall judgments on the predicted set. There can be other features that help the calibrator better judge set predictions. In order to incorporate arbitrary number of features and avoid manual partitioning of the data and training separate calibrators (which quickly becomes infeasible as the number of features grows), a general multi-variate regressor should be employed. The multi-variate extension of isotonic regression exists [32], but it is not well suited to our problem because some features such as cardinality do not have a monotonic relationship with the calibrated confidence (see Figure 1c). [21] proposes KNN and regression trees as calibrators for general structured prediction problem.

2.3 Calibrator Model Training

In this work, we choose Gradient Boosted Trees (GB) [11] as the calibrator model. Similar to regression trees, GB as a multi-variate regressor automatically partitions the prediction's feature space into regions and outputs (approximately) the average prediction accuracy in each region as the calibrated confidence score. GB often produces smoother output than trees and generalizes better. GB is also very powerful in modeling complex feature interactions automatically by building many trees on top of the features. To leverage its power we also use the binary representation of the set prediction $\mathbf{y}$ itself as features for GB. This way GB can discover additional rules concerning certain label interactions that are not described by the manually designed features (for example, "if two conflicting labels A and B are both predicted, the prediction is never correct, therefore lower the confidence score"). It is also possible to use instance features x during calibration, but we do not find it helpful because BR was already built on x.

There are two commonly used GB variants [11]. The first variant, GB-MSE, uses the tree ensemble score as the output, and MSE as the training objective. The second variant, GB-KL, adds a sigmoid transformation to the ensemble score and uses KL-divergence as the training objective. GB-MSE has the advantage of directly minimizing MSE, which matches the evaluation metric used for calibration (see section 2.1). But it has the disadvantage that its output is not bounded between 0 and 1 and one has to clip its output in order to treat that as a confidence score.

GB-KL has the advantage of providing bounded output, but its training objective does not directly match the evaluation metric used for calibration; note, however, that minimizing KL-divergence also encourages the model output to match the average prediction accuracy, hence achieves the calibration effect. It may appear that one could get the best of both worlds by having sigmoid transformation and MSE training objective at the same time. Unfortunately, adding sigmoid makes MSE a non-convex function of the ensemble scores, thus hard to optimize. In this paper, we choose GB-MSE as our GB calibrator and shall simply call it GB from now on. In supplementary material, we show that GB-KL has very similar performance.

Each BR set prediction is transformed to a feature vector (containing original BR confidence score, set cardinality, set prior probability, and set binary

representation) and the binary correctness of the prediction is used as the regression target. Since the goal of GB calibrator is to objectively evaluate BR's prediction accuracy, it is critical that the calibration data to be disjoint from the BR classifier training data. Otherwise, when BR over-fits its training data, the calibrator will see over-optimistic results on the same data and learn to generate over-confident scores. Similarly, it is also necessary to further separate the label calibration data and the set calibration data, since the product of the calibrated label probabilities is used as input to the set calibrator training.

Imposing Partial Monotonicity Imposing monotonicity is a standard practice in univariate calibration methods such as isotonic regression [31] and Platt scaling [39, 28] as it avoids over-fitting and leads to better interpretability. Imposing (partial) monotonicity for a multi-variate calibrator is more challenging. Certain features considered in calibration are expected to be monotonically related to the confidence. For example, the confidence should always increase with the popularity (prior probability) of the predicted set, if all other features of the prediction are unchanged. The same is true for BR score. The rest of the features, including the cardinality of the set and the binary representation of the set, do not have monotonic relations with confidence. Therefore the calibration function is partially monotonic. We have done additional experiments on imposing partial monotonicity for the GB calibrator but did not observe significant improvement (details and experiment results are in supplementary material).

