Computational Intelligence, Volume 000, Number 000, 2011

Improving Multi-label Classification by Avoiding Implicit Negativity with Incomplete Data

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Many real world problems require multi-label classification, in which each training instance is associated with a set of labels. There are many existing learning algorithms for multi-label classification; however, these algorithms assume implicit negativity, where missing labels in the training data are automatically assumed to be negative. Additionally, many of the existing algorithms do not handle incremental learning in which new labels could be encountered later in the learning process. A novel multi-label adaptation of the backpropagation algorithm is proposed that does not assume implicit negativity. In addition, this algorithm can, using a naïve Bayesian approach, infer missing labels in the training data. This algorithm can also be trained incrementally as it dynamically considers new labels. This solution is compared with existing multi-label algorithms using data sets from multiple domains and the performance is measured with standard multi-label evaluation metrics. It is shown that our algorithm improves classification performance for all metrics by an overall average of 7.4% when at least 40% of the labels are missing from the training data, and improves by 18.4% when at least 90% of the labels are missing.

Key words: multi-label classification, implicit negativity, backpropagation, missing labels

1. INTRODUCTION

Traditionally, many classification problems have dealt with single-label classification, meaning each training instance is associated with only one class or label. In single-label classification, the task is to learn some target function $f : X \rightarrow L$ that predicts the correct label for each new instance. However, in multi-label classification, each training instance can be associated with more than one label. The task is to learn some target function $f : X \rightarrow 2^L$ that predicts the correct set of labels (of unknown size) for each new instance.

There are many interesting problems that require multi-label classification. For example, in gene classification, genes can perform more than one function (Zhang and Zhou, 2006). In text categorization, a document can contain multiple topics such as outdoors, sports, and recreation (Schapire and Singer, 2000). Images can be labeled by the multiple objects they may contain Boutell et al. (2004). Web sites can be given several labels for the different topics they represent (Tsoumakas et al., 2008). Music and movies can belong to more than one genre (Trohidis et al., 2008). The list of multi-label classification problems continues to grow and it is imperative that we have good multi-label classification solutions for these various problems.

The existing methods for multi-label classification follow two main strategies: *problem transformational methods* and *algorithm adaptation methods* (Tsoumakas and Katakis, 2007). Problem transformational methods involve transforming a multi-label classification problem into one or more single-label classification problems. Algorithm adaptation methods involve modifying specific learning algorithms to directly handle multi-label problems. Much research has been done to show that many of these methods are successful in solving various multi-label problems.

However, all these multi-label learning algorithms assume that each training instance

will have all the correct positive labels provided and that any label not listed is negative. We call this assumption *implicit negativity*. We will define our set of multi-label data to be $\{(x_i, Y_i)|i = 1, 2, \ldots, m\}$, where $Y_i \subseteq L$ is the set of all correct positive labels for x_i and $L = \{\lambda_j|j = 1, 2, \ldots, q\}$ is the set of all possible labels. Let Y_i' be the provided set of positive labels for a training instance x_i. Existing multi-label learning algorithms assume that $Y_i' = Y_i$, or that the provided set of positive labels is always equal to the true set of all positive labels for a training instance x_i. In reality, this is not always the case. Gathering training data is constantly an issue in machine learning and getting training data with all the correct positive labels listed can be very difficult in many domains. Often Y_i' is only a subset of Y_i and is therefore missing positive labels. Algorithms that assume implicit negativity struggle with these incomplete positive label sets because it is automatically implied that those missing positive labels are negative and the model is trained incorrectly. It should be noted that there is also the case involving noise, where $\lambda_j \in Y_i'$ but $\lambda_j \notin Y_i$. However, dealing with noise is beyond the scope of this thesis.

Removing the assumption of implicit negativity helps to avoid training the model incorrectly when positive labels are missing. However, eliminating this assumption requires negative labels, in addition to the positive labels. This can potentially create a class imbalance problem between the positive and negative examples of each label because negative labels are generally even harder to acquire than positive labels. One approach to dealing with this is to have the learning algorithm take advantage of label correlations in the data to infer what the missing positive and negative labels are for each training instance. Let $\bar{Y}_i$ be the true set of all negative labels for a training instance x_i and let $\bar{Y}_i'$ be the provided set of negative labels for a training instance x_i. When the learning algorithm encounters a new training instance x_i with positive labels Y_i' and negative labels $\bar{Y}_i'$, it should be able to infer Y_i and $\bar{Y}_i$.

Another issue to consider in multi-label learning is that during incremental training, often the complete set of all possible labels L may not be known *a priori*. In these situations, the learning algorithm must be able to dynamically account for new labels as they are encountered. Let L' be the set of all possible labels that are known at the start of training. When the learning algorithm encounters a new label $\lambda \notin L'$, it should be able to dynamically add λ to L' and start learning this new label without disrupting what has previously been learned.

We propose a novel variation of the backpropagation algorithm called the BAIN (Backpropagation for Avoiding Implicit Negativity) algorithm that does not assume implicit negativity. The BAIN algorithm only trains the output nodes explicitly labeled (as positive or negative) in the training data, while ignoring the labels not mentioned. The BAIN algorithm can also dynamically add new output nodes for previously unseen labels during incremental training. Since the BAIN algorithm does not assume implicit negativity, it is now reliant on explicitly given negative and positive labels. The BAIN algorithm uses a naïve Bayes method to infer missing positive and negative labels in the training data.

BAIN is compared to popular multi-label learning algorithms, including BP-MLL (Zhang and Zhou, 2006), Binary Relevance (Tsoumakas and Katakis, 2007) and ML-kNN (Zhang and Zhou, 2005). Four experiments with two different types of data sets are outlined. Standard multi-label evaluation metrics such as *Hamming loss, accuracy, precision, recall, one-error, coverage,* and *ranking loss* (Schapire and Singer, 2000; Zhang and Zhou, 2006) are used to evaluate the effectiveness of our new BAIN algorithm compared to existing multi-label algorithms. It is shown that the BAIN algorithm is robust to missing labels in the training data and outperforms existing multi-label learning methods as the amount of missing data increases.

Section 2 provides a simple review of multi-label classification methods as well as a review of related research. Section 3 explains in detail the BAIN algorithm. Section 4 provides a description of the data sets, evaluation metrics, and algorithms used in the experiments.

Section 5 describes the four experiments designed to evaluate the BAIN algorithm and presents the results. Finally, Section 6 outlines our conclusions and future work.

2. RELATED WORK

Problem transformational methods and algorithm adaptation methods are the two main strategies for handling multi-label classification. Here we review a few of the most popular methods. For a more comprehensive review of problem transformational and algorithm adaptation methods, there are several excellent surveys on multi-label classification (Tsoumakas et al., 2010; Tsoumakas and Katakis, 2007; de Carvalho and Freitas, 2009). In addition, we will consider other work that has been done to solve the specific problems of implicit negativity, inferring missing labels, and incremental learning.

2.1. Problem Transformational Methods

Problem transformational methods involve transforming a multi-label classification problem into one or more single-label classification problems. One approach is to treat each unique non-singleton set of labels in the training data as an additional label in the set of all possible labels L (Tsoumakas and Katakis, 2007; de Carvalho and Freitas, 2009). For example, given a data set with the possible labels $L = \{A, B, C, D\}$ and training set:

$$x_1 \rightarrow A$$
$$x_2 \rightarrow A, B$$
$$x_3 \rightarrow A, C, D$$
$$x_4 \rightarrow D$$

The set of possible labels becomes $L = \{A, B, C, D, \{A, B\}, \{A, C, D\}\}$ and the problem is now a single-label classification problem and any standard learning algorithm can be used. This method is called Label Powerset and does not work well when there are a large number of possible labels because it is difficult to get enough data to support every combination of labels that might be encountered.

Another strategy is to split this problem into several binary classification problems, one for each label (Tsoumakas and Katakis, 2007; de Carvalho and Freitas, 2009). So the data set mentioned previously becomes four new data sets:

$L_A = \{A, \bar{A}\}$	$L_C = \{C, \bar{C}\}$	$L_B = \{B, \bar{B}\}$	$L_D = \{D, \bar{D}\}$
$x_1 \rightarrow A$	$x_1 \rightarrow \bar{C}$	$x_1 \rightarrow \bar{B}$	$x_1 \rightarrow \bar{D}$
$x_2 \rightarrow A$	$x_2 \rightarrow \bar{C}$	$x_2 \rightarrow B$	$x_2 \rightarrow \bar{D}$
$x_3 \rightarrow A$	$x_3 \rightarrow C$	$x_3 \rightarrow \bar{B}$	$x_3 \rightarrow D$
$x_4 \rightarrow \bar{A}$	$x_4 \rightarrow \bar{C}$	$x_4 \rightarrow \bar{B}$	$x_4 \rightarrow D$

This method is called Binary Relevance and any standard binary classifier can now be used for each label. A common criticism of this method is that, rather than a single model, multiple learning models are needed. This can be inefficient for problems with large label sets. Another common criticism is that as labels are separated, correlations between labels are not considered which can weaken the system's expressive power (Zhang and Zhou, 2006).

