

Context-Aware MIML Instance Annotation

Forrest Briggs, Xiaoli Z. Fern, Raviv Raich

School of Electrical Engineering & Computer Science, Oregon State University, Corvallis, Oregon, 97331

Email: briggssf@eecs.oregonstate.edu, xfern@eecs.oregonstate.edu, raich@eecs.oregonstate.edu

Abstract—In multi-instance multi-label (MIML) instance annotation, the goal is to learn an instance classifier while training on a MIML dataset, which consists of bags of instances paired with label sets; instance labels are not provided in the training data. The MIML formulation can be applied in many domains. For example, in an image domain, bags are images, instances are feature vectors representing segments in the images, and the label sets are lists of objects or categories present in each image. Although many MIML algorithms have been developed for predicting the label set of a new bag, only a few have been specifically designed to predict instance labels. We propose MIML-ECC (ensemble of classifier chains), which exploits bag-level context through label correlations to improve instance-level prediction accuracy. The proposed method is scalable in all dimensions of a problem (bags, instances, classes, and feature dimension), and has no parameters that require tuning (which is a problem for prior methods). In experiments on two image datasets, a bioacoustics dataset, and two artificial datasets, MIML-ECC achieves higher or comparable accuracy in comparison to several recent methods and baselines.

I. INTRODUCTION

Instance annotation for multi-instance multi-label (MIML) data is a recent and little-studied problem for supervised classification. A MIML dataset consists of bags of instances paired with sets of labels. For example, in an image domain, a bag is an image, the instances in the bag are feature vectors describing regions, and the label set for a bag indicates which objects or categories the image contains. There are many algorithms that train a classifier on a MIML dataset to predict the label set for a new bag (e.g., the original formulation of MIML by [33]). In contrast, MIML instance annotation aims to train a classifier on a MIML dataset to **predict the instance labels**. For example, we train a classifier on images paired with sets of objects they contain, then predict the class label for each region of a new image.

MIML instance annotation differs from the traditional MIML problem of label set prediction (e.g., M^3 MIML [30]), and multi-label classification (MLC, e.g., binary relevance). In particular, it is commonly assumed that each instance only belongs to one class, thus the predictions to be made are single labels for instances, not label sets. An appropriate objective for MIML instance annotation is to maximize instance-level accuracy (the fraction of correctly classified instances). However, it is not possible to train a model that directly optimizes accuracy on the training data, because instance labels are not available for training. Sometimes it

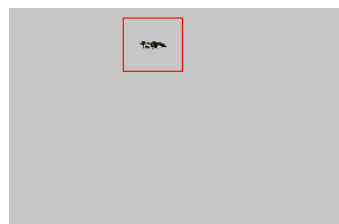


Figure 1. Inductive instance annotation without context – “What class is the region of pixels inside the red box?”

is possible to modify a MIML or MLC algorithm that is designed for label set prediction, to predict instance labels. The problem with this approach is that the model is optimized for label set accuracy, not instance accuracy. Domain-specific instance annotation problems (e.g., for images) have been widely explored, however, to our knowledge only two prior studies have specifically considered the general domain-independent MIML instance annotation problem [3, 4]. Briggs et al. [3, 4] proposed rank-loss Support Instance Machines (SIM), a collection of SVM-style algorithms that learn a linear instance classifier by minimizing a rank loss objective on bag-level labels.

Prior work [3, 4] has observed that the rank-loss SIM algorithms, as well as several other baseline methods, achieve lower accuracy for inductive classification of instances (predicting instance labels for previously unseen bags) in comparison to transductive classifications (predicting instance labels for bags with known label sets). We hypothesize that one way to improve the performance of inductive classification is to exploit the contextual information provided by other instances in the same bag.

Figure 1 illustrates the importance of using context in inductive instance annotation. The region of pixels inside the red box is an instance. A MIML instance annotation classifier might be asked to predict the class label of this instance. Without the context provided by the rest of the image, it is hard to classify, even for a human. Figure 2 shows the rest of the image. With this context available, it is much easier to recognize the instance. The situation illustrated by Fig. 1 is how inductive MIML instance annotation is posed in prior work [3, 4]. It is not as important to use the context provided by other instances in the same bag for transductive classification, because the bag label set is already known, and provides a similar kind of context. Consider the same example in Fig. 1. If we know that the

image contains labels “cow” and “grass,” we do not need to see the rest of the image to conclude that the label for this instance should be “cow.”



Figure 2. Inductive instance annotation with context – “What class is the region of pixels inside the red box?” This image is from the VOC12 data.

This paper proposes a new algorithm for MIML instance annotation designed to improve inductive instance classification accuracy by exploiting the context provided by other instances in the same bag. In particular, we capture the context by modeling label correlations in the bag label set. The proposed algorithm is a multi-instance multi-label ensemble of classifier chains, called MIML-ECC (Sec. IV). MIML-ECC has no “tuning” parameters (which are necessarily selected by a heuristic in prior work) (Sec. V-D), and is asymptotically efficient in all dimensions of a problem (number of bags, instances, classes, and feature dimension) (Sec. IV-D). The training algorithm is closely related to EM (Sec. IV-C), and the classification algorithm selects the maximum a posteriori (MAP) instance label as estimated by the ensemble (Sec. IV-B). Experiments show that MIML-ECC achieves higher accuracy than several recent methods and baselines, including Hamming, rank, and ambiguous-loss SVMs, and comparable accuracy to a recent graphical model (Sec. V-E). Further experiments show that the chain structure outperforms binary relevance (Sec. V-F), and an ensemble of chains outperforms a single chain (Sec. V-G).

II. PROBLEM STATEMENT

Our goal is to learn an instance-level classifier by training on a MIML dataset consisting of n bags paired with their corresponding label sets $\{(B_1, Y_1), \dots, (B_n, Y_n)\}$, where B_i is a bag, $Y_i \subseteq \mathcal{Y} = \{1, \dots, c\}$ is its label set, and c is the total number of classes. Each bag B_i contains n_i instances, i.e., $B_i = \{\mathbf{x}_{i1}, \dots, \mathbf{x}_{in_i}\}$, $\mathbf{x} \in \mathcal{X} = \mathbb{R}^d$.