2.4 Calibration Results

We test the proposed GB calibrator for BR set predictions on 6 commonly used multi-label datasets (see Table 1 for details). Each dataset is randomly split into training, calibration, validation and test subsets. BR model with logistic regression base learners is trained on training data; isotonic regression label calibrators and GB set calibrators are trained on (different parts of) calibration data. All hyper parameters in BR and calibrators are tuned on validation data. Calibration

Table 1: Datasets characteristics; label sets = number of label combinations in training set; cardinality = average number of labels per instance; inst/label = the average number of training instances per label. Datasets are obtained from `http://mulan.sourceforge.net/datasets-mlc.html`, `http://cocodataset.org` and `https://www.kaggle.com/c/wise-2014/data`

Dataset	BIBTEX	OHSUMED	RCV1	TMC	WISE	MSCOCO
domain	bkmark	medical	news	reports	articles	image
labels	159	23	103	22	203	80
label sets	2,173	968	622	1,104	2,782	19,597
features	1,836	12,639	47,236	49,060	301,561	4,096
instances	7,395	13,929	6,000	28,596	48,643	123,287
cardinality	2.40	1.68	3.21	2.16	1.45	2.90
inst/label	89	811	150	2,244	278	3,572

results are reported on test data.

For comparison, we consider the following calibrators:

- uncalib: use the uncalibrated BR probability as it is;
- isotonic: calibrate the BR probability with isotonic regression;
- card isotonic: for each label set cardinality, train one isotonic regression;
- tree: use the features considered by GB, train a single regression tree.

To make a fair comparison, for all methods, individual label probabilities have already been calibrated by isotonic regressions. We focus on their abilities to calibrate set predictions. BR prediction is made by thresholding each label's probability (calibrated by isotonic regression) at 0.5. This corresponds to the set with the highest BR score.

Table 2: BR prediction calibration performance in terms of MSE (the smaller the better) and sharpness (the bigger the better). Bolded numbers are the best.

Dataset	uncentainty	uncalib		isotonic		card isotonic		tree		GB	
		MSE	sharp	MSE	sharp	MSE	sharp	MSE	sharp	MSE	sharp
BIBTEX	0.133	0.193	0.007	0.140	0.002	0.109	0.038	0.086	0.065	**0.068**	**0.072**
OHSUMED	0.232	0.226	0.015	0.221	0.013	**0.182**	**0.051**	0.211	0.039	0.189	0.047
RCV1	0.247	0.175	0.077	0.175	0.075	0.159	0.093	0.134	**0.129**	**0.123**	0.126
TMC	0.212	0.192	0.019	0.192	0.020	0.192	0.022	0.194	0.029	**0.180**	**0.032**
WISE	0.249	0.252	0.017	0.234	0.017	0.151	0.098	0.166	0.093	**0.147**	**0.102**
MSCOCO	0.227	0.158	0.075	0.151	0.075	0.150	0.076	0.163	0.070	**0.143**	**0.083**

The evaluation metrics we use are MSE, sharpness and alignment error, as described in Section 2.1. Following the standard practice, we use 10 equal-width buckets to estimate sharpness and alignment error. One issue with evaluation by bucketing is that using different number of buckets leads to different estimations of alignment error and sharpness (but not MSE and uncertainty, whose computations do not depends on bucketing). In fact, increasing the number of buckets will increase both the estimated alignment error and sharpness by the same amount, due to Eq 1. Using 10 buckets often produces negligible alignment error (relative to MSE), and the comparison effectively focuses on sharpness. This amounts to maximizing sharpness subject to a very small alignment error [14], which is often a reasonable goal in practice. All calibrators are able to achieve small alignment error (on the order of 10^{-3} and contributing to less than 10% of the MSE), so we do not report that. The results are summarized in Table 2. All calibrators improve upon the BR uncalibrated probabilities. Our GB calibrator achieves the overall best MSE and sharpness calibration performance, due to use of additional features extracted from set predictions.

3 Rerank Multi-label Predictions

Now we aim to improve BR's prediction accuracy, by fixing some of the prediction mistakes BR made due to ignoring label dependencies. Our solution is based on the calibrator we just developed. Traditionally, the only role of a calibrator is to map an uncalibrated confidence score to a calibrated confidence score. In that sense the calibrator usually does not affect the classification, only the confidence. In fact, popular univariate calibrators such as isotonic regression and Platt scaling implement monotonic functions, thus preserve the ranking/argmax of predictions. For our multi-variate GB calibrator, however, this is not the case. Even if we constrain the calibrated confidence to be monotonically increasing with the BR prediction scores, there are still other features that may affect the ranking; in particular the argmax predictions before and after calibration might be different $\mathbf{y}$ sets. If indeed different, the prediction based on calibrated confidence takes into account label dependencies and other constraints (which BR does not), and is more likely to be the correct set (even when the calibrated confidence is not very high in absolute terms). Table 3 shows two such examples on the MSCOCO image dataset. Therefore we can also use GB as a multi-label wrapper on top of BR to rerank its predictions. We name this method as ***BR-rerank***.