Classifier Chains (CC) is a more sophisticated problem transformational method that extends the binary relevance method (Read et al., 2011). The idea is to chain the individual binary models together such that the output of the first model is input to the next model and so on. It is claimed that this chaining method helps to preserve the correlations between labels but determining optimal chain order is an important consideration. Dual Layer Voting

is another problem transformational method that combines binary relevance with a pairwise method (Madjarov et al., 2011). A layered network of classifiers is built where the first layer is composed of binary classifiers, and the second layer is composed of pairwise classifiers. When classifying a new instance, the model uses the result of the binary layer to determine if the pairwise layer should be consulted based on some threshold. There has also been a study that compares three different problem transformational approaches on hierarchical multi-label problems using decision trees as the base algorithm (Vens et al., 2008), which found that a label powerset method is the superior method for hierarchical multi-label problems.

2.2. Algorithm Adaptation Methods

Algorithm adaptation methods involve modifying specific learning algorithms to directly handle multi-label problems. One of the first algorithms to be adapted to multi-label classification was the C4.5 algorithm (Clare and King, 2001). The C4.5 algorithm was modified to allow multiple labels in the leaves of the tree and the entropy formula was changed to consider both the class membership and non-class membership of each label. The AdaBoost algorithm was extended for multi-label classification resulting in the Adaboost.MH and the Adaboost.MR algorithms (Schapire and Singer, 2000). Adaboost.MH focuses on label classification, while Adaboost.MR focuses on label ranking.

ML-kNN is a multi-label classification algorithm adapted from the kNN algorithm (Zhang and Zhou, 2005). This adaptation uses the kNN algorithm independently for each label; so fundamentally it is a problem transformational method. However, it differs from a normal problem transformational method because it makes use of prior and posterior probabilities as it recombines the results. There also exists an SVM algorithm adapted for multi-label classification that is also in reality a problem transformational method (Godbole and Sarawagi, 2004). This SVM adaptation does, however, use a kind of meta-learning strategy to consider the dependencies among the different labels.

BP-MLL (Backpropagation for Multi-Label Learning) is a modified version of the backpropagation algorithm (Zhang and Zhou, 2006). The error function is modified to consider label correlations where labels belonging to an instance should be ranked higher than those not belonging to that instance. ML-RBF is an extension of the RBF neural network algorithm that handles multi-label classification (Zhang, 2009). ML-RBF selects hidden nodes by conducting a clustering analysis on instances of each possible label. Information encoded in the hidden nodes corresponding to all classes is exploited to optimize the weights corresponding to each label.

Multi-label classification can be thought of as a specific case of structured output learning. Structured output learning is a classification task in which the output space consists of structured objects, such as trees, strings, sequences, or graphs. The goal is to learn the entire structure of the output, where multiple instances are inter-related. There are several structured learning algorithms that have been used for multi-label classification (Taskar et al., 2003; Tsochantaridis et al., 2005; Bielza et al., 2011). These methods combine the advantages of kernel-based and probabilistic classifiers. The kernel-based component can deal with high dimensional feature spaces and provides strong generalization guarantees, while the probabilistic component is able to represent label correlations and exploit problem structure. Bakir et al. provide a comprehensive review of structured output learning (2007).

2.3. Implicit Negativity

Most of these multi-label classification methods work well for the specific tasks they were developed for. However, each of these methods assumes implicit negativity, and will

likely perform poorly when applied to tasks where not all the correct positive labels are provided.

The Weakened Implicit Negatives (WIN) algorithm was proposed in order to deal with the issue of implicit negativity for backpropagation (Whiting and Ventura, 2004). The WIN algorithm uses a separate probabilistic neural network component that learns a target output value for each output node in the network. When a label is missing for a given training instance, the WIN algorithm uses the learned target output value during error calculation instead of assuming it to be zero. Training time is alternated between learning the network weights and learning the target output values. How often each component alternates must be provided as a parameter. This method was shown to be effective at learning toy problems and a few real world problems with incomplete data; however, the algorithm was not compared to any of the standard multi-label algorithms nor with any of the standard multi-label evaluation metrics. Additionally, using a separate probabilistic neural network on top of backpropagation increases the computational complexity, which could be problematic for problems with large numbers of labels. Finally, the WIN algorithm was designed for the specific case where $|Y_i'| = 1$ and $|\bar{Y}_i'| = 0$. In other words, there is exactly one positive label provided for each training instance and all other labels are unknown.

In the broader field of structured output learning, there exists several methods that deal with missing labels for sequence labeling and part of speech tagging (Tsuboi et al., 2008; Smola et al., 2005; Suzuki et al., 2007). Each method uses a probabilistic model for which the parameters must be optimized to match the training data. These methods deal with missing labels by marginalizing out the the unknown labels so as to maximize the likelihood of a set of possible label structures which are consistent with the given data. These methods are only applied to sequence labeling and part of speech tagging and it is unclear how they would adapt to multi-label classification.

However, a multi-label active learning algorithm was proposed that is based on similar probabilistic ideas (Qi et al., 2009). This method avoids the tedious process of labeling thousands of images with possibly hundreds of labels by using a Bayesian error bound to actively annotate only a subset of labels and then later deal with the missing labels. This approach then uses the Maximum Entropy Method to learn a function that can classify new instances (Zhu et al., 2005). This method handles missing labels by integrating out the unlabeled part yielding the marginal distribution of the labeled part. This technique was shown to be effective with small data sets. However, this algorithm is computationally inefficient for problems with large sets of possible labels.

2.4. Inferring Missing Labels

Removing the assumption of implicit negativity helps to avoid training the model incorrectly when positive labels are missing. However, to compensate, negative labels are needed in addition to the positive labels. Inferring those missing positive and negative labels is needed to help fill in the gaps in the training data. That is to say, when the learning algorithm encounters a new training instance x_i with a set of incomplete positive labels Y_i' and negative labels $\bar{Y}_i'$, it should be able to infer the true set of positive labels Y_i and negative labels $\bar{Y}_i$. This is similar to the class imbalance problem because there will likely be fewer negative examples of each label compared to positive examples of each label.

A common solution to class imbalance is to either oversample the minority class or under-sample the majority class (Guo et al., 2008). This solution is not the most effective because over-fitting becomes a problem with oversampling and loss of crucial data is a problem with under-sampling. Another method is to use data generation strategies where new data instances for the minority class are generated by interpolating between the existing data instances (Guo and Viktor, 2004; Han et al., 2005). In multi-label classification, class

imbalance has been studied (Chen and Lu, 2006). However, the research does not deal with class imbalance between positive and negative examples caused by missing data. Rather, the research deals with class imbalance between different labels when one label is more rare than another.

There is little research that deals with inferring missing labels for multi-label problems. The active annotation algorithm mentioned in the previous section indirectly infers missing labels as part of the training process (Qi et al., 2009). However, there is no algorithm that we are aware of that explicitly tries to predict missing labels in the training data by considering label correlations in the data that is provided.

2.5. Incremental Learning

Most of these multi-label learning algorithms are not incremental learners and specifically do not deal with the case of the complete set of all possible labels being unknown *a priori*. There are learning algorithms that deal with incremental learning for neural networks and handle the issue of new incoming labels (Bruzzone and Fernández Prieto, 1999; Polikar et al., 2001). However, these incremental algorithms are not designed for multi-label classification. There is an active annotation algorithm that claims to be the first incremental multi-label algorithm (Hua and Qi, 2008; Qi et al., 2009). This algorithm allows for introducing new labels and is able to dynamically update the model to account for these new incoming labels. This solution is similar to our approach, except our solution is a backpropagation solution, while theirs is a Bayesian model.

3. METHODS

Multi-label learning is a complicated problem with many potential issues. We propose a novel variation of the backpropagation algorithm called the BAIN (Backpropagation for Avoiding Implicit Negativity) algorithm that addresses multi-label learning and deals with the issues previously mentioned. Specifically, the BAIN algorithm:

- Does not assume implicit negativity
- Uses label correlations in the training data to infer missing labels
- Can learn incrementally and dynamically incorporate previously unseen labels

These issues are nontrivial when it is difficult to get data with all the correct labels for each training instance or when new data is being gathered and additional labels could appear. The BAIN algorithm is implemented by taking the initial set of training data and building a standard feed-forward neural network with each output node representing a label. The neural network is then trained using standard backpropagation with a few key differences.