We assume that each instance \mathbf{x} in B_i has a single label $y \in \mathcal{Y}$. The instance labels are not available in the training data; and we only have ambiguous information about them provided through the bag label sets.

We consider instance annotation in both transductive and inductive modes, which differ in what information is available at the classification stage. The transductive classifier is defined as:

$$y = f(\mathbf{x}, B, Y) : \mathcal{X} \times 2^{\mathcal{X}} \times 2^{\mathcal{Y}} \rightarrow \mathcal{Y} \quad (1)$$

The notation $f(\mathbf{x}, B, Y)$ indicates that we are given all of the instances in a bag B , its label set Y , and the goal is to

Table I
FRAMEWORKS FOR SUPERVISED CLASSIFICATION

Framework	Training Dataset	Classifier
SISL	$(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)$	$y = f(\mathbf{x}) : \mathcal{X} \rightarrow \mathcal{Y}$
MIL	$(B_1, y_1), \dots, (B_n, y_n)$	$y = F(B) : 2^{\mathcal{X}} \rightarrow \{0, 1\}$
MLC	$(\mathbf{x}_1, Y_1), \dots, (\mathbf{x}_n, Y_n)$	$Y = f(\mathbf{x}) : \mathcal{X} \rightarrow 2^{\mathcal{Y}}$
MIML	$(B_1, Y_1), \dots, (B_n, Y_n)$	$Y = F(B) : 2^{\mathcal{X}} \rightarrow 2^{\mathcal{Y}}$
ALC/SLL	$(\mathbf{x}_1, Y_1), \dots, (\mathbf{x}_n, Y_n)$	$y = f(\mathbf{x}) : \mathcal{X} \rightarrow \mathcal{Y}$

predict the label y for a specific instance \mathbf{x} in B .

The inductive mode classifies an instance without the bag label set given. Prior work [3] on MIML instance annotation formulates the inductive classifier as $f(\mathbf{x}) : \mathcal{X} \rightarrow \mathcal{Y}$, which ignores any contextual information from the bag containing \mathbf{x} . We instead formulate the inductive classifier as

$$y = f(\mathbf{x}, B) : \mathcal{X} \times 2^{\mathcal{X}} \rightarrow \mathcal{Y} \quad (2)$$

The difference is that when classifying an instance \mathbf{x} , we know that it is part of a bag B , and can use the contextual information of B to improve the prediction.

A. Related Problems

There are many other formulations of supervised classification that are related to MIML instance annotation. The main difference between these frameworks is the structure of training data (instance or bag, single- or multi-label), and the input to and type of prediction made by the classifier (instance-level or bag-level, single or multi-label). Refer to Table I for a statement of the training data and inductive classifier in each framework.

The most common supervised classification formulation is single-instance single-label (SISL). Most standard methods such as support vector machines, decision trees, and logistic regression are for SISL. Multiple-instance learning (MIL) is a framework where the training data consists of bags of instances paired with a single binary label, and the classifier maps bags to binary labels. Multi-label classification (MLC) [22] pairs single instances with sets of labels, and the goal is to predict a label set given a new instance.

Ambiguous label classification (ALC) [8] and superset label learning (SLL) [16] have the same structure of training data as MLC, but assume only one label in the set is correct and the rest are “distractors.” The goal is to learn a classifier to predict a single label for a new instance. MIML instance annotation can be reduced to ALC/SLL by pairing each instance with its bag label set. However, this reduction can be undesirable as it discards the context of the bag.

III. BACKGROUND

A key observation motivating our approach is that the context provided by a bag’s label set is useful for classifying instances. In the previous example, knowing that there is “grass” in the image can help for predicting the label “cow” for the given instance, because the labels “cow” and “grass” are correlated. A natural way to exploit such context is to follow a classifier-chain approach, which has been

previously developed for MLC to exploit label correlation. Below we begin with a review of classifier chains for MLC. We then discuss some design patterns in MIL and MIML algorithms that learn an instance-level model from bag-level labels, which provide inspiration for our algorithm.

A. Classifier Chains for Multi-Label Classification

Originally introduced for MLC, classifier chains [22] exploit label correlation by building a chain of binary classifiers. Given an instance \mathbf{x} , we denote its label set Y as a binary vector: $Y = [Y^1, \dots, Y^c]$, where $Y^j = 1$ if the label set for instance \mathbf{x} contains class j . We use $Y^{1:j-1} = [Y^1, \dots, Y^{j-1}]$ to refer to the first $j-1$ elements of Y . The key idea of classifier chains is to use a chain factorization of the conditional joint distribution of Y :

$$P(Y|\mathbf{x}) = P(Y^1|\mathbf{x}) \prod_{j=2}^c P(Y^j|\mathbf{x}, Y^{1:j-1}) \quad (3)$$

During training, one binary model $P(Y^j|\mathbf{x}, Y^{1:j-1})$ is learned for each class j , which depends on \mathbf{x} , and all of the preceding classes $1, \dots, j-1$. Let \oplus denote vector concatenation. The basic training algorithm is:

MLC Probabilistic Classifier Chain – Train

for $j = 1, \dots, c$:

$$\mathcal{D}_j = \{\dots, (\mathbf{x}_i \oplus Y_i^{1:j-1}, Y_i^j), \dots\}_{i=1}^n$$

train classifier $P(Y^j|\mathbf{x}, Y^{1:j-1})$ on \mathcal{D}_j

For each class j , a binary supervised classification problem \mathcal{D}_j is created (this is a standard SISL problem, not an MLC problem). This 2-class problem has n instances like the original MLC problem. Each instance consists of the original feature vector \mathbf{x}_i concatenated with part of the corresponding label vector $[Y_i^1, \dots, Y_i^{j-1}]$, and paired with the binary label Y_i^j . The binary model for class j , namely $P(Y^j|\mathbf{x}, Y^{1:j-1})$, can be learned using any binary probabilistic classifier, e.g., logistic regression or Random Forest (RF) [2].