To do so, we use a two stage prediction pipeline. For each test instance x, we first list the top K label set candidates $\mathbf{y}$ by highest BR uncalibrated scores. This can be done efficiently using a dynamic programming procedure which takes advantage of the label independence assumption made in BR, described in [23], and included in the supplementary material of this paper for the sake of completeness. Although the label independence assumption does not hold in practice, we find empirically that when K is reasonably large (e.g., $K = 50$), the correct $\mathbf{y}$ is often included in the top-K list. The chance that the correct answer is included in the top-K list is commonly called "oracle accuracy", and it is an upper bound of the final prediction accuracy. Empirically, we observe the oracle accuracy to be much higher than the final prediction accuracy, indicating that the candidate generation stage is not a bottleneck of final performance.

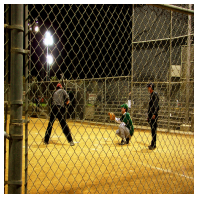
Prediction stage two: send the top set candidates with their scores and additional features to the GB calibrator, and select the one with the highest calibrated confidence as the final prediction. The calibrator has to be trained on more than top-1 BR candidates (on a separate calibration dataset) to evaluate correctly prediction candidates, so we train the GB calibrator on top-K candidates.

3.1 Conceptual Comparison with Related Multi-label Classifiers

Although the proposed BR-rerank classifier has a very simple design, it has some advantages over many existing multi-label classifiers. Here we make some conceptual comparisons between BR-rerank and related multi-label classifiers.

BR-rerank can be seen as a stacking method in which a stage-1 model provides initial estimations and a stage-2 model uses these estimations as input and makes the final decision. There are other stacking methods proposed in the literature, and the two most well-known ones are called 2BR [15, 34] and DBR [25]. The

Table 3: Predictions made by standard BR vs predictions made by reranking BR predictions based on calibrated confidence. For each image, the top row shows the top-5 set prediction candidates generated by BR. Numbers after "BR" are uncalibrated confidence. Numbers after "BR-rerank" are calibrated confidence. Top image: BR predicts {`person,baseball bat`} with confidence 0.58. BR-rerank predicts the correct set {`person, baseball bat, baseball glove`} with confidence 0.17. Bottom image: BR predicts {`person, remote, toothbrush`} with confidence 0.70. BR-rerank predicts the correct set {`person, remote`} with confidence 0.18.

	**y** candidates	person, baseball bat	**person, baseball bat, baseball glove**	person, handbag, baseball bat	person, sports ball, baseball bat	person, handbag, baseball bat, baseball glove
	BR	0.58*	0.35	0.02	0.02	0.01
	BR-rerank	0.16	0.17*	0.04	0.08	0.03

	**y** candidates	person, remote, toothbrush	**person, remote**	person, toothbrush	person	person, tennis racket, remote, toothbrush
	BR	0.70*	0.24	0.03	0.01	0.01
	BR-rerank	0.16	0.18*	0.05	0.02	0.01

stage-1 models in 2BR and DBR are also BR models just as in BR-rerank. The stage-2 models in 2BR and DBR work differently. In 2BR, the stage-2 model predicts each label ℓ with a separate binary classifier which takes as input the original instance feature vector x as well as all label probabilities predicted by the stage-1 model. In DBR, the stage-2 model predicts each label ℓ with a separate binary classifier which takes as input the original instance feature vector