3.1. Avoiding Implicit Negativity

When certain labels are encountered in the training data, only the weights of the outputs nodes corresponding to those labels are trained, while the other output nodes are ignored. The assumption of implicit negativity is simply not made. Negative examples must be explicitly labeled as negative in the training data. For example, given a data set with the possible labels $L = \{A, B, C, D\}$ and training set:

$$
\begin{aligned}
&x_1 \rightarrow A, \bar{C} \\
&x_2 \rightarrow A, B \\
&x_3 \rightarrow A, \bar{B}, C, D \\
&x_4 \rightarrow \bar{B}, D
\end{aligned}
$$

When training the neural network on x_1, only the weights corresponding to output nodes A and C are trained, while B and D are ignored. For x_2, only the weights corresponding to output nodes A and B are trained, while C and D are ignored.

This is done by changing how the error term is calculated for each network output node. Let K and H be the set of output nodes and the set of hidden nodes, respectively, for the neural network. Let o_k, t_k, and δ_k be the actual output value, target output value, and error term, respectively, for an output node $k \in K$. In standard backpropagation, the error term δ_k is calculated for each k as follows:

$$\delta_k \leftarrow o_k(1 - o_k)(t_k - o_k)$$

The error term δ_h for each hidden node $h \in H$ can then be calculated:

$$\delta_h \leftarrow o_h(1 - o_h) \sum_{k \in K} w_{kh}\delta_k$$

where o_h is the output value for hidden node h and w_{kh} is the weight between hidden node h and output node k. The network weights are then updated as follows:

$$w_{ji} \leftarrow w_{ji} + \eta\delta_j x_{ji}$$

where η is the learning rate, x_{ji} is the input value to node j from unit i, and w_{ji} denotes the corresponding weight.

In the BAIN algorithm, the assumption of implicit negativity is removed by changing how the error term δ_k is calculated:

$$\delta_k \leftarrow \begin{cases} 0, \text{ if } t_k \text{ is unknown} \\ o_k(1 - o_k)(t_k - o_k), \text{ otherwise} \end{cases}$$

When using standard backpropagation for multi-label classification, t_k is automatically assumed to be zero when its value is unknown. However, by setting δ_k to zero when t_k is unknown, the weights that connect each hidden node to the kth output node are prevented from changing due to multiplication by zero. The kth output node is also prevented from affecting the error term for each hidden node. In this way the kth output node is ignored when there is no explicitly given label for that node.

It should be noted that the BAIN algorithm relies on having at least one explicit negative label per training instance and could perform poorly when no negative labels are provided. However, it may not be unreasonable to require that there be at least one negative label provided for each training instance when using the BAIN algorithm, because there are usually far more negative labels per instance than positive labels.

3.2. Inferring Missing Labels

The goal is to take advantage of label correlations in the data to infer the missing positive and negative labels for each training instance. To do this, a naïve Bayes approach is used. Naïve Bayes is simple and fast, allowing us to avoid unreasonable computational overhead in training the actual multi-label model. The naïve Bayes classifier takes the form:

$$\mathit{classify}(w_1, w_2, ..., w_n) = \underset{g}{\operatorname{argmax}}\ p(G = g) \prod_{j=1}^{n} p(W_j = w_j | G = g)$$

We consider the problem of inferring missing labels as a classification problem. A missing label can be classified as either positive or negative. The other known labels are used as the input features. In our case, w_j ranges over the set of labels $Y_i' \cup \bar{Y}_i'$—all the provided labels (both positive and negative) for a given training instance x_i, $n = |Y_i' \cup \bar{Y}_i'|$ (number of labels), and G is the missing label we are trying to infer, which can be either positive or

negative. The missing label is inferred only when there is confidence in the prediction. This means that the argmax is only taken when the difference is larger than a certain threshold θ, otherwise the label is left unknown. Hence, our method to infer a missing label G can be defined as follows:

$$G = \begin{cases} 1, \text{ if } f_G(1, Y_i', \bar{Y}_i') - f_G(-1, Y_i', \bar{Y}_i') > \theta \\ -1, \text{ if } f_G(-1, Y_i', \bar{Y}_i') - f_G(1, Y_i', \bar{Y}_i') > \theta \\ unknown, \text{ otherwise} \end{cases}$$

where

$$f_G(g, Y_i', \bar{Y}_i') = p(G = g) \prod_{\lambda \in Y_i'} p(\lambda | G = g) \prod_{\lambda \in \bar{Y}_i'} p(\bar{\lambda} | G = g)$$

To clarify, inferring that $G = 1$ means that the training instance should be considered a positive example of label G and inferring $G = -1$ means that the training instance should be considered a negative example of label G. This method is applied iteratively to each missing label G in each training instance x_i. The probabilities can be estimated from the training data based on the assumption that there exist other training instances that are not missing the label G.

For example, given a data set with the possible labels $L = \{A, B, C, D\}$ and training set:

$$\begin{array}{l} x_1 \rightarrow A, B, \bar{C}, \bar{D} \\ x_2 \rightarrow \bar{A}, \bar{B}, C, D \\ x_3 \rightarrow A, \bar{C}, \bar{D} \\ x_4 \rightarrow \bar{A}, \bar{B}, C, D \\ x_5 \rightarrow A, B, C, \bar{D} \end{array}$$

Information about B is missing from x_3 and must be inferred. For training instance x_3, $Y_3' = \{A\}$ and $\bar{Y}_3' = \{C, D\}$, hence $f_B(1, Y_3', \bar{Y}_3')$ and $f_B(-1, Y_3', \bar{Y}_3')$ can be estimated as follows:

$$f_B(1, Y_3', \bar{Y}_3') = p(B)p(A|B)p(\bar{C}|B)p(\bar{D}|B)$$

$$f_B(-1, Y_3', \bar{Y}_3') = p(\bar{B})p(A|\bar{B})p(\bar{C}|\bar{B})p(\bar{D}|\bar{B})$$

where $p(B)$ and $p(\bar{B})$ are shorthand for $p(B = 1)$ and $p(B = -1)$, respectively. The probability terms on the right hand side of each equation are estimated by counting the occurrences of each label in the training set. For instance, $p(B) = 0.5$ because positive B occurs twice out of the four total times B occurs. Here $p(A|B) = 1.0$ because every time B is positive, so is A. By counting occurrences in this manner, the rest of the probability terms are estimated: $p(\bar{B}) = 0.5$, $p(\bar{C}|B) = 0.5$, $p(\bar{D}|B) = 1.0$, $p(A|\bar{B}) = 0.0$, $p(\bar{C}|\bar{B}) = 0.0$, and $p(\bar{D}|\bar{B}) = 0.0$. The equations can then be evaluated as follows:

$$f_B(1, Y_3', \bar{Y}_3') = 0.5 * 1.0 * 0.5 * 1.0 = 0.25$$

$$f_B(-1, Y_3', \bar{Y}_3') = 0.5 * 0.0 * 0.0 * 0.0 = 0.0$$

If $(0.25 - 0.0) > \theta$, then it can be safely inferred that the missing label B is positive.

if $\lambda_j \notin L'$ **then**
  $L' \leftarrow L' \cup \{\lambda_j\}$
  $o_j = createOutputNode(\lambda_j)$
  $outputNodes \leftarrow outputNodes \cup \{o_j\}$
  for all $h \in hiddenNodes$ **do**
    $addWeight(h, o_j)$
  end for
end if

FIGURE 1. Psuedocode for dynamically incorporating a new label into the neural network during incremental training.

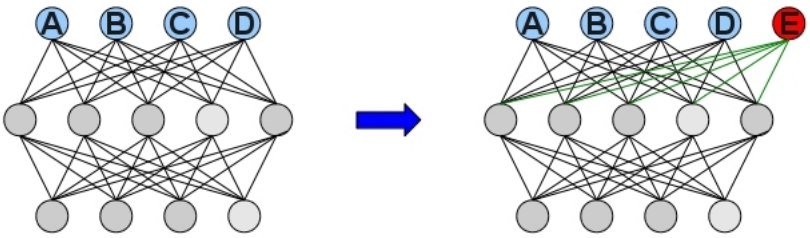


FIGURE 2. Dynamically adding a new label to the neural network during incremental training.

3.3. Incremental Learning

In incremental learning, all the possible labels that might be encountered during training are not always known *a priori*. Recall that L' is the set of all possible labels that are known at the start of training. If a previously unknown label λ is encountered where $\lambda \notin L'$, then there would be no output node in the network that corresponds to that label. To accommodate a new incoming label, a new output node is simply added to the output layer that corresponds to that label. The weights to the hidden layer are initialized randomly and the model can now begin learning this new label. Pseudocode for accommodating new incoming labels is shown in Figure 1.