To classify a new instance \mathbf{x} with a probabilistic classifier chain, one can evaluate $P(Y|\mathbf{x})$ for all 2^c possible label vectors Y , and pick one that minimizes a set-level loss function. However, this approach may be intractable unless c is small. An alternative is to greedily construct a single value of Y . A basic greedy algorithm [9] is:

MLC Probabilistic Classifier Chain – Classify

$Y = []$

for $j = 1, \dots, c$:

$$Y = Y \oplus I[P(Y^j|\mathbf{x} \oplus Y) > 0.5]$$

return Y

In ensembles of classifier chains (ECC) [22], there are multiple chains, each of which is learned as above, but factorizing the classes in a different random order. When classifying with ECC, each chain votes. ECC reduces the sensitivity to the specific order of the chain and is generally observed to improve accuracy over a single chain.

B. From Instance to Bag Labels

A central problem in MIL and MIML is that labels are only provided at the bag level. Learning an instance classifier from bag label sets requires an assumption about the relationship between the observed label sets and the hidden instance labels. A common assumption in MIL is that if any instance is positive, the bag label is positive, otherwise it is negative. The corresponding assumption in MIML is that the bag label set is equal to the union of instance labels. Prior algorithms approximate these assumptions using different formulations, e.g., the max model.

In the MIL setting, the max model is: $F(B) = \max_{\mathbf{x} \in B} f(\mathbf{x})$, i.e. the bag-level output F is the max over the instance-level outputs f on all instances in the bag.

For probabilistic MIL classifiers, the max model has also been called the “most-likely-cause estimator” [17],

$$P(y = 1|B, \theta) = \max_{\mathbf{x} \in B} p(y = 1|\mathbf{x}, \theta) \quad (4)$$

The equivalent formulation for MIML [30, 3] applies the same principle for each class $j = 1, \dots, c$:

$$F_j(B) = \max_{\mathbf{x} \in B} f_j(\mathbf{x}) \quad (5)$$

Given a model for connecting bag labels with instance labels, the output of a bag-level classifier can sometimes be expressed as a function of a single instance in the bag or representing the bag. For example, assuming the max model for MIL we have:

$$F(B_i) = \max_{\mathbf{x} \in B_i} f(\mathbf{x}) = f(\hat{\mathbf{x}}_i) \quad (6)$$

$$\hat{\mathbf{x}}_i = \arg \max_{\mathbf{x} \in B_i} f(\mathbf{x}) \quad (7)$$

where $\hat{\mathbf{x}}_i$ is referred to as the support instance (or “witness instance” [1]) for bag B_i . We can define support instances similarly for MIML, except that one support instance is defined for each class and each bag.

Many existing algorithms for MIL (e.g., MI-SVM [1] and EM-DD [31]) and MIML (e.g., SIM [4]) alternate between computing support instances based on a current classifier, and training a SISL classifier on the support instances. Our proposed algorithm follows the same pattern.

IV. PROPOSED METHODS

Our goal is to learn a classifier that predicts the label of a given instance, using its feature vector \mathbf{x} and the context provided by the bag B containing \mathbf{x} . We propose the MIML-ECC algorithm, which is motivated by the observation that the prediction of whether an instance belongs to a particular class can be influenced by the presence/absence of some other classes in the bag. To capture the label correlation, we assume an ordered chain structure such that whether an instance belongs to a particular class depends on whether the bag contains classes earlier in the chain. Table II summarizes notation for the proposed method.

Table II
SUMMARY OF NOTATION

Notation	Meaning
\oplus	vector concatenation operator
B_i	i 'th bag of instances in the training data
Y_i	label set for bag B_i , $Y_i \subseteq \{1, \dots, c\}$
n	number of bags in the training set
n_i	number of instances in bag B_i
$\pi(j)$	the j 'th class in some permutation π
$\pi_l(j)$	the j 'th class in the permutation for chain l
$Y_i^{\pi_l(j)}$	the j 'th bit (0 or 1) of the label set Y_i in order π_l
$Y_i^{\pi_l(1):\pi_l(j-1)}$	the first $j-1$ bits of the label set Y_i in order π_l
$\mathbf{x} \in B_i$	an instance in bag B_i , a vector in \mathbb{R}^d
f_{jl}	instance-level score function for class $\pi_l(j)$
F_{jl}	bag-level score function for class $\pi_l(j)$
$\hat{\mathbf{x}}_{ijl}$	support-instance for bag i , chain l , class $\pi_l(j)$
y^k	indicator variable for instance \mathbf{x} in class k

A. Training

A classifier chain for MLC is a chain of SISL classifiers. At a high level, our method can be viewed as building an ensemble of L chains of MIL classifiers. Each chain $l = 1, \dots, L$ in the ensemble views the classes $1, \dots, c$ in a different order π_l , such that $\pi_l(j)$ is the j 'th class in the order for chain l . We will use F_{jl} to denote the MIL classifier for the j -th class in chain l , which predicts the presence/absence of class $\pi_l(j)$ in the label set of a bag given the bag and $Y^{\pi_l(1):\pi_l(j-1)}$, the presence/absence information of the first $j-1$ classes in chain l . The training algorithm viewed in terms of MIL classifiers is:

MIML-ECC – Train (Bag-Level View)

Input: MIML dataset $\{(B_1, Y_1), \dots, (B_n, Y_n)\}$

Output: MIL classifiers F_{jl}

for $l = 1, \dots, L$:

$\pi_l = \text{random-permutation}([1, \dots, c])$

for $j = 1, \dots, c$:

$\mathcal{D}_{jl} = \{\dots, (B_i \oplus Y_i^{\pi_l(1):\pi_l(j-1)}, Y_i^{\pi_l(j)}), \dots\}_{i=1}^n$

train MIL Classifier F_{jl} on \mathcal{D}_{jl}

Each MIL dataset \mathcal{D}_{jl} constructed in the algorithm pairs the bag B_i (and the context $Y_i^{\pi_l(1):\pi_l(j-1)}$) with one bit of the label vector $Y_i^{\pi_l(j)}$. In a standard MIL formulation, there are only bags of instances, so it is a modification of MIL to allow the context $Y_i^{\pi_l(1):\pi_l(j-1)}$, which is a vector in \mathbb{R}^{j-1} , to be associated with the bag rather than an instance. However, in practice we simply append this vector to the end of all of the instance features.