x as well as the binary absence/presence information of all other labels. The absence/presence of label ℓ itself is not part of the input to avoid learning a trivial mapping. During training, the absence/presence information is obtained from the ground truth; during prediction, it is obtained from the stage-1 model's prediction. Clearly for DBR there is some inconsistency on how stage-2 inputs are obtained. BR-rerank and 2BR do not suffer from such inconsistency. All three stacking methods BR-rerank, 2BR, and DBR try to incorporate label dependencies into final classification. However, both 2BR and DBR have a critical flaw: when their stage-2 models make the final decision for a particular label, they do not really take into account the *final decisions* made for other labels by the stage-2 model; they instead only consider the *initial estimations* on other labels made by the stage-1 model, which can be quite different. As a result, the final set predictions made by 2BR and DBR may not respect the label dependencies/constraints these models have learned. By contrast, the stage-2 model in BR-rerank directly evaluates the final set prediction (based on its binary representation and other extracted features) to make sure that the final set prediction satisfies the desired label dependencies/constraints. For example, in the RCV1 dataset, each instance has at least one label. But DBR predicted the empty set on 6% of the test instances. By contrast, BR-rerank never predicted empty set on this dataset.

Many multi-label methods avoid the label independence assumption made in BR and model the joint distribution $p(\mathbf{y}|x)$ in more principled ways. Examples include Conditional Random Fields (CRF) [13], Conditional Bernoulli Mixtures (CBM) [23], and Probabilistic Classifier Chains (PCC) [30, 7, 22, 24]. Despite the joint estimation formulation, CRF, CBM, and PCC in practice often produce over-confident set prediction confidence scores, due to overfitting. Their prediction confidence must also be post-calibrated.

The pair-wise CRF model [13] captures pairwise label interactions by estimating 4 parameters for each label pair. However, because the model needs to assign dedicated parameters to different label combinations, modeling higher order label dependencies becomes infeasible. The BR-rerank approach we propose relies on boosted trees to automatically build high order interactions as tree learns their splits on the binary representation of the label set – there is no need to allocate parameters in advance. There is another CRF model designed specifically to capture exclusive or hierarchical label relations [9]; this works only when the label dependency graph is *strict* and *a priori* known.

CBM is a latent variable model and represents the joint as a mixture of binary relevance models. However, it is hard to directly control the kinds of dependencies CBM learns, or to enforce constraints in the prediction. For example, CBM often predicts the empty set even on dataset where empty prediction is not allowed. There is no easy way to enforce the cardinality constraint in CBM.

PCC decomposes the joint $p(\mathbf{y}|x)$ into a product of conditional probabilities $p(y_1|x)p(y_2|x, y_1) \cdots p(y_L|x, y_1, .., y_{L-1})$, and reduces a multi-label problem to L binary problems, each of which learns a new label given all previous labels. However, different label chaining orders can lead to different results, and to find

the best order is often a challenge. In BR-rerank, all labels are treated as features in the GB calibrator training and they are completely symmetric.

The Structured Prediction Energy Network (SPEN) [1] uses deep neural networks to efficiently encode arbitrary relations between labels, which to large degree avoids parameterization issue associated with pair-wise CRF, but it cannot generate a confidence score for its MAP prediction as computing the normalization constant is intractable. The Predict-and-Constraint method (PC) [2] specifically handles cardinality constraint (but not other label constraints or relations) during learning and prediction. Deep value network (DVN) [18] trains a neural network to evaluate prediction candidates and then uses back-propagation to find the prediction that leads to the maximum score. The idea is similar to our BR-rerank idea. The difference is: DVN could only use the binary encoding of the label set, but not any higher level features extracted from the label set, such as cardinality and prior set probability. That is because its gradient based inference makes it very difficult to directly incorporate such features. There are methods that seek to rank labels [3, 12]. Our method differs from theirs in that we rank label sets as opposed to individual labels, and we take into account label dependencies in the label set.