As an example, if the initial training set had the possible labels $L' = \{A, B, C, D\}$, then the network would have four output nodes, one corresponding to each label. If a new label E is encountered during incremental training, E would be added to L' and a fifth output node would be dynamically created in the network with randomly initialized weights as shown in Figure 2. The BAIN algorithm can now train the network as if that output node had been known from the start. In fact, the resulting solution will be identical to the solution obtained if label E was known from the beginning. This is because no assumption of implicit negativity is made and that output node would have been ignored if the training instances did not explicitly mention E.

4. EXPERIMENTAL SETUP

Four experiments are designed to validate our proposed solution. The first experiment involves several well-known multi-label data sets that have been used in other studies and are publicly available (Tsoumakas et al., 2011). These data sets do not have missing labels; however, this enables us to artificially remove both positive and negative labels from the

TABLE 1. Data sets that are used for experimentation.

Data Set	Domain	Instances	Nominal Attributes	Numeric Attributes	Labels	Label Cardinality	Density
corel5k	text	5000	499	0	374	2.028	0.009
medical	text	978	1449	0	45	1.245	0.028
emotions	music	593	0	72	6	1.859	0.311
eron	text	1702	1001	0	53	3.378	0.064
genbase	biology	662	1186	0	27	1.252	0.046
mediamill	video	43907	0	120	101	4.376	0.043
scene	images	2407	0	294	6	1.074	0.179
yeast	biology	2417	0	103	14	4.237	0.303
triclass	artificial	1500	0	2	8	3.00	0.375
classoverlap	artificial	1500	0	2	8	1.578	0.197
DARCI	images	2101	0	102	211	3.535	0.017
Average		5706.09	375.91	63.18	77.55	2.506	0.143

data sets and then compare the results with the complete data sets. The percentage of labels that are removed can be adjusted, which allows us to evaluate how the algorithm performs with different numbers of missing labels. The second experiment involves the DARCI data set (Norton et al., 2010), which is a real world data set with a large percentage of missing labels. This second experiment shows how our solution performs with actual problems that have missing labels. The third experiment involves the specific case where there is only one positive label provided for each instance. This allows us to compare BAIN with the WIN algorithm (Whiting and Ventura, 2004), which is a multi-label learning algorithm that deals with that specific case. The fourth experiment tests how well our algorithm can learn incrementally. Using the data sets from the first set of experiments, we explicitly leave out labels and training instances from the training data and then later introduce them. The final result is then compared to a model that is trained with all the training data from the start.

4.1. Data Sets

Eight of the ten data sets used in the experiments are publicly available as part of the open source Mulan project (Tsoumakas et al., 2011). These data sets represent a variety of domains and a range of statistical properties. The remaining two data sets (triclass and classoverlap) are simple artificially generated toy problems (Whiting and Ventura, 2004). The attributes of each data set can be seen in Table 1. The table introduces two potentially unfamiliar terms used for quantifying properties of multi-label data sets. *Label Cardinality* refers to the average number of labels per instance. *Density*, or label density, is equivalent to the label cardinality divided by the number of possible labels. This metric gives an indication of how often labels are used throughout the data set.

The DARCI data set consists of 2,101 images that are labeled with adjectives that describe each image. The DARCI data set has 102 numerical features and currently 211 possible labels with a label cardinality of 3.535 and density of 0.017. Each image has, on average, only 4.7% of both positive and negative labels; the rest are unknown. Additionally, data is

TABLE 2. Parameters used for the neural network based algorithms BAIN, BPMLL, WIN, and binary relevance. The number of hidden nodes for binary relevance are shown as hidden nodes per model, where the number of models is equal to the number of possible labels in the data set.

			Number of Hidden Nodes	
Data Set	**Epochs**	**Learning Rate**	**BAIN, WIN, BP-MLL**	**Binary Relevance**
corel5k	100	.01	256	2
medical	100	.01	128	10
emotions	100	.01	96	10
eron	100	.01	128	10
genbase	100	.01	256	10
mediamill	100	.01	128	10
scene	100	.01	96	10
yeast	100	.05	96	10
triclass	100	.10	16	2
classoverlap	100	.10	16	2
DARCI	200	.01	128	10

continually being collected, and new labels (or adjectives) are continually being added. This makes the DARCI data set ideal for testing our solution as it is a real world example of the problems we are trying to solve.

4.2. Algorithms

For a baseline comparison in the first three experiments, popular multi-label algorithms which include BP-MLL (Zhang and Zhou, 2006), Binary Relevance (Tsoumakas and Katakis, 2007) and ML-kNN (Zhang and Zhou, 2005) are used. Two versions of the BAIN algorithm are also compared. The first is the full algorithm as described in Chapter 3. The second is a version that does not infer missing labels and is referred to as BAIN_nopred. This allows us to evaluate how effective our method is at inferring missing labels, as opposed to only removing the assumption of implicit negativity. Additionally, an untrained model that is random in its label predictions will be used to provide an overall baseline for comparison.

The number of k-nearest neighbors for the ML-kNN algorithm is the same for each data set at $k = 5$. The binary relevance method uses standard single-label backpropagation as its base algorithm. The various parameters used by each neural network based algorithm for each data set can be seen in Table 2. These parameters are not necessarily optimal for each algorithm; reasonable parameters were chosen based on simple trial runs with each data set in order to increase the overall score across all metrics. The neural network parameters were calibrated with the BPMLL algorithm and then used for all neural network based algorithms. The number of hidden nodes for binary relevance were chosen so that the total number of connections from all the resulting neural networks are roughly the same as in the single BPMLL network. Previous studies have shown that choosing hidden nodes this way for binary relevance reduces training time while still allowing binary relevance to perform better than BPMLL (Skabar et al., 2006; Heath et al., 2010).

4.3. Evaluation Metrics

Empirically evaluating multi-label problems is more complicated than evaluating single-label problems, as there are different degrees of correctness. Multi-label evaluation metrics fall into two main categories: *prediction-based* and *ranking-based*. Prediction-based metrics evaluate how well the algorithm predicts the actual set of correct labels for each instance. Ranking-based metrics evaluate how well the algorithm ranks the labels relative to one another. The correct labels should be ranked higher than the incorrect labels. The same notation as established in Chapter 1 will be used to formalize our evaluation metrics. In addition, given an instance x_i, the set of predicted labels is denoted as Z_i, while the predicted rank of a label λ is denoted as $r_i(\lambda)$. We will use the following standard multi-label prediction-based evaluation metrics (Tsoumakas et al., 2010) with 10-fold cross validation as we compare each algorithm:

Hamming Loss is the average percentage of correct labels not predicted and incorrect labels predicted.

$$HammingLoss = \frac{1}{m}\sum_{i=1}^{m}\frac{|Y_i \Delta Z_i|}{q}$$

where Δ is the set symmetric difference operator and q is the total number of possible labels.

Accuracy is the average percentage of true positives out of the total true positives, false positives, and false negatives.

$$Accuracy = \frac{1}{m}\sum_{i=1}^{m}\frac{|Y_i \cap Z_i|}{|Y_i \cup Z_i|}$$

Precision is the average percentage of predicted labels that were correct.

$$Precision = \frac{1}{m}\sum_{i=1}^{m}\frac{|Y_i \cap Z_i|}{|Z_i|}$$

Recall is the average percentage of correct labels that were predicted.

$$Recall = \frac{1}{m}\sum_{i=1}^{m}\frac{|Y_i \cap Z_i|}{|Y_i|}$$

We will use the following standard multi-label ranking-based evaluation metrics (Schapire and Singer, 2000; Zhang and Zhou, 2006) with 10-fold cross validation as we compare each algorithm:

One-Error is the percentage of top ranked labels that are not in the set of correct labels.

$$OneError = \frac{1}{m}\sum_{i=1}^{m}\delta_i(\operatorname*{argmin}_{\lambda \in L} r_i(\lambda))$$

where

$$\delta_i(\lambda) = \begin{cases} 1, \text{ if } \lambda \notin Y_i \\ 0, \text{ otherwise} \end{cases}$$

Coverage is how far, on average, we need to go down the list of predicted labels in order to

cover all the correct labels. It is normalized between 0 and 1.

$$Coverage = \frac{1}{m}\sum_{i=1}^{m}\frac{\omega_i - |Y_i|}{q - |Y_i|}$$

where

$$\omega_i = \max_{\lambda \in Y_i} r_i(\lambda)$$

Ranking Loss is the average percentage of incorrect labels that are ranked higher than correct labels.

$$RankingLoss = \frac{1}{m}\sum_{i=1}^{m}\frac{1}{|Y_i||\bar{Y}_i|}|\{(\lambda_a, \lambda_b) : r_i(\lambda_a) > r_i(\lambda_b), (\lambda_a, \lambda_b) \in Y_i \times \bar{Y}_i\}|$$

Each of these seven metrics tell us different things about the performance of the multi-label algorithm. In order to provide a single metric that at least partially captures all these different aspects, an additional metric is added that averages the previous seven together. For the metrics that are to be minimized instead of maximized, one minus the value is done in the averaging. This metric is called the *Overall Average*.