Because our goal is ultimately to predict instance labels, we instantiate this template with a MIL classifier that internally builds an instance-level model. The instance-level models are SISL probabilistic classifiers f_{jl} for $j = 1, \dots, c$ and $l = 1, \dots, L$. We assume f_{jl} maps the input $\mathbf{x} \oplus Y^{\pi_l(1):\pi_l(j-1)}$ to an output in $[0, 1]$ (as is the case for a RF). Recall that $\mathcal{Y} = \{1, \dots, c\}$; we encode the label $y \in \mathcal{Y}$ of instance \mathbf{x} with c binary indicator variables y^1, \dots, y^c

where $y^j = I[y = j]$, and interpret $f_{jl} : \mathbb{R}^{d+j-1} \rightarrow [0, 1]$ as the posterior probability $P(y^{\pi_l(j)} | \mathbf{x}, Y^{\pi_l(1):\pi_l(j-1)})$. MIL classifiers F_{jl} can be obtained from the instance-level classifiers using the max model, taking into account the context $Y^{\pi_l(1):\pi_l(j-1)}$:

$$F_{jl}(B_i \oplus Y^{\pi_l(1):\pi_l(j-1)}) = \max_{\mathbf{x} \in B_i} f_{jl}(\mathbf{x} \oplus Y^{\pi_l(1):\pi_l(j-1)}) \quad (8)$$

Similar to the MIL algorithm EM-DD, and rank-loss SIM for MIML, we define the bag-level model in terms of a support instance. In MIML-ECC, there is a different support instance for each bag, class, and chain. The bag-level model in terms of support instances is

$$F_{jl}(B_i \oplus Y^{\pi_l(1):\pi_l(j-1)}) = f_{jl}(\hat{\mathbf{x}}_{ijl} \oplus Y_i^{\pi_l(1):\pi_l(j-1)})$$

$$\hat{\mathbf{x}}_{ijl} = \arg \max_{\mathbf{x} \in B_i} f_{jl}(\mathbf{x} \oplus Y_i^{\pi_l(1):\pi_l(j-1)})$$

The support instance $\hat{\mathbf{x}}_{ijl}$ is the instance in bag B_i that is most representative of class $\pi_l(j)$, according to the classifiers in chain l .

The MIML-ECC training algorithm alternates K times between updating support instances according to the max model, then training SISL classifiers on binary datasets that pair support instances with bits of the label set. In the first iteration, there are no instance classifiers f_{jl} to compute support instances from, so we start by setting the support instances to the average of the instances in each bag, as in [3, 4]. The instance-level view of the training algorithm is:

MIML-ECC – Train (Instance-Level View)

Input: MIML dataset $\{(B_1, Y_1), \dots, (B_n, Y_n)\}$

Output: SISL classifiers f_{jl}

for $l = 1, \dots, L$:

$\pi_l = \text{random-permutation}([1, \dots, c])$

for $k = 1, \dots, K$:

if $k = 1$ then:

for $i = 1, \dots, n$: for $j = 1, \dots, c$:

$\hat{\mathbf{x}}_{ijl} = \frac{1}{n_i} \sum_{\mathbf{x} \in B_i} \mathbf{x}$

if $k > 1$ then:

for $i = 1, \dots, n$: for $j = 1, \dots, c$:

$\hat{\mathbf{x}}_{ijl} = \arg \max_{\mathbf{x} \in B_i} f_{jl}(\mathbf{x} \oplus Y_i^{\pi_l(1):\pi_l(j-1)})$

for $j = 1, \dots, c$:

$\mathcal{D}_{jl} = \{\dots, (\hat{\mathbf{x}}_{ijl} \oplus Y_i^{\pi_l(1):\pi_l(j-1)}, Y_i^{\pi_l(j)}), \dots\}_{i=1}^n$

train SISL classifier f_{jl} on \mathcal{D}_{jl}

B. Classification

In the training phase, instance-level binary classifiers $f_{jl}(\mathbf{x} \oplus Y^{\pi_l(1):\pi_l(j-1)})$ are obtained for every class j and chain l . The output of f_{jl} can be considered an estimate of the posterior $P(y^{\pi_l(j)} | \mathbf{x}, Y^{\pi_l(1):\pi_l(j-1)})$, so we consider a probabilistic framework for instance classification based on the maximum a-posteriori (MAP) approach. This is how MIML-ECC approximately optimizes instance accuracy, the desired performance measure for MIML instance annotation.

1) *Transductive Mode*: In the transductive mode, we condition on the bag and its label set, and predict instance labels according to

$$f(\mathbf{x}, B, Y) = \arg \max_{j \in Y} P(y^j | \mathbf{x}, B, Y) = \arg \max_{j \in Y} P(y^j | \mathbf{x}, Y)$$

This prediction rule assumes that bag label set Y provides all of the contextual information that is relevant to predicting the label for \mathbf{x} , i.e. the label is conditionally independent of the other instances in the bag B given Y .

During training we introduced random orders π for the purpose of constructing an ensemble. Now we take a Bayesian approach and assume that π is random variable from a uniform prior $P(\pi)$, so each chain in the ensemble corresponds to one i.i.d. sample $\pi_l \sim P(\pi)$ for $l = 1, \dots, L$. We estimate the probability for instance \mathbf{x} to have label $y = k$ as $P(y^k | \mathbf{x}, Y) = E_\pi [P(y^k | \mathbf{x}, Y, \pi)]$ using L samples, one for each chain in the ensemble.

$$P(y^k | \mathbf{x}, Y) \approx \frac{1}{L} \sum_{l=1}^L \sum_{\{j: \pi_l(j)=k\}} P(y^{\pi_l(j)} | \mathbf{x}, Y^{\pi_l(1):\pi_l(j-1)}, \pi_l)$$

The algorithm for classification in the transductive mode is:

MIML-ECC – Classify (Transductive)

Input: instance \mathbf{x} , label set Y

Output: label y

for $j = 1, \dots, c: y^j = 0$

for $l = 1, \dots, L:$

 for $j = 1, \dots, c:$

$y^{\pi_l(j)} = y^{\pi_l(j)} + f_{jl}(\mathbf{x} \oplus Y^{\pi_l(1):\pi_l(j-1)})$

$y = \arg \max_{j \in Y} y^j$

2) *Inductive Mode*: In the inductive setting, the bag label set is not given, so the posterior required for classification conditions only on the instances from bag B (and not the bag label set). Therefore, we predict the instance label as the class with the highest posterior probability

$$y = f(\mathbf{x}, B) = \arg \max_{j=1, \dots, c} P(y^j | \mathbf{x}, B) \quad (9)$$

The probability $P(y^j | \mathbf{x}, B)$ is not directly modeled by the instance-level classifiers f_{jl} ; instead we estimate this probability by marginalizing $P(y^j | \mathbf{x}, Y, B)$ over the latent variable Y . This process requires a probabilistic model for Y given B , which we develop below.