3.2 Classification Results

We test the proposed BR-rerank classifier on 6 popular multi-label datasets (see Table 1 for details). All datasets used in experiments contain at least a few thousands instances. We do not take datasets with only a few hundred instances as their testing performance tends to be quite unstable. We also do not consider datasets with extremely large number of labels as our method is not designed for extreme classification (our method aims to maximize set accuracy but on extreme data it is very unlikely to predict the entire label set correctly due to large label set cardinality and annotation noise). We compare BR-rerank with many other well-known multi-label methods: Binary Relevance (BR) [35], 2BR [15, 34], DBR [25], pair-wise Conditional Random Field (CRF) [13], Conditional Bernoulli Mixture (CBM) [23], Probabilistic Classifier Chain (PCC) [30], Structured Prediction Energy Network (SPEN) [1], PD-Sparse (PDS) [38], Predict-and-Constrain (PC) [2], Deep value network (DVN) [18], Multi-label K-nearest neighbors (ML-KNN) [41], and Random k-label-sets (RAKEL) [36].

For evaluation, we report set accuracy and instance F1, defined as:

$$\text{set accuracy} = \frac{1}{N}\sum_{n=1}^{N}\mathbb{I}(\mathbf{y}^{(n)} = \hat{\mathbf{y}}^{(n)}); \quad \text{instance F1} = \frac{1}{N}\sum_{n=1}^{N}\frac{2\sum_{l=1}^{L} y_l^{(n)}\hat{y}_l^{(n)}}{\sum_{l=1}^{L} y_l^{(n)} + \sum_{l=1}^{L}\hat{y}_l^{(n)}},$$

where $\mathbf{y}^{(n)}$ and $\hat{\mathbf{y}}^{(n)}$ are the ground truth and predicted label set for the n-th instance, and $\mathbb{I}(\mathbf{y}^{(n)} = \hat{\mathbf{y}}^{(n)})$ returns 1 when the prediction is perfect and 0 otherwise.

To make a fair comparison, we use logistic regressions as the underlying learners for BR as

Table 5: Training time of different methods, measured in seconds. All algorithms run multi-threaded on a server with 56 cores.

Dataset	BIBT	OHSUM	RCV1	TMC	WISE	MSCO
BR	4	3	7	8	80	1380
BR-rerank	9	6	10	11	88	1393
CBM	64	210	70	224	1320	8520
CRF	353	268	1223	771	16363	14760

Table 4: Prediction performance in terms of set accuracy (top) and instance F1 (bottom). Numbers are shown as percentages. Bold numbers are the best ones on each dataset. "-" means the method could not finish within 24 hours on a server with 56 cores and 256G RAM or 4 NVIDIA Tesla V100 GPUs. The ranking indicates for each method, on average over datasets, what position its performance is (lower is better). Our BR-rerank has the best average ranking on both measures. Note also that BR is not the worst as one might naively assume. Hyper parameters for all methods have been tuned on validation set.

Dataset	BR	*BR-rerank*	2BR	DBR	CBM	CRF	SPEN	PDS	DVN	PC	PCC	Rakel	MLKNN
BIBTEX	16.6	21.5	16.1	20.2	22.9	**23.3**	14.8	16.1	16.2	20.3	21.4	18.3	8.4
OHSUMED	36.6	**42.0**	37.5	37.6	40.5	40.4	29.1	34.8	18.6	29.5	38.0	39.3	25.4
RCV1	44.5	53.2	42.3	45.8	**55.3**	53.8	27.5	40.8	13.7	39.7	48.7	46.0	46.2
TMC	30.4	**33.3**	32.1	31.7	30.8	28.2	26.7	23.4	20.3	23.0	31.3	27.6	18.9
WISE	52.9	60.5	51.8	55.8	**61.0**	46.4	-	52.4	28.3	-	55.9	3.5	2.4
MSCOCO	34.7	**35.9**	33.7	32.0	31.1	35.1	34.1	25.0	29.9	31.1	32.1	32.6	29.1
ranking	6.3	1.8	6.7	5.7	3.3	3.8	10.0	9.8	11.2	10.0	4.5	6.8	11.0