When comparing one learning model to another, it is important to have confidence that one model truly outperforms the other. One way to do this is to measure how statistically significant the difference is between their performance on each metric. This significant difference can be measured using the *paired permutation test*. The paired permutation test outputs a *p-value* between 0 and 1; the higher the *p*-value, the less statistically significant the difference is between two models. It is common convention that a *p*-value less than 0.05 means that it can be said with confidence that one model outperforms the other. The paired permutation test can only compare two models at a time; hence, for each metric, the paired permutation test is only calculated between the BAIN algorithm and the next best performing algorithm.

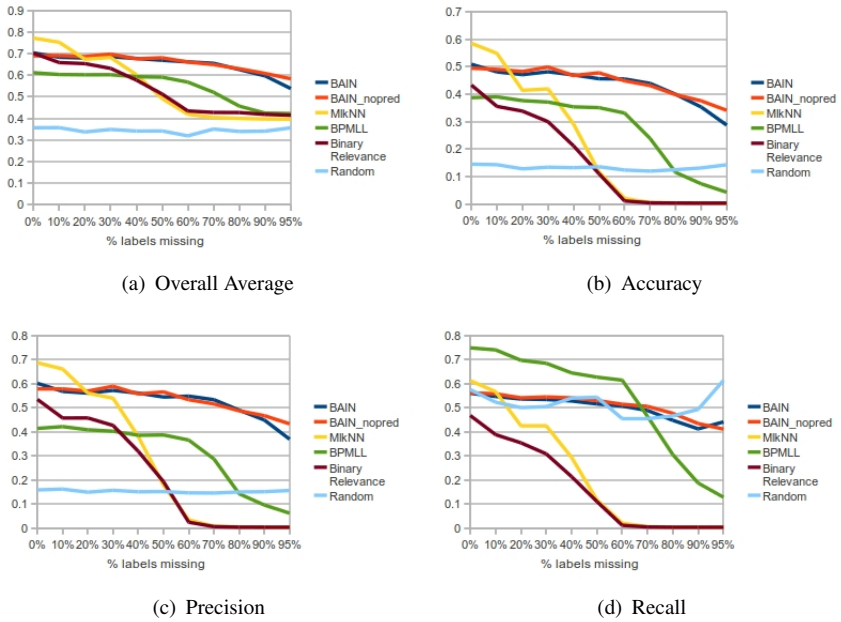
5. RESULTS

This chapter presents the results of the four experiments described in Chapter 4. The first experiment involves artificially removing an incremental percentage of labels in the training data. The second experiment uses the DARCI data set, which is a real world problem with a high percentage of missing labels. The third experiment considers the case where each training instance has exactly one positive label with all other labels unknown. The fourth experiment evaluates how well the BAIN algorithm can learn incrementally. Finally, the on-line multi-label Bayesian algorithm described in Section 2.3 is compared to the BAIN algorithm.

5.1. Artificially Removing Labels

The first experiment involves the ten data sets described in Section 4.1. Each algorithm is run on each data set using 10-fold cross validation. For each fold, a certain percentage of the labels are artificially removed from the training data. The model is trained with this modified training data and then evaluated using test data that still has all the labels present. The percentage of labels that are removed changes in 10% increments from 0% to 90%. An additional run at 95% is also performed because 95% is close to the percentage of missing labels in the DARCI data set. The results from all ten data sets are averaged for each algorithm and for each evaluation metric. The results for overall average, accuracy, precision and recall can be seen in Figure 3. The results for Hamming loss, one-error, coverage, and

ranking loss can be seen in Figure 4. The paired permutation test was performed for each of these metrics between the best version of BAIN (BAIN_nopred) and the best other algorithm (non-BAIN). The paired permutation test results for each metric can be seen in Figures 5 and 6.



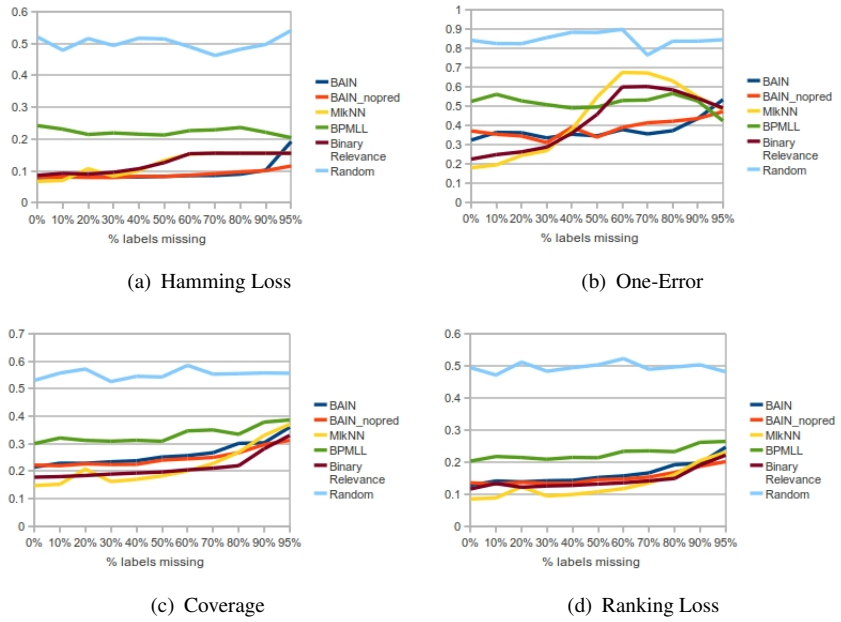
(a) Overall Average (b) Accuracy

(c) Precision (d) Recall

FIGURE 3. Average results of 10 different data sets as the percentage of missing labels increases (higher is better for these metrics). As more labels are removed, the performance of the other algorithms decreases rapidly, while the BAIN algorithm appears much more robust to missing labels and its performance decreases much more slowly.

When all labels are present, the BAIN algorithm does well, but is not the best. However, as labels are removed, the performance of the other algorithms decreases rapidly, while the BAIN algorithm appears much more robust to missing labels and its performance decreases much more slowly. In some cases, as with the MLkNN algorithm, when the percentage of labels missing reaches a threshold it stops predicting any labels as evidenced by the precision and recall dropping to zero. By the time 95% of the labels are missing, the BAIN algorithm outperforms all other algorithms for almost every metric, and does so by a considerable margin for accuracy, precision, and recall as shown in Figure 3. It should be mentioned that for recall, the random baseline ends up performing the best. This is because recall only measures the percentage of all the positive labels that are predicted. As more labels are missing, each algorithm predicts fewer labels, while the random baseline will always predict around 50% of the labels.

It is important to note that there is little difference in performance between the original BAIN algorithm and the BAIN algorithm without the naïve Bayes label prediction (BAIN_nopred). However, at the 95% missing labels threshold BAIN_nopred actually performs better and hence is the version of BAIN used in the paired permutation tests. These results show that our naïve Bayes method for inferring missing labels yields little benefit and even hurts our performance when the amount of missing labels exceeds 95%. In practice, it would therefore be better to not include the naïve Bayes approach as it requires more processing time, without any benefit.



(a) Hamming Loss

(b) One-Error

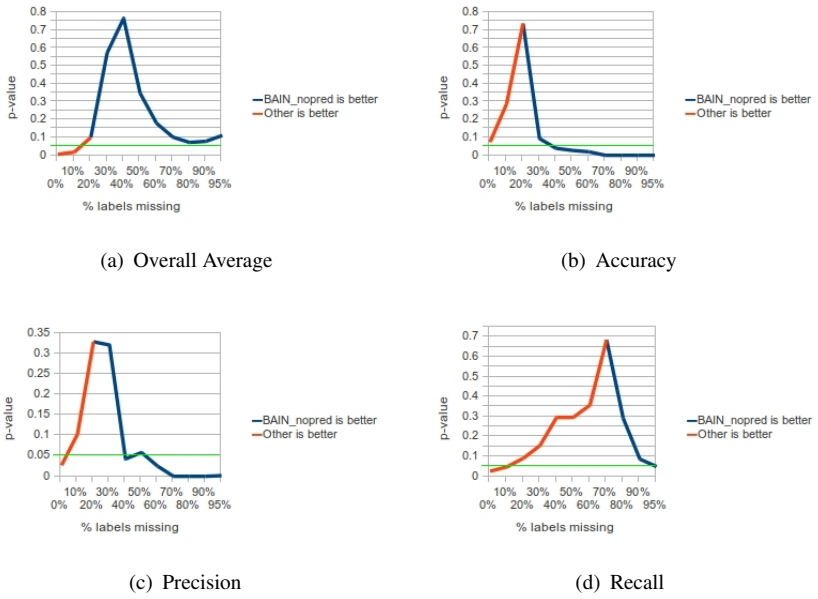
(c) Coverage

(d) Ranking Loss

FIGURE 4. Average results of 10 different data sets as the percentage of missing labels increases (lower is better for these metrics). The BAIN algorithm outperforms almost all other algorithms by the time 95% of the labels are missing.