Assumption 1: Given an order π , an instance \mathbf{x} and the bag-level labels $Y^{\pi(1):\pi(j-1)}$, $y^{\pi(j)}$ is conditionally independent of any other instances in the same bag B ,

$$P(y^{\pi(j)} | \mathbf{x}, B, Y^{\pi(1):\pi(j-1)}, \pi) = P(y^{\pi(j)} | \mathbf{x}, Y^{\pi(1):\pi(j-1)}, \pi)$$

For training, we defined the relation between instance labels and bag label sets according to the max model. The max model is also part of our assumptions for inference, although we will rewrite it in probability notation.

Assumption 2: Bag label sets and instance labels are linked via the max model,

$$P(Y^{\pi(j)} | B, Y^{\pi(1):\pi(j-1)}, \pi) = \max_{\mathbf{x} \in B} P(y^{\pi(j)} | \mathbf{x}, Y^{\pi(1):\pi(j-1)}, \pi)$$

Similar to a classifier chain for MLC, the conditional distribution of the bag label set is factored as a chain in the order π as

$$P(Y | B, \pi) = P(Y^{\pi(1)} | B, \pi) \prod_{j=2}^c P(Y^{\pi(j)} | B, Y^{\pi(1):\pi(j-1)}, \pi)$$

Recall that Assumption 2 defines the conditional probability for $Y^{\pi(j)}$ in terms of the instance-level probabilities for $y^{\pi(j)}$, while Assumption 1 defines the instance-level probabilities for $y^{\pi(j)}$ in terms of $Y^{\pi(1):\pi(j-1)}$.

We estimate $P(y^j | \mathbf{x}, B)$ by sampling as follows. For a given π , we apply Assumption 1 to obtain $P(y^{\pi(j)} | \mathbf{x}, B, \pi)$

$$\begin{aligned} &= E_{Y^{\pi(1):\pi(j-1)} | B, \pi} [P(y^{\pi(j)} | \mathbf{x}, Y^{\pi(1):\pi(j-1)}, B, \pi)] \\ &= E_{Y^{\pi(1):\pi(j-1)} | B, \pi} [P(y^{\pi(j)} | \mathbf{x}, Y^{\pi(1):\pi(j-1)}, \pi)] \end{aligned} \quad (10)$$

Because π is a permutation, computing $P(y^{\pi(j)} | \mathbf{x}, B, \pi)$ for $j = 1, \dots, c$ implies computing $P(y^j | \mathbf{x}, B, \pi)$ for all j .

Finally, we average the posterior estimates over multiple samples from a uniform prior on π :

$$P(y^j | \mathbf{x}, B) = E_\pi [P(y^j | \mathbf{x}, B, \pi)] \quad (11)$$

As in the transductive mode, each chain in the ensemble gives one sample of $\pi_l \sim P(\pi)$ to estimate the expectation. The inductive classification algorithm is:

MIML-ECC – Classify (Inductive)

Input: bag $B = \{\mathbf{x}_1, \dots, \mathbf{x}_{n_i}\}$

Output: instance labels y_1, \dots, y_{n_i}

01: for $i = 1, \dots, n_i$: for $j = 1, \dots, c$:

02: $y_i^j = 0$

03: for $l = 1, \dots, L$:

04: $Y = []$

05: for $j = 1, \dots, c$:

06: for $i = 1, \dots, n_i$:

07: $y_i^{\pi_l(j)} = y_i^{\pi_l(j)} + f_{jl}(\mathbf{x}_i \oplus Y)$

08: $p_j = \max_{i=1, \dots, n_i} f_{jl}(\mathbf{x}_i \oplus Y)$

09: $Y = Y \oplus \text{Bernoulli}(p_j)$

10: for $i = 1, \dots, n_i$:

11: $y_i = \arg \max_{j=1, \dots, c} y_i^j$

Line 7 updates the estimate of $y_i^{\pi_l(j)}$ based on one sample of the expectation (10). Line 8 applies the max model (Assumption 2). In lines 4 through 8, the pseudocode variable Y stores $Y^{\pi_l(1):\pi_l(j-1)}$. Line 9 samples $Y^{\pi_l(j)}$ from a $\text{Bernoulli}(p_j)$ distribution, and appends it to the current label vector.

C. Similarities with EM

The proposed training algorithm is a heuristic, and is not proven to converge over multiple support instances updates. However, it is closely related to prior work using support instances with expectation maximization (EM). We discuss this similarity with prior algorithms to provide evidence that MIML-ECC can be expected to improve in accuracy as the number of support instance updates K increases.

EM-DD [31] is a widely used algorithm for MIL (single-labeled bags of instances), in the spirit of EM (a formal proof is not given). The ‘‘E-step’’ consists of computing support instances, and the ‘‘M-step’’ maximizes likelihood in a model involving the support instances. EM-DD also uses the max model to define the support instances. The main difference in how support instances are treated in MIML-ECC is that each bag has a different support instance for each class and chain. Recall that MIML-ECC trains SISL classifiers f_{jl} in each iteration. If the base SISL classifier maximizes log-likelihood (e.g., logistic regression), there is a direct correspondence with the M-step of EM-DD. In our implementation of MIML-ECC, f_{jl} is a RF using the Gini split criteria, which greedily minimizes squared-loss $\mathcal{L}_2(y, p) = (y - p)^2$ on the training data [6]. If the entropy split criteria were used instead, the RF would greedily maximize likelihood. Gini and entropy are very similar for binary problems.