Dataset	BR	*BR-rerank*	2BR	DBR	CBM	CRF	SPEN	PDS	DVN	PC	PCC	Rakel	MLKNN
BIBTEX	35.9	42.2	36.7	40.1	45.3	46.2	38.6	40.4	47.3	**47.5**	40.9	38.3	23.0
OHSUMED	62.9	**67.5**	62.9	61.5	67.2	65.6	58.8	66.4	60.0	60.5	61.7	62.3	48.6
RCV1	77.0	78.8	77.5	72.8	**80.3**	75.0	66.5	76.7	36.3	71.7	75.6	76.1	72.3
TMC	65.8	66.8	**67.9**	66.1	65.2	64.4	66.2	64.0	65.5	61.7	64.9	63.6	52.2
WISE	68.3	75.4	69.1	69.9	**76.0**	60.7	-	73.6	62.3	-	69.7	6.2	5.6
MSCOCO	73.0	73.2	72.6	69.6	70.0	**73.9**	73.2	64.8	72.7	72.7	69.6	71.7	68.2
ranking	6.3	2.5	5.5	7.3	4.0	5.7	8.3	6.8	7.5	8.8	7.5	8.7	12.0

well as the stage-1 models in BR-rerank, 2BR and DBR. We use gradient boosting as the underlying learners in PCC as well as the stage-2 models in BR-rerank, 2BR and DBR. Each dataset is randomly split into training, validation and test subsets. All classifiers are trained on the training set, with hyper parameters tuned on validation set. Supplementary material contains implementations and hyper parameters tuning details. For BR-rerank and 2BR, since the stage-2 model uses stage-1 model's out-of-sample prediction as input, the stage-1 model and stage-2 model are trained on different parts of the training data. For DBR, since the stage-2 model training only takes the ground truth labels as input, both stage-1 model and stage-2 model are trained on the whole training set.

Test performance is reported in Table 4. As expected, by reranking BR-independent-prediction candidates, BR-rerank outperforms BR significantly. We also observe that generally BR-rerank only needs to rerank the top-10 candidates from BR in order to achieve the best performance (supplementary material

shows how its performance changes as K increases). On each dataset, we rank all algorithms by performance, and report each algorithm's average ranking across all datasets. BR-rerank has the best average ranking with both metrics, followed by CBM and CRF. We emphasize that with slightly better performance, BR-rerank is noticeably simpler to use than CBM and CRF. CBM and CRF require implementing dedicated training and prediction procedures, while BR-rerank can be ran by simply combining existing machine learning libraries such as LIBLINEAR [10] for BR and Xgboost [4] for GB. BR-rerank is also much faster than CBM and CRF. Its running time is determined mostly by its stage one, the BR classifier training. See Table 5 for a comparison.

4 Other Related Work and Discussion

There are many other approaches to multi-label classification. Some of them focus on exploiting label structures [27, 19, 6, 42]. Several approaches adapt existing machine learning models, such as Bayesian network [40], recurrent neural networks [26, 29], and determinantal point process [37].

The idea of first generating prediction candidates and then reranking them using richer features has been considered in several natural language processing tasks, including parsing [8] and machine translation [33]. Here we show that the reranking idea, with properly designed models and features, is well suited for multi-label classification as well. Generative Adversarial Nets (GANs) [16] also employ two models, one for generating samples and one for judging these samples. GANs are usually trained in an unsupervised fashion, and are mainly used for generating new samples. By contrast, our BR-rerank is trained in supervised fashion, and its main goal is to do classification. Also the two models in GANs are trained simultaneously, while the two models in BR-rerank are trained in separate stages.

Besides isotonic regression and Platt scaling, there are also some recent developments on binary, multi-class, and structured prediction calibration methods [20, 17, 21, 5]. Our work instead focuses on how to design the calibrator model and features for the BR multi-label classifier and how to take advantage of the calibrated confidence to get better multi-label predictions.

5 Conclusion

We improve BR's confidence estimation and prediction through a simple post calibration and reranking procedure. We take the BR predicted set of labels and its uncalibrated confidence as features, extract more features from the prediction that capture label constraints, such as the label set cardinality and prior probability, and apply gradient boosted trees (GB) as a calibrator to map the features to a better-calibrated confidence score. GB not only uses these manually designed features but also builds trees on binary label features to automatically model label interactions. This allows the calibrator to better separate good predictions from bad ones, yielding new confidence scores that are not only well

aligned with accuracy but also sharp. We further demonstrate that using the new confidence scores we are able to rerank BR's prediction candidates to the point it outperforms state-of-the-art classifiers. Our code and data are available at `https://github.com/cheng-li/pyramid`.