The paired permutation test results (Figures 5 and 6) show BAIN_nopred compared to the best non-BAIN algorithm. It should be noted that the best non-BAIN algorithm at each interval is used in the permutation test. For example, with precision, MLkNN is used at 0% missing labels and BPMLL is used at 95% missing labels. This puts BAIN at a disadvantage for the paired permutation test, which makes the results more significant when BAIN performs better. The red line indicates that the other algorithm is performing better than BAIN on average across all datasets, while the blue line indicates that BAIN is performing better on average across all datasets. When all labels are present, the p-value is below 0.05 and red for all metrics, which means that the BAIN algorithm starts off performing worse than the best other algorithm. However, as the percentage of missing labels increases, the p-values also increase, which means there is less and less confidence in the difference between BAIN and the best other algorithm. At some threshold the p-values change to blue, indicating that BAIN is now the best performing algorithm. This transition can be seen in Figures 3 and 4 when the BAIN algorithm crosses with the best other algorithm.

By the time 95% of the labels are missing, the p-values are blue and less than 0.05 for accuracy, precision, and recall. This means that we can confidently say that the BAIN algorithm outperforms the other algorithms for those metrics. For the ranking-based metrics and Hamming loss, however, the p-values are still quite high. This means that, even though the BAIN algorithm is performing better on those metrics, there is still uncertainty in how significant that difference is. This uncertainty can be expected for ranking-based metrics because a complete ranking is much more challenging to get correct than the binary prediction of labels. With coverage and ranking loss, that uncertainty is more prominent, which is why their p-values take longer to change to blue. With Hamming loss and one-error, the p-values drop close to 0.05 at around 50% - 60% missing labels with BAIN performing better; however, the p-values then go back up. This indicates that, for Hamming loss and one-error, there is a certain range of missing labels that BAIN confidently performs better at. At this



(a) Overall Average (b) Accuracy

(c) Precision (d) Recall

FIGURE 5. Paired permutation test results between BAIN_nopred and the best other algorithm corresponding to the metrics in Figure 3. The green line at 0.05 denotes statistical significance. When 95% of the labels are missing, the p-value is below 0.05 for accuracy, precision and recall, which means that there is high confidence that the difference between BAIN and the best other algorithm is statistically significant for those metrics.

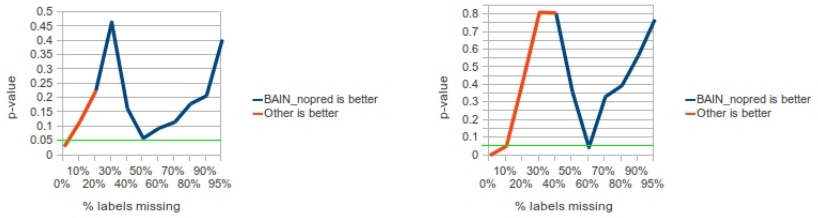
point, it is not clear why that particular range of missing labels (50% - 60%) is better for BAIN on Hamming loss and one-error.

5.2. The DARCI Data Set

The second experiment involves the DARCI data set, which is a real world problem that has missing labels. As mentioned before, approximately 95.3% of the labels are missing in the DARCI data set. This makes evaluation more challenging because the test sets used at each fold are also missing labels. The evaluation metrics can only be applied to labels that are actually known. While this limitation does not give us a complete measure of performance, it stills gives us general insight into how well each algorithm performs relative to one another. The results for overall average, accuracy, precision, and recall can be seen in Figure 7. The results for Hamming loss, one-error, coverage, and ranking loss can be seen in Figure 8. The paired permutation test was performed between the best BAIN (BAIN_nopred) and the best non-BAIN algorithm and the results for each metric can be seen in Table 3.

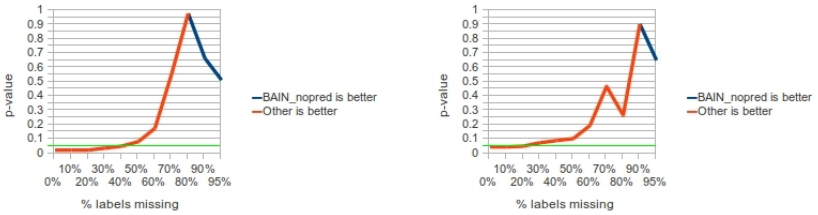
The results show that BAIN without label prediction is the clear winner in every metric. Normal BAIN and BPMLL are the next best and perform equally well overall, with BPMLL doing better on Hamming loss and one-error and BAIN doing better on accuracy and recall. MLkNN and binary relevance, however, perform no better than random overall. All algorithms do better than random with Hamming loss and all the ranking based metrics. The paired permutation test results show p-values less than 0.05 for all metrics, which means that the difference in performance between BAIN without label prediction and the best other algorithm is statistically significant.

With the DARCI data set, it appears that inferring missing labels hurts the performance



(a) Hamming Loss

(b) One-Error



(c) Coverage

(d) Ranking Loss

FIGURE 6. Paired permutation test results between BAIN_nopred and the best other algorithm corresponding to the metrics in Figure 4. The green line at 0.05 denotes statistical significance. The p-value is never below 0.05 when BAIN is better, which means that there is little confidence in how significant the difference is between BAIN and the best other algorithm for these metrics.

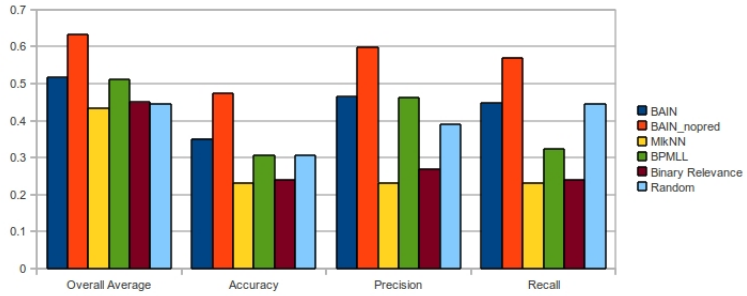


FIGURE 7. Results of the DARCI data set for overall average, accuracy, precision, and recall (higher is better for these metrics). BAIN without label prediction performs better on every metric than all the other algorithms.

of the BAIN algorithm, whereas in the previous experiment it didn't seem to affect the performance. A reason for this could be due to the previously mentioned limitation of not having a test set without missing labels. A full test set may reveal that label prediction makes no difference for the DARCI data set. A more likely explanation, however, could be the fact that our naïve Bayes method for inferring missing labels relies on at least some of the labels being present in order to make any kind of accurate inference on the labels that are missing. Having only 5% of the labels present in the data simply may not be enough for an accurate prediction and hence many of the predictions are inaccurate and the resulting performance is worse. There is evidence from the previous experiment to support this. If we refer back to

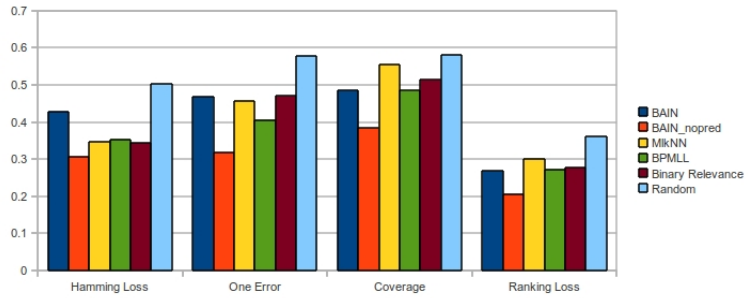


FIGURE 8. Results of the DARCI data set for Hamming loss, one-error, coverage, and recall (lower is better for these metrics). BAIN without label prediction performs better on every metric than all the other algorithms.

TABLE 3. Paired permutation test results between BAIN_nopred and the best non-BAIN algorithm for the DARCI data set corresponding to Figures 7 and 8. The best non-BAIN method for Hamming loss is binary relevance, while BPMLL is the best non-BAIN method for all other metrics. The p-values are below 0.05 for all metrics, which means that there is high confidence that the difference between BAIN and the best other algorithm is statistically significant.

