Risk Consistent Multi-Class Learning from Label Proportions

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Abstract
This study addresses a multiclass learning from label proportions (MCLLP) setting in which training instances are provided in bags and only the proportion of each class within the bags is provided. Most existing MCLLP methods impose bag-wise constraints on the prediction of instances or assign them pseudo-labels; however, none of these methods have a theoretical consistency. To solve this problem, a risk-consistent method is proposed for instance classification using the empirical risk minimization framework, and its estimation error bound is derived. An approximation method is proposed for the proposed risk estimator, to apply it to large bags, by diverting the constraints on bags in existing research. The proposed method can be applied to any deep model or loss and is compatible with stochastic optimization. Experiments are conducted on benchmarks to verify the effectiveness of the proposed method.

1. Introduction
In recent years, with the development of machine learning models, such as deep models, there has been focus on finding and studying in detail methods to learn from weakly supervised information (Zhou, 2017). Weakly supervised learning aims to learn from such information, and various settings have been investigated. Some examples are semi-supervised (Chapelle et al., 2006; Sakai et al., 2017), noisy label (Natarajan et al., 2013; Han et al., 2018), multi-instance (Amores, 2013; Ilse et al., 2018), partial label (Feng et al., 2020; Lv et al., 2020), complementary label (Ishida et al., 2017), positive unlabeled (du Plessis et al., 2014), positive confidence (Ishida et al., 2018), similar unlabeled (Bao et al., 2018), and similar dissimilar (Shimada et al., 2021) learning.

In this study, we examine learning from label proportions (LLP) (Quadrianto et al., 2009), a type of weakly supervised learning. LLP is a learning method for classifying instances in bags given their class proportions or quantities in each bag. LLP has been used in many cases where supervised information for instances is unavailable owing to unobservable information or privacy issues, such as in image and video analysis (Chen et al., 2014; Lai et al., 2014; Ding et al., 2017; Li & Taylor, 2015), applications in physics (Dery et al., 2017; Musicant et al., 2007), medical applications (Hernández-González et al., 2018; Bortsova et al., 2018), and activity analysis (Poyiadzi et al., 2018).

We particularly focus on multiclass LLP (MCLLP), on which previously research has been conducted on two main types of learning methods. In the first method, restrictions are imposed on bag-level predictions. A related milestone in MCLLP is Deep LLP (DLLP) (Ardehaly & Culotta, 2017), which can be applied to any model, including deep learning. By DLLP, instance class prediction can be learned by restricting the mean statistics of the prediction in a bag to be close to a given label proportion. In the second method, pseudo-labels are assigned to instances using the label proportions given to a bag. Methods for assigning pseudo-labels based on the optimal transport theory and other techniques have been investigated (Dulac-Arnold et al., 2019). However, the above two described learning methods lack the statistical theoretical background for per-instance prediction, and the theoretical understanding for MCLLP is not developed well.
In many studies on weakly supervised learning, empirical risk minimization (ERM) (Vapnik, 1998) has played an important role in learning correctly from such weak supervisory information (Sakai et al., 2017; Feng et al., 2020; Ishida et al., 2017; du Plessis et al., 2014; Shimada et al., 2021; Bao et al., 2018). Similarly, the ERM framework has been used in binary LLP and its statistical background has been clarified (Yu et al., 2015; Lu et al., 2019b). Only recently, Jianxin Zhang (2022) conducted a theoretical analysis of MCLLP with label noise framework. However, the statistical background of MCLLP is still lacking.

Motivated by the above, in this study, an MCLLP learning method is established with a statistical background. Specifically, the ERM framework, which is commonly used in supervised learning, is adopted, and the convergence of an MCLLP classifier is demonstrated. One of the difficulties in applying ERM to MCLLP is its computational complexity. If the possible combinations for a given label can be enumerated, the order is \(O(K^{C-1})\) for bag size \(K\) and number of classes \(C\), making it difficult to apply a risk estimator to large bags. To solve this problem, we propose an approximation method using bag-wise loss, which is extensively used in existing research, and show experimentally its effectiveness.

The contributions of this research are as follows:

- We propose a risk-consistent method for MCLLP, which has a loss estimator equivalent to the typical multiclass classification. We analyze the estimation error bound.

- We propose an approximation method to apply the proposed estimator to bags with many instances.

2. Formulations and Related Studies

In this section, we introduce ordinary multiclass classification, partial label learning (PLL), and label proportions learning, and subsequently present the review of some related studies.