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References

1. Belanger, D., McCallum, A.: Structured prediction energy networks. In: Proceedings of the International Conference on Machine Learning (2016)
2. Brukhim, N., Globerson, A.: Predict and constrain: Modeling cardinality in deep structured prediction. arXiv preprint arXiv:1802.04721 (2018)
3. Bucak, S.S., Mallapragada, P.K., Jin, R., Jain, A.K.: Efficient multi-label ranking for multi-class learning: application to object recognition. In: Computer Vision, 2009 IEEE 12th International Conference on. pp. 2098–2105. IEEE (2009)
4. Chen, T., Guestrin, C.: Xgboost: A scalable tree boosting system. In: Proceedings of the 22nd acm sigkdd international conference on knowledge discovery and data mining. pp. 785–794. ACM (2016)
5. Chen, T., Navrátil, J., Iyengar, V., Shanmugam, K.: Confidence scoring using whitebox meta-models with linear classifier probes. arXiv preprint arXiv:1805.05396 (2018)
6. Chen, Y.N., Lin, H.T.: Feature-aware label space dimension reduction for multi-label classification. In: NIPS. pp. 1529–1537 (2012)
7. Cheng, W., Hüllermeier, E., Dembczynski, K.J.: Bayes optimal multilabel classification via probabilistic classifier chains. In: ICML-10. pp. 279–286 (2010)
8. Collins, M., Koo, T.: Discriminative reranking for natural language parsing. Computational Linguistics **31**(1), 25–70 (2005)
9. Deng, J., Ding, N., Jia, Y., Frome, A., Murphy, K., Bengio, S., Li, Y., Neven, H., Adam, H.: Large-scale object classification using label relation graphs. In: Computer Vision–ECCV 2014, pp. 48–64. Springer (2014)
10. Fan, R.E., Chang, K.W., Hsieh, C.J., Wang, X.R., Lin, C.J.: Liblinear: A library for large linear classification. Journal of machine learning research **9**(Aug), 1871–1874 (2008)
11. Friedman, J.H.: Greedy function approximation: a gradient boosting machine. Annals of statistics pp. 1189–1232 (2001)
12. Fürnkranz, J., Hüllermeier, E., Mencía, E.L., Brinker, K.: Multilabel classification via calibrated label ranking. Machine learning **73**(2), 133–153 (2008)
13. Ghamrawi, N., McCallum, A.: Collective multi-label classification. In: Proceedings of the 14th ACM international conference on Information and knowledge management. pp. 195–200. ACM (2005)