	Overall Average	**Accuracy**	**Precision**	**Recall**
***p*-value**	0.00098	0.00098	0.00098	0.00098
	Hamming Loss	**One-Error**	**Coverage**	**Ranking Loss**
***p*-value**	0.00293	0.00098	0.00098	0.00098

Figure 3 and Figure 4, we can see that the performance of BAIN at 95% missing labels is worse than BAIN without label prediction for every metric except recall.

5.3. Only One Positive Label

The third experiment involves the specific case where each training instance has exactly one positive label with all other labels being unknown. This allows us to compare the BAIN algorithm to the WIN algorithm, which was designed for this specific case, in addition to the other algorithms previously used. Using the same ten data sets from Section 4.1 and 10-fold cross validation, we artificially remove all labels except for one randomly chosen positive label from each instance of the training data. The algorithms are then evaluated using the fully labeled test set. This experiment will only use the version of BAIN without label prediction (BAIN_nopred) as it was shown in the previous two experiments to perform better than BAIN with label prediction. To further demonstrate BAIN's reliance on at least some explicitly given negative labels, the BAIN algorithm will also be run on the ten data sets where a randomly chosen negative label is provided for each instance in addition to the positive label. The results from all ten data sets are averaged over each algorithm and for each metric. The results for overall average, accuracy, precision, and recall can been seen in Figure 9. The results for Hamming loss, one-error, coverage, and ranking loss can be seen in Figure 10. The paired permutation test results between BAIN with one positive label and the best non-BAIN algorithm can be seen in Table 4. The paired permutation test results between the best non-BAIN algorithm and BAIN with one positive and one negative label can be seen in Table 5.

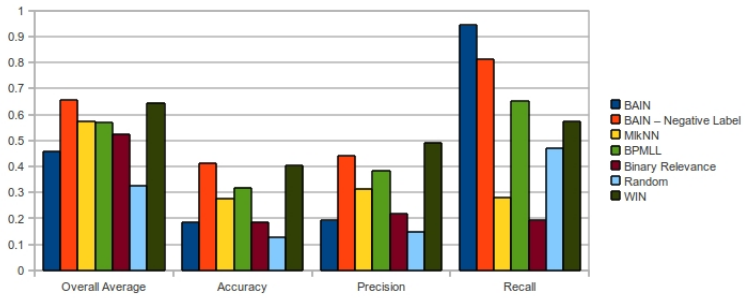


FIGURE 9. Results for overall average, accuracy, precision, and recall when there is only one positive label for each training instance (higher is better for these metrics). With the exception of recall, BAIN performs worse than the other algorithms. However, when BAIN is given at least one negative label per training instance, it performs comparable to the WIN algorithm.

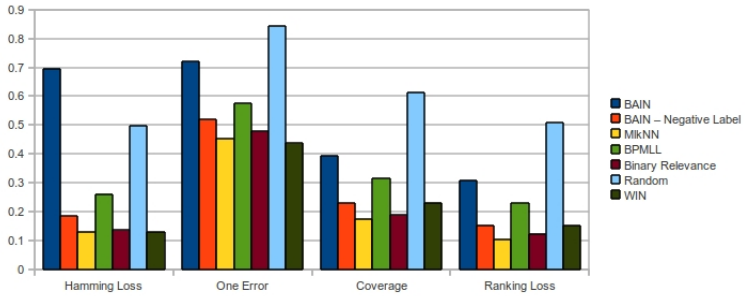


FIGURE 10. Results of Hamming loss, one-error, coverage and ranking loss when there is only one positive label for each training instance (lower is better for these metrics). BAIN performs worse than the other algorithms. However, when at least one additional negative label per training instance is given to BAIN, its performance increases to be competitive with the other algorithms.

The results show that the BAIN algorithm, although better than random, performs worse than the other algorithms for all metrics except recall. This experiment exposes BAIN's main weakness of relying on at least some explicitly given negative labels being present in the training data. The other algorithms do not suffer from this weakness as they automatically assume any missing label to be negative. However, if at least one negative label per training instance is present, then the performance of BAIN improves considerably and is comparable to the WIN algorithm. The paired permutation test results in Table 5 show no significant difference between BAIN with a single negative label and the best non-BAIN algorithm for all metrics except recall, where BAIN is superior. Adding an explicit negative label makes no difference to the other algorithms because that label is already assumed to be negative. In general, explicit negative labels are harder to acquire than positive labels. However, it may not be unreasonable to require that there be at least one negative label provided for each training instance when using the BAIN algorithm. This is because there are usually far more negative labels per instance than positive labels. Table 1 shows that the average density of all the data sets we have used is 0.143, which means that only 14.3% of the possible labels are positive, while the remaining 85.7% are negative.

TABLE 4. Paired permutation test results between BAIN with only one positive label and the best non-BAIN algorithm corresponding to Figures 9 and 10. BPMLL is the best non-BAIN algorithm for recall, MLkNN is the best non-BAIN algorithm for coverage and ranking loss, while WIN is the best non-BAIN algorithm for all other metrics. All the *p*-values are less than 0.05, which means that there is high confidence that the difference between BAIN and the best non-BAIN algorithm is statistically significant, with BAIN performing worse.

	Overall Average	**Accuracy**	**Precision**	**Recall**
***p*-value**	0.00098	0.00684	0.00293	0.00293
	Hamming Loss	**One-Error**	**Coverage**	**Ranking Loss**
***p*-value**	0.00098	0.00684	0.00293	0.00293

TABLE 5. Paired permutation test results between BAIN with a negative label and the best non-BAIN algorithm corresponding to Figures 9 and 10. BPMLL is the best non-BAIN algorithm for recall, MLkNN is the best non-BAIN algorithm for coverage and ranking loss, while WIN is the best non-BAIN algorithm for all other metrics. With the exception of recall, none of the *p*-values are less than 0.05, which means that there is little confidence that the difference between BAIN with a negative label and the best non-BAIN algorithm is statistically significant.

	Overall Average	**Accuracy**	**Precision**	**Recall**
***p*-value**	0.49902	0.70996	0.21973	0.01660
	Hamming Loss	**One-Error**	**Coverage**	**Ranking Loss**
***p*-value**	0.15723	0.10645	0.13184	0.06934

5.4. Incremental Learning

The fourth experiment is designed to evaluate the incremental learning capabilities of the BAIN algorithm and again involves 10-fold cross validation and the ten data sets described in Section 4.1. The incrementally trained model is compared with a model that was trained with the entire data set from the start. Due to the iterative nature of backpropagation, labels that are introduced later in the training process have less influence on the resulting model. Hence, in order for the performance of the two models to be comparable, we do the incremental training in a specific way that allows new labels just as much influence as the labels known from the beginning.

To illustrate this, consider an example with the possible labels $L = \{A, B, C, D\}$ and training set:

$$T = \begin{cases} x_1 \to A, \bar{B}, \bar{C}, \bar{D} \\ x_2 \to \bar{A}, \bar{B}, C, D \\ x_3 \to A, B, \bar{C}, \bar{D} \\ x_4 \to \bar{A}, \bar{B}, C, \bar{D} \end{cases}$$

First, the training data is shuffled and split in half.

$$T_1 = \begin{cases} x_2 \to \bar{A}, \bar{B}, C, D \\ x_3 \to A, B, \bar{C}, \bar{D} \end{cases}$$

$$T_2 = \begin{cases} x_1 \to A, \bar{B}, \bar{C}, \bar{D} \\ x_4 \to \bar{A}, \bar{B}, C, \bar{D} \end{cases}$$

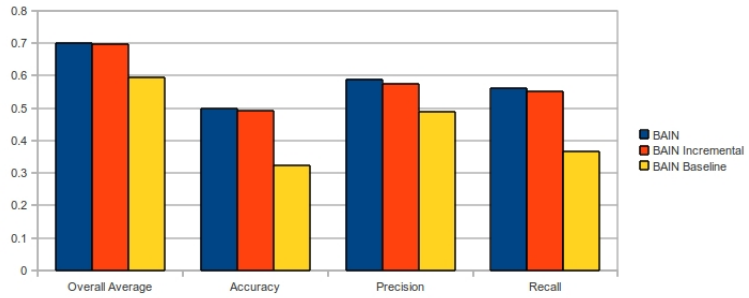


FIGURE 11. Results of incremental training versus non-incremental for overall average, accuracy, precision, and recall (higher is better for these metrics). The BAIN that has been trained incrementally performs comparable to the BAIN that has been trained with all the data from the start.