D. Asymptotic Complexity

MIML-ECC implemented with RF as the base SISL classifier is asymptotically efficient in all important dimensions of problem size. The size of a MIML dataset is determined by the number of bags n , the total number of instances in all bags m , the number of classes c , and the instance feature dimension d . MIML-ECC has several parameters which affect its runtime: the number of chains L , the number of trees in each RF T , and the number of support-instance updates K . Note that the runtime to train a RF on a SISL dataset of n instances with feature dimension d is $O(T(\log d)(n \log n))$, and to classify it is $O(\log n)$. It follows from the loop-structure of the pseudocode that the training time for MIML-ECC is

$$O\left(LKT(m(\log n)(\log d) + cn \log n \log(d + c))\right) \quad (12)$$

An efficient implementation of MIML-ECC classifies all instances in a bag at once, rather than treating each instance classification problem separately, in order to share redundant work. Using this optimization, the classification time is $O(LTc \log n)$ per instance. In Section V-I we provide empirical run time of our algorithm.

V. EXPERIMENTS

Our experiments compare MIML-ECC to prior and baseline methods on two vision datasets, an audio dataset, and

Table III
MIML DATASETS USED IN OUR EXPERIMENTS

Dataset	Classes	Dimension	Bags	Instances
MSRCv2	23	48	591	1,758
VOC 2012	20	48	1,053	4,142
Birdsong	13	38	548	4,998
Carroll	26	16	166	717
Frost	26	16	144	565

two artificial datasets. Our experimental setup is identical to the setup used in [4] and [16], hence results are directly comparable (e.g., the same features and folds for cross validation are used). Therefore we report new results for MIML-ECC and baseline methods, and compare to previously reported results from the aforementioned prior work.

A. Datasets

The datasets used in our experiments are summarized in Table III. Datasets have been preprocessed through feature rescaling (which does not affect RF), to improve results for SVM style-classifiers, by the same process in [8, 3, 4].

1) *Vision Datasets*: We consider two vision datasets, Microsoft Research Cambridge v2 (MSRCv2) [25], and PASCAL Visual Object Recognition Challenge (2012 ‘‘Segmentation’’) [11]. Both datasets contain images of objects with pixel-level labeling of regions. MSRCv2 provides a single class label for each pixel. VOC provides a segmentation of each image into objects and a label for each object. Here bags are images labeled with a list of objects, instances are objects / regions of pixels, described by a 48-D feature vector. Single-label images are removed to make the learning problem more challenging.

2) *Bioacoustics Dataset*: This dataset was introduced by [5], applying a MIML formulation for label set prediction to a real-world application of classifying bird song collected in field conditions. Each bag is a 10 second audio recording labeled with the set of species it contains. Each instance is an utterance of bird sound obtained by an automatic segmentation algorithm. This dataset has also been used in work on MIML instance annotation and superset label learning [3, 4, 16]. For instance annotation, [3] introduced two variants of this dataset, ‘‘filtered’’ and ‘‘unfiltered.’’ Our experiments use the filtered variant, as does [16].

3) *Artificial Datasets*: We use the same artificial MIML datasets as [3, 4], which are generated to simulate correlations between labels by using letter correlation in English words. The datasets are generated based on the words in two poems, ‘‘Jabberwocky’’ by Lewis Carroll [7], and ‘‘The Road Not Taken’’ by Robert Frost [13], hence they are referred to as Carroll and Frost. Each bag is a word, its letters are instances, and the bag label set is the union of instance labels. The instance features are sampled randomly from the UCI Letter Recognition dataset [12].

B. Prior & Baseline Methods

We compare MIML-ECC with a number of prior methods that can be applied to MIML instance annotation.

1) *M³MIML*: Originally intended for label-set prediction, M³MIML is a MIML support-vector machine algorithm, which builds one linear instance-level model per class by minimizing a heuristic relaxation of bag-level hinge loss, and connecting instance labels with bag label sets by the max model. Although not intended for this purpose, the learned instance-level models can be used for instance annotation.

2) *Rank-loss SIM*: Rank-loss SIM was introduced by [3], and refers to a class of instance annotation algorithms which learn one linear instance-level model per class by minimizing a bag-level rank-loss objective. Different variants of rank-loss SIM consider different models for connecting bag-level output with instance-level outputs, and apply different procedures for optimizing the rank-loss objective. We consider SIM-Heuristic using a softmax model and SIM-CCCP with the max model, with random Fourier kernel features [20] to achieve nonlinear classification by approximating an RBF kernel. These models are chosen for comparison because they achieved the best accuracy in [4].

3) *CLPL*: Like the other SVM-style algorithms, Convex Learning from Partial Labels (CLPL) [8] learns one linear instance-level model per class, but uses an ALC formulation instead of MIML. CLPL minimizes a loss function which can be seen as an upper bound to the 0/1 loss on the true-unknown label, which is part of the candidate label set.

4) *LSB-CMM*: Logistic Stick-Breaking Conditional Multinomial Model (LSB-CMM) [16] is a recent hybrid generative / discriminative graphical model for SLL that have been used (by reduction) to solve the instance annotation problem. In particular, the same Birdsong and MSRCv2 datasets were used in [16] to evaluate its instance annotation accuracy. We compare to the results reported in [16] on these two datasets.

5) *SISL Random Forest and SVM*: We also consider SISL algorithms, which have an unfair advantage of learning directly from instance labels. Results with these SISL algorithms are presented for the inductive mode as an empirical upper bound on the accuracy that can be achieved on these datasets. For this comparison, we use a SISL RF (with 1000 trees), and refer to prior results from [4] with a SISL multi-class linear SVM.

C. Transductive and Inductive

In the transductive mode, there is no cross-validation (the whole dataset is used for training and testing). However, because MIML-ECC is a randomized algorithm, we run 10 repetitions and report the average accuracy \pm the standard deviation over repetitions. Most of the other algorithms we compare to are not randomized, so in the transductive mode there is no uncertainty associated with the accuracy result.