2.1. Ordinary Multiclass Classification

In \(k\)-classification, let \(\mathcal{X}\) be the space of instances and \(\mathcal{Y} = \{1, \ldots, c\}\) be the space of labels. In multiclass classification, it is assumed that \((x, y) \in \mathcal{X} \times \mathcal{Y}\) is sampled independently from the probability distribution, \(p(x, y)\). Subsequently, the classifier, \(f: \mathcal{X} \to \mathbb{R}^K\), is learned to minimize

\[
R(f) = \mathbb{E}_{(x,y) \sim p(x,y)}[l(f(x), y)]
\]

where \(l: \mathbb{R}^k \times \mathcal{Y} \to \mathbb{R}_{\geq 0}\) is the multiclass loss function, which measures the effectiveness of the classifier for predicting, given the labels. Typically, the true distribution, \(p(x, y)\), cannot be observed. Therefore, the training data, \(\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n\), are used, and the empirical loss (Vapnik, 1998) is minimized.

\[
\hat{R}(f) = \frac{1}{n} \sum_{i=1}^n l(f(x_i), y_i)
\]

A learning method is risk-consistent when it has the same risk estimator as \(R(f)\).

2.2. Partial Label Learning

Partial Label Learning (PLL) refers to a method that learns multiclass classification, where multiple label candidates are given for each instance and only one of them is correct. This setting occurs when multiple annotators are labeled or when labeling is performed by selecting a set of labels (Jin & Ghahramani, 2003; Cour et al., 2011). The problem of MCLLP can also be regarded as a setting of PLL in which all labels given to a bag are considered as partial labels.

Let \(S\) denote a set of candidate labels given to a sample \((x, y)\). The conditions commonly assumed in PLL can be expressed as follows:

\[
p(y \in S|x, y) = 1
\]

Although there have been considerable studies on PLL, they relied on specific models and data structures, and in many cases, there was no theoretical basis (Chen et al., 2013; Nguyen & Caruana, 2008; Yao et al., 2020). Recently, Lv et al. (2020) proposed PRODEN, a PLL method that can be applied to any model, particularly deep learning models, to gradually update the labels of instances during training. They also theoretically showed that the learning method is classifier-consistent, i.e., on increasing the sample size, the classifier converges to that trained with normal labels. Furthermore, Feng et al. (2020) showed that the PRODEN estimator is also risk-consistent under some conditions.

2.3. Label Proportions Learning

LLP is a task of classifying instances in which the proportion or number of classes of instances is assigned to each bag. In this study, LLP is formulated using a multiset of labels, instead of a proportion of labels. The multiset is denoted as \(\{\cdot, \cdot\}\), which is different from tuple \((\cdot, \cdot)\) in that it ignores the order of elements.

Let \(K\) be the number of instances in a bag and \(\mathcal{X}^K = \{(X^{(1)}, \ldots, X^{(K)})|X^{(k)} \in \mathcal{X}\}\) be the space of the instance sets of size \(K\), and \(\mathcal{Y}^K = \{\{Y^{(1)}, \ldots, Y^{(K)}\}|Y^{(k)} \in \mathcal{Y}\}\) be the space of the label multisets of size \(K\). Subsequently, learning is performed from \((X, S) \sim P(\mathcal{X}^K, \mathcal{S}^K)\). Similar to the PLL constraints, LLP assumption for a labeled bag sample \((X, Y) \in \mathcal{X}^K \times \mathcal{Y}^K\) with a label multiset \(S \in \mathcal{S}^K\)
can be expressed as
\[ P_r\left(\left\{|Y^{(1)},...,Y^{(K)}|\right\} = S \mid X, S\right) = 1 \]

To solve the LLP problem, various models and methods have been studied, e.g., support vector machine (Rüping, 2010; Yu et al., 2013; Qi et al., 2017; Cui et al., 2016; Shi et al., 2019; Chen et al., 2017; Wang et al., 2015; Lu et al., 2019a), clustering (Stolpe & Morik, 2011), Bayesian network (Hernández-González et al., 2013; 2018), random forest (Shi et al., 2018), graphs (Poyiadzi et al., 2018), and linear models (Wang & Feng, 2013; Cui et al., 2017; Pérez-Ortiz et al., 2016).

Studies on MCLLP, which can be applied to deep learning models developed in recent years, can be classified into two policies: policy of constraints on predictions for bags and policy of assigning pseudo-labels to instances.

A typical method of restricting predictions to bags is DLLP (Ardehaly & Culotta, 2017). It has been shown experimentally that by restricting the predicted average of the instances to be close to the given class fraction of a bag, the classifier can learn to predict each instance class. Let \( p_0(Y^{(i)}|X^{(i)}) \in \mathbb{R}^C \) be a vector of the predicted class of instance, \( X^{(i)} \), by a model with parameter \( \theta \) that satisfies \( \Sigma_{c=1}^C p_0(c|X^{(i)}) = 1 \). In addition, let \( p_S \in \mathbb{R}^C \) be a vector representing the class proportions for the set of labels, \( S = \{Y^{(1)},...,Y^{(K)}\} \).

\[ p_S(c) = \frac{|\{j \in \{1,...,K\}| Y^{(j)} = c\}|}{|S|} \]

In DLLP, the cross-entropy between the bag label fraction, \( p_S \), and the predicted average vector of the instances, \( \bar{p}_X = \frac{1}{K} \Sigma_{k=1}^K p_0(Y^{(k)}|X^{(k)}) \), is taken.

\[ L_{prop} = -p_S^T \log(\bar{p}_X) \]

Based on this direction, some studies added consistency regularization (Tsai & Lin, 2020), contrastive learning (Yang et al., 2021), and semi-supervised learning using generative adversarial networks (Liu et al., 2019).