Some labels are randomly chosen and removed from each instance of the first half of the training data (the same labels are chosen for each fold). (In the actual experiment, we removed 5 labels).

$$T_1 = \begin{cases} x_2 \rightarrow \bar{A}, \bar{B} \\ x_3 \rightarrow A, B \end{cases}$$

$$T_2 = \begin{cases} x_1 \rightarrow A, \bar{B}, \bar{C}, \bar{D} \\ x_4 \rightarrow \bar{A}, \bar{B}, C, \bar{D} \end{cases}$$

Each instance of the first half of the training data is then added to the second half with only the removed labels provided. This is to ensure that the model will eventually see the labels that were removed.

$$T_1 = \begin{cases} x_2 \rightarrow \bar{A}, \bar{B} \\ x_3 \rightarrow A, B \end{cases}$$

$$T_2 = \begin{cases} x_1 \rightarrow A, \bar{B}, \bar{C}, \bar{D} \\ x_4 \rightarrow \bar{A}, \bar{B}, C, \bar{D} \\ x_2 \rightarrow C, D \\ x_3 \rightarrow \bar{C}, \bar{D} \end{cases}$$

The BAIN algorithm is trained using T_1 and is unaware that the removed labels exist. After initial training, the model is then trained with T_2. The removed labels are introduced to the model at the same time and the model must learn incrementally as described in Section 3.3.

This incrementally trained model is then compared with a model that was trained with the entire data set from the start. A version of BAIN that does not learn incrementally is also used as a baseline comparison. Most multi-label learning algorithms that do not handle new incoming labels will either crash, or ignore the new label. This version of BAIN just ignores any new labels during training. During evaluation, the removed labels are never predicted and are always ranked at the bottom. The results from all ten data sets are averaged for each model. The results for overall average, accuracy, precision and recall can be seen in Figure 11. The results for Hamming loss, one-error, coverage, and ranking loss can be seen in Figure 12. The paired permutation test results between the incrementally trained BAIN and the BAIN trained with all the data from the start can be seen in Table 6. The paired permutation test results between the incrementally trained BAIN and the non-incremental baseline BAIN can be seen in Table 7.

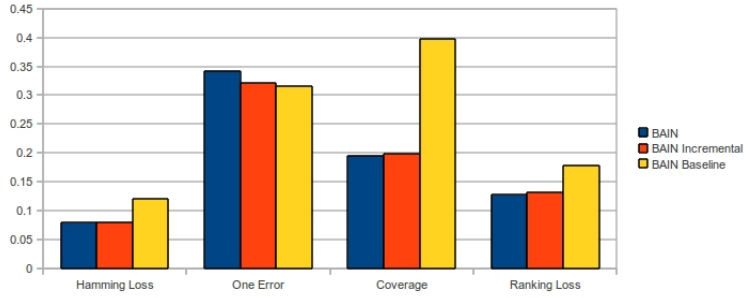


FIGURE 12. Results of incremental training versus non-incremental for Hamming loss, one-error, coverage, and recall (lower is better for these metrics). The BAIN that has been trained incrementally performs comparable to the BAIN that has been trained with all the data from the start.

TABLE 6. Paired permutation test results between the BAIN that has been trained incrementally and the BAIN that has been trained with all the data from the start corresponding to Figures 11 and 12. All the p-values are high, indicating that there is no significant difference between their performances.

	Overall Average	**Accuracy**	**Precision**	**Recall**
***p*-value**	0.55176	0.72363	0.50293	0.31348
	Hamming Loss	**One-Error**	**Coverage**	**Ranking Loss**
***p*-value**	0.62402	0.26465	0.55567	0.09277

TABLE 7. Paired permutation test results, corresponding to Figures 11 and 12, between the BAIN that has been trained incrementally and the baseline BAIN that cannot handle new incoming labels. With the exception of one-error and ranking loss, the p-values are low, which means there is high confidence that the difference between these two models is statistically significant.

	Overall Average	**Accuracy**	**Precision**	**Recall**
***p*-value**	0.03613	0.03223	0.10254	0.08691
	Hamming Loss	**One-Error**	**Coverage**	**Ranking Loss**
***p*-value**	0.07324	0.89941	0.00488	0.24707

As expected, the results show little significant difference in performance between the model that was trained incrementally and the model that was trained with all the data from the start. The BAIN algorithm can handle new incoming labels during incremental training, and the resulting model achieves similar performance to a model trained with the new labels from the beginning. The non-incremental baseline model performs worse than the incremental model for every metric except one-error. The paired permutation test results for these two models in Table 7 show a significant difference for all metrics except for one-error, ranking loss, recall, precision, and Hamming loss, although Hamming loss, precision, and recall are close to 0.05. The reason one-error actually performs slightly better is because one-error only measures when the top ranked label is a false positive. The five removed labels are never

given the chance to be false positives and are never ranked at the top and hence never count against one-error. With the exception of one-error, the results clearly show that accounting for new incoming labels during incremental training significantly improves the performance.

5.5. Comparing with the Bayesian Model

The on-line Bayesian multi-label learning algorithm (Qi et al., 2009) discussed in Section 2.3 was not included in the previous experiments because it is strictly an on-line learning method and its inefficiency on problems with a large number of possible labels. However, in their paper, the authors use the yeast and scene data sets, which are two of the data sets used in our experiments (see Table 1). We can, therefore, compare our results on those data sets with the results achieved in their paper. The authors use the $F1$ score to evaluate their algorithm, which is defined as:

$$F1 = \frac{2pr}{p + r}$$

where p and r are precision and recall respectively.

Using their Bayesian active learning approach on the yeast data set, they were able to achieve an $F1$ score of 0.58. The BAIN algorithm, using ten-fold cross validation with all the labels provided, achieved an $F1$ score of 0.64. However, on the scene data set, they had an $F1$ score of 0.91, while the BAIN algorithm only achieved 0.70. Clearly there are trade-offs between the two algorithms. The results indicate that the Bayesian algorithm may be better for data sets with a small number of possible labels, while the BAIN algorithm can better handle problems with a large number of possible labels. The Bayesian algorithm is strictly an on-line learner, so if the training has to be restarted, it can become intractable to retrain the model with the whole training set. The BAIN algorithm is more flexible as it can learn incrementally or with all the data at once.

6. CONCLUSIONS AND FUTURE WORK

The BAIN algorithm is successful at improving multi-label classification performance for problems where the labeling is incomplete. We have shown that, compared to other multi-label algorithms, the BAIN algorithm is more robust in performance as the percentage of missing labels increases. On the DARCI data set, which is a real world problem that has missing labels, we have shown that the BAIN algorithm successfully performs better than other multi-label learning algorithms. We have also shown that the BAIN algorithm can learn incrementally and handle new labels that were previously unknown with hardly any loss of performance.

The naïve Bayes method to infer missing labels was shown to be ineffective and even detrimental in the case of the DARCI data set. Either the labels that are inferred are redundant and make little difference, or there are not enough provided labels to accurately infer the missing labels. In either case, it is clear that the BAIN algorithm without this label inference method is the better choice. Further research would be useful in discovering other methods that could be more effective than the naïve Bayes approach.

The BAIN algorithm was shown to perform poorly when there are no explicitly given negative labels in the training data. However, one negative label provided per training instance is enough to significantly increase BAIN's performance to be competitive with the WIN algorithm. This requirement may not be unreasonable as there are far more possible negative labels than positive labels for each training instance. Additional research needs to be done on multiple real-world data sets with missing labels to better determine how plausible that requirement is. The WIN algorithm performed well when only one positive label

was provided per training instance. Additional research could extend the WIN algorithm to handle data sets with any number of provided labels, both positive and negative. The BAIN algorithm could be extended to overcome its weakness of requiring at least some explicitly given negative labels. However, there would likely be a trade-off because the point of the BAIN algorithm is to avoid assumptions about missing data.

The BAIN algorithm was shown to have trade-offs compared to the on-line multi-label Bayesian model (Qi et al., 2009). The BAIN algorithm can handle problems with a large number of possible labels, while the Bayesian model is inefficient on these problems. This is likely because the Bayesian algorithm explicitly attempts to model the higher order relationships between labels. While this is a significant advantage on problems with a small number of possible labels (such as the scene data set), it is too slow for large sets of possible labels. Additional research needs to be done to see how the BAIN algorithm could benefit from trying to model these higher order relationships.

Removing the assumption of implicit negativity is effective in improving multi-label classification performance for the backpropagation algorithm. Other multi-label algorithms, such as MLkNN, could be modified to remove that assumption, or adapted in other ways to handle missing labels. Instead of trying to infer the missing labels for each training instance, active learning approaches could be used to provide additional training instances for the labels not adequately represented in the current data set. Additional research could be done to find other applications where BAIN could be useful. For example, the BAIN algorithm might be applicable to the frequent itemset mining problem (Bodon, 2006; S. and Vyas, 2010). There are many opportunities for future research in this area; the BAIN algorithm provides a stepping stone as a simple yet effective solution to problems with missing labels.

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