In the inductive mode, we use 10-fold cross validation, except for the VOC dataset, for which there is a pre-specified partition into “train” and “val” sets. Results with 10-fold cross-validation are reported as average accuracy over all

fold \pm standard deviation in accuracy. A different random instantiation of MIML-ECC is used in each fold, so we do not run multiple repetitions on top of cross-validation. However, because there is only one fold for the VOC dataset, we report results \pm standard deviation over 10 repetitions for MIML-ECC (and the randomized baseline method SISL Random Forest) on VOC.

M³MIML, CLPL, and rank-loss SIM-Heuristic/CCCP all build one instance-level model per class $f_j(\mathbf{x})$. In the inductive mode, these models are used to predict an instance label by the rule $f(\mathbf{x}) = \arg \max_{j=1, \dots, c} f_j(\mathbf{x})$. In the transductive mode, the rule is $f(\mathbf{x}, Y) = \arg \max_{j \in Y} f_j(\mathbf{x})$ (hence when the bag label set Y is known, it is used to constrain the instance-label predictions). This constraint provides some context for instance-label prediction, so there is not as much benefit to be had from looking at other instances in the transductive mode.

D. Parameter Selection

All of the rank-loss SIM algorithms, CLPL, M³MIML, and SISL SVM have a regularization parameter (either λ or C). When random kernel features are used to approximate the RBF kernel, there is also a kernel parameter γ , and a parameter D which controls the approximation accuracy. In prior work, these parameters are optimized post-hoc by a grid search as described in [4]. This means the experiment is run once for each parameter setting in a grid, and the best test accuracy over all parameters is reported. Post-hoc selection is not feasible without using instance labels to compute which parameter setting has the best accuracy, but it has been accepted in prior work on MIML instance annotation because it is an unsolved problem. Results using post-hoc selection can be interpreted as the highest accuracy that can be achieved using an oracle to select meta-parameters.

An important practical advantage of MIML-ECC compared to the above prior methods is that it does not have regularization parameters that must be tuned. Note that MIML-ECC has parameters L, K , and T . The accuracy of the algorithm tends to increase as these parameters increases up to a limit. So the parameter choices primarily depend on the time budget for training and testing. Our experiments set $L = 20, K = 20, T = 100$, which provides a good tradeoff between runtime and accuracy.

LSB-CMM [16] has some parameters which can affect accuracy, but in their experiments these parameters are set to standard values for all datasets.

E. Results

MIML instance annotation algorithms are evaluated based on accuracy, which is the fraction of correctly classified instances. These experiments compare multiple classifiers on multiple datasets, so following the recommendations of [10], we summarize results using wins, ties, and losses, and average ranks. Table IV lists the accuracy and average

Table IV
 INSTANCE ANNOTATION ACCURACY RESULTS († – RESULTS FROM [4], ‡ – RESULTS FROM [16])

(a) Transductive accuracy \pm standard deviation over 10 repetitions for MIML-ECC and SIM-RF

Algorithm	Carroll	Frost	Birdsong	MSRCv2	VOC	Avg Rank
Proposed Methods						
MIML-ECC ($L = 20, K = 20, T = 100$)	.803 \pm .006	.831 \pm .004	.779 \pm .003	.805 \pm .007	.624 \pm .004	1.8
Prior Methods						
† CLPL	.672	.688	.742	.678	.598	4.0
† M ³ MIML	.454	.532	.651	.547	.533	5.0
† SIM-CCCP _{max} + kernel	.807	.780	.829	.798	.623	2.2
† SIM-Heuristic _{softmax} + kernel	.794	.819	.833	.766	.634	2.0
Baseline Methods						
SIM-RF ($K = 20, T = 100$)	.763 \pm .014	.787 \pm .015	.791 \pm .010	.799 \pm .007	.618 \pm .003	

(b) Inductive accuracy \pm standard deviation over 10-fold cross validation or 10 repetitions for VOC

Algorithm	Carroll	Frost	Birdsong	MSRCv2	VOC	
Proposed Methods						
MIML-ECC ($L = 20, K = 20, T = 100$)	.618 \pm .059	.646 \pm .048	.666 \pm .052	.611 \pm .038	.43 \pm .004	1
Prior Methods						
† CLPL	.464 \pm .058	.506 \pm .063	.620 \pm .038	.431 \pm .036	.345	3.6
† M ³ MIML	.288 \pm .041	.313 \pm .041	.433 \pm .073	.317 \pm .055	.396	4.2
† SIM-CCCP _{max} + kernel	.618 \pm .042	.576 \pm .065	.630 \pm .040	.519 \pm .044	.343	2.6
† SIM-Heuristic _{softmax} + kernel	.596 \pm .041	.587 \pm .066	.642 \pm .039	.506 \pm .038	.337	2.8
‡ LSB-CMM	–	–	.715	.459	–	
Baseline Methods						
SIM-RF ($K = 20, T = 100$)	.522 \pm .079	.589 \pm .040	.645 \pm .055	.575 \pm .045	.444 \pm .002	
MIML-ECC ($L = 1, K = 20, T = 2000$)	.530 \pm .047	.598 \pm .040	.644 \pm .044	.580 \pm .047	.425 \pm .003	
SISL Methods (uses instance labels)						
† SISL SVM (multi-class, linear)	.772 \pm .049	.753 \pm .038	.772 \pm .032	.638 \pm .045	.440	
SISL Random Forest ($T = 1000$)	.809 \pm .049	.807 \pm .076	.805 \pm .033	.729 \pm .050	.511 \pm .002	

rank results in transductive and inductive modes. Average ranks are computed by sorting the accuracy of MIML-ECC, and the prior methods M³MIML, CLPL, SIM-Heuristic, and SIM-CCCP on each dataset, then averaging the position in the sorted list over all datasets. We do not include LSB-CMM in the ranking because there are only 2 datasets with comparable results.

In the inductive mode, MIML-ECC ties with SIM-CCCP _{max} with RBF kernel on the Carroll dataset, and wins in all other comparisons. Results are not as decisive in the transductive mode, but MIML-ECC still achieves the best average rank over all datasets. This is consistent with our expectation because the known label sets provide a surrogate for context to the other algorithms.

It should be noted that due to the use of post-hoc selection in experiments for CLPL, M³MIML and SIM, they are actually given an unfair advantage compared to MIML-ECC, which does not use the test data ground truth in training or parameter selection.