14. Gneiting, T., Balabdaoui, F., Raftery, A.E.: Probabilistic forecasts, calibration and sharpness. Journal of the Royal Statistical Society: Series B (Statistical Methodology) **69**(2), 243–268 (2007)
15. Godbole, S., Sarawagi, S.: Discriminative methods for multi-labeled classification. In: Pacific-Asia conference on knowledge discovery and data mining. pp. 22–30. Springer (2004)
16. Goodfellow, I., Pouget-Abadie, J., Mirza, M., Xu, B., Warde-Farley, D., Ozair, S., Courville, A., Bengio, Y.: Generative adversarial nets. In: Advances in neural information processing systems. pp. 2672–2680 (2014)
17. Guo, C., Pleiss, G., Sun, Y., Weinberger, K.Q.: On calibration of modern neural networks. arXiv preprint arXiv:1706.04599 (2017)
18. Gygli, M., Norouzi, M., Angelova, A.: Deep value networks learn to evaluate and iteratively refine structured outputs. arXiv preprint arXiv:1703.04363 (2017)
19. Hsu, D., Kakade, S., Langford, J., Zhang, T.: Multi-label prediction via compressed sensing. In: NIPS. vol. 22, pp. 772–780 (2009)
20. Kuleshov, V., Fenner, N., Ermon, S.: Accurate uncertainties for deep learning using calibrated regression. arXiv preprint arXiv:1807.00263 (2018)
21. Kuleshov, V., Liang, P.S.: Calibrated structured prediction. In: Advances in Neural Information Processing Systems. pp. 3474–3482 (2015)
22. Kumar, A., Vembu, S., Menon, A.K., Elkan, C.: Learning and inference in probabilistic classifier chains with beam search. In: Machine Learning and Knowledge Discovery in Databases, pp. 665–680. Springer (2012)
23. Li, C., Wang, B., Pavlu, V., Aslam, J.A.: Conditional bernoulli mixtures for multi-label classification. In: Proceedings of the 33rd International Conference on Machine Learning. pp. 2482–2491 (2016)
24. Liu, W., Tsang, I.: On the optimality of classifier chain for multi-label classification. In: Advances in Neural Information Processing Systems. pp. 712–720 (2015)
25. Montañes, E., Senge, R., Barranquero, J., Quevedo, J.R., del Coz, J.J., Hüllermeier, E.: Dependent binary relevance models for multi-label classification. Pattern Recognition **47**(3), 1494–1508 (2014)
26. Nam, J., Mencía, E.L., Kim, H.J., Fürnkranz, J.: Maximizing subset accuracy with recurrent neural networks in multi-label classification. In: Advances in Neural Information Processing Systems. pp. 5413–5423 (2017)
27. Park, S.H., Fürnkranz, J.: Multi-label classification with label constraints. In: ECML PKDD 2008 Workshop on Preference Learning. pp. 157–171 (2008)
28. Platt, J., et al.: Probabilistic outputs for support vector machines and comparisons to regularized likelihood methods. Advances in large margin classifiers **10**(3), 61–74 (1999)
29. Qin, K., Li, C., Pavlu, V., Aslam, J.: Adapting RNN sequence prediction model to multi-label set prediction. In: Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long and Short Papers). pp. 3181–3190 (2019)
30. Read, J., Pfahringer, B., Holmes, G., Frank, E.: Classifier chains for multi-label classification. Machine learning **85**(3), 333–359 (2011)
31. Robertson, T.: Order restricted statistical inference. Tech. rep. (1988)
32. Sasabuchi, S., Inutsuka, M., Kulatunga, D.: A multivariate version of isotonic regression. Biometrika **70**(2), 465–472 (1983)
33. Shen, L., Sarkar, A., Och, F.J.: Discriminative reranking for machine translation. In: HLT-NAACL 2004 (2004)

34. Tsoumakas, G., Dimou, A., Spyromitros, E., Mezaris, V., Kompatsiaris, I., Vlahavas, I.: Correlation-based pruning of stacked binary relevance models for multi-label learning. In: Proceedings of the 1st international workshop on learning from multi-label data. pp. 101–116 (2009)
35. Tsoumakas, G., Katakis, I.: Multi-label classification: An overview. Int J Data Warehousing and Mining **2007**, 1–13 (2007)
36. Tsoumakas, G., Vlahavas, I.: Random k-labelsets: An ensemble method for multil-abel classification. In: ECML. pp. 406–417. Springer (2007)
37. Xie, P., Salakhutdinov, R., Mou, L., Xing, E.P.: Deep determinantal point process for large-scale multi-label classification. In: ICCV. pp. 473–482 (2017)
38. Yen, I.E., Huang, X., Zhong, K., Ravikumar, P., Dhillon, I.S.: Pd-sparse: A primal and dual sparse approach to extreme multiclass and multilabel classification. In: Proceedings of the 33nd International Conference on Machine Learning (2016)
39. Zadrozny, B., Elkan, C.: Transforming classifier scores into accurate multiclass probability estimates. In: KDD. pp. 694–699. ACM (2002)
40. Zhang, M.L., Zhang, K.: Multi-label learning by exploiting label dependency. In: KDD. pp. 999–1008. ACM (2010)
41. Zhang, M.L., Zhou, Z.H.: Ml-knn: A lazy learning approach to multi-label learning. Pattern recognition **40**(7), 2038–2048 (2007)
42. Zhou, T., Tao, D., Wu, X.: Compressed labeling on distilled labelsets for multi-label learning. Machine Learning **88**(1-2), 69–126 (2012)