The comparison with LSB-CMM on two datasets is less conclusive. MIML-ECC outperforms LSB-CMM by a margin of 15.2% on the MSRCv2 dataset, but LSB-CMM is slightly better (by a margin of 4%) on the Birdsong dataset.

F. Ensemble of Chains vs. Binary Relevance (SIM-RF)

MIML-ECC is motivated by the idea that bag-level label correlations captured through the chain structure are useful

for predicting instance labels. However, it is possible that the improved performance we observe compared to prior linear/kernel algorithms is not due to exploiting label correlations, but instead to using a RF as the base-classifier. To address this hypothesis, we consider an additional comparison against a baseline that we call SIM-RF, which is the same as MIML-ECC in all details except it does not use a chain or model correlations. SIM-RF is equivalent to running MIML-ECC with one chain ($L = 1$) but omitting all of the concatenation of label set bits, i.e. $\oplus Y^{\pi_1:\pi(j-1)}$. SIM-RF is also equivalent to binary relevance with each class modeled by a MIL classifier which alternates between computing support instances and training an RF on them.

MIML-ECC achieves better accuracy than SIM-RF most of the time. The win-loss count is 4-1 in favor of MIML-ECC for both transductive and inductive modes. The comparison to SIM-RF suggests that the chain structure is actually critical, and the improved performance of MIML-ECC compared to prior methods cannot be attributed only to switching from a linear or kernel SVM classifier to RF.

G. Single Chain vs. Ensemble of Chains

We want to know how much benefit the ensemble provides compared to a single chain. The results we reported so far are obtained with $L = 20, K = 20, T = 100$, i.e., 20 chains and 100 trees and 20 iterations of support instance updates. To understand the impact of using multiple chains with a

Table V
 RUNTIME FOR TRAINING AND CLASSIFICATION WITH MIML-ECC, PER
 FOLD OF CROSS-VALIDATION OR PER REPETITION (SECONDS)

Mode	Carroll	Frost	Birdsong	MSRCv2	VOC
Transductive	104.9	84.4	251.8	304.5	798.0
Inductive	69.4	57.8	135.5	202.8	2895.8

fair comparison, we run MIML-ECC with one chain order ($L = 1$), and $K = 20, T = 2000$, so the total number of decision trees that vote on an instance label is the same. Table IV (b) lists results for 1-chain MIML-ECC in the inductive mode (see Baseline Methods). In this comparison, MIML-ECC with multiple chains achieves higher accuracy on all datasets than MIML-ECC with a single chain. These results suggest that given a fixed time budget, it is better to have multiple chains, each with less trees, than a single chain with more trees. Recall that when predicting instance scores for class j , each chain can only use the presence/absence of other classes which come before j in the chain. Using multiple chains with random orders increases the chance that relevant classes are available for use as context (at least in some of the chains).

H. Comparison to SISL

SISL methods achieve better accuracy in inductive experiments than MIML instance annotation, ALC and SLL (Table IV (b)), which is expected because they are trained on unambiguously labeled instances. This improved accuracy must be weighed against the greater human effort required to obtain instance labels compared to bag label sets.

I. Empirical Runtime

Table V lists empirical runtimes for training plus classification with MIML-ECC (with $L = 20, K = 20, T = 100$), on each dataset, averaged over the number of repetitions or folds of cross-validation. The runtime is on the order of seconds or minutes for all datasets. In our experiments, training is parallelized using threads, and classification is done sequentially.¹

VI. RELATED WORK

Graphical models for MIML sometimes include instance labels as hidden variables. Inference over these hidden variables can be used for instance annotation. In addition to LSB-CMM, some recent examples of graphical models for MIML include Dirichlet-Bernoulli Alignment [28] and Exponential Multinomial Mixture model [27]. [29] proposed MLMIL, a conditional random field for MIML which uses Gibbs sampling to infer instance labels.

[24] developed a MIML SVM algorithm which uses a bag-level kernel. Their algorithm predicts instance labels by applying the bag-level classifier to a bag of one instance.

¹Code is C++ compiled with GCC 4.0 (most speed optimizations enabled). Experiments ran on a Mac Pro with 2x 2.4 GHz Quad-Core Intel Xeon processor and 16 GB 1066 MHz DDR3 memory, with OS X 10.8.1.

[23] proposed a MIML instance annotation algorithm which alternates between sampling random instance labels and training a Semantic Texton Forest (a specialization of RF to images). [19] proposed a MIML algorithm which alternates between assigning instance labels and training a maximum margin classifier. [15] considers the problem of selecting a set of instances explaining each label, which is different from instance annotation, where the goal is to label all instances.

Prior work on multi-instance (single-label) learning has considered the case where instance labels are not independent, and encoded instance-label relationships through a graph [14, 32]. These approaches can be viewed as a different way to model instance-label correlations.

Several formulations besides the max model have been used for MIL and MIML to relate instance and bag labels. Different formulations encode different assumptions about instance labels. One version of the Diverse Density algorithm for MIL [18] used a Noisy-OR model $P(y = 1|B, \theta) = 1 - \prod_{x \in B} (1 - P(y = 1|x, \theta))$. [17] points out that the max model makes fewer independence assumptions than the Noisy-OR model, although both generate similar probabilities in many cases. In later work the EM-DD [31] algorithm replaced Noisy-OR with max. [21] proposed Multiple-Instance Logistic Regression, which uses a smooth softmax approximation to max. [3, 4] used a multi-class softmax model. [26] propose a model where the bag-label probability is the average of the instance-label probabilities.

VII. CONCLUSION & FUTURE WORK

We proposed MIML-ECC, an algorithm for context-aware MIML instance annotation. Experiments on image, audio, and artificial datasets show that MIML-ECC achieves better accuracy than other recent algorithms.

MIML-ECC exploits context through correlations, which can be summarized by statements like “if A is present, B is also likely to be present.” However, MIML-ECC cannot exploit a different kind of context, which can be summarized as “if one A is present, there are likely to be more A’s.” For example, consider Fig 2. It might be easy to recognize some of the larger cows in the image, but harder to recognize the small ones. However, after recognizing one cow, it we might expect to find more cows. MIML-ECC will not exploit this kind of context because it can only use information about the presence or absence of other classes to inform its prediction.

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