As a pseudo-label approach, Relax-OT (ROT) (Dulac-Arnold et al., 2019) was proposed to assign pseudo-labels based on entropy regularization and the optimal transport (OT) theory. Based on this approach, Liu et al. (2021) proposed to combine other MCLLP methods such as DLLP and OT pseudo-labeling. Despite numerous MCLLP studies, its statistical background is still lacking. Only recently, Jianxin Zhang (2022) proposed to utilize label noise correction framework (Patrini et al., 2017) and showed its statistical consistency. This method uses a nonparametrically estimated label transition matrix to estimate the true risk, on the other hand we utilize deformation of ERM formula to estimate it.

For the theoretical analysis of LLP, generalization error analysis has been conducted in several studies on binary classification. In a pioneering study, Quadrianto et al. (2009) proposed a method for solving LLP using MeanMap, which is the average output of a bag with an exponential family model, and analyzed the Rademacher complexity of MeanMap; however, they did not discuss its classification performance. Patrini et al. (2014) extended their investigation and analyzed the generalization error in two terms: “bag Rademacher complexity” and “label proportion complexity.” Yu et al. (2015) introduced “empirical proportion risk minimization,” and analyzed it under the only assumption that bags are mainly composed of one class. Lu et al. (2019b) and Lu et al. (2021) analyzed the generalization error using the ERM framework, and Scott & Zhang (2020) analyzed it using mutual contamination models. However, it is difficult to extend these methods to multiclass classification, and it has not yet been achieved.

As explained thus far, for MCLLP, it is empirically known that the class of each instance can be predicted by constraining its predicted average. However, a statistical theoretical background of MCLLP is lacking in the most of previous studies. In the next section, we propose a statistical learning method for MCLLP that can be applied to large datasets and various models, particularly deep learning models, using the ERM framework.

3. Learning from Label Proportions

In this section, we present the derivation of a risk-consistent loss estimator and the analysis of its estimation error bound. Subsequently, the derivation of the method to approximate this estimator for its use for large bags is described. This method is model-independent and can be applied to large datasets owing to the stochastic optimization.

3.1. Risk Estimation

Here, some assumptions about the bag generation process and labels are introduced. First, it is assumed that the probability distribution of a bag satisfies the following:

\[ P(x) = \frac{1}{K} \Sigma_{i=1}^K P(X^{(i)}) \]

Second, independence of the instances labels is assumed as follows:

\[ P(Y|X) = \Pi_{i=1}^K P(Y^{(i)}|X^{(i)}) \]

Finally, it is assumed that the label set given to a bag is independent of the instance set, under the given label of the instance. This is expressed as

\[ P(S|X,Y) = P(S|Y) \]
Let \( L(f(X), Y) = \sum_{k=1}^{K}[l(f(X^{(k)}), Y^{(k)})] \) and \( \mathcal{Y}_{s(i)}^{K} \) be all possible label candidates generated by \( S \):

\[
\mathcal{Y}_{s(i)}^{K} = \{ (Y^{(1)}, ..., Y^{(K)}) \in \mathcal{Y}^{K} | \{Y^{(1)}, ..., Y^{(K)}\} = S \}
\]

Thus, \( R(f) \) can be transformed as follows:

\[
R(f) = \frac{1}{K} \mathbb{E}_{(X,Y) \sim P(X,Y)}[L(f(X), Y)] = \frac{1}{K} \int_{\mathcal{X}^{K}} \sum_{Y \in \mathcal{Y}^{K}} P(X) P(Y|X) L(f(X), Y) dX
\]

\[
= \frac{1}{K|S^K|} \int_{\mathcal{X}^{K}} \sum_{Y \in \mathcal{Y}^{K}} P(X) \sum_{S \in S^K} P(S|X) \sum_{Y \in \mathcal{Y}^{K}} \frac{P(Y|X)}{P(S|X)} L(f(X), Y) dX
\]

Here, the following holds for \( P(S|Y) \).

\[
P(S|Y) = \begin{cases} 1 & \text{if } \{Y^{(1)}, ..., Y^{(K)}\} = S \\ 0 & \text{otherwise.} \end{cases}
\]

Therefore, for \( P(S|X) \), the following holds:

\[
P(S|X) = \sum_{Y \in \mathcal{Y}^{K}} P(S|Y) P(Y|X) = \sum_{Y \in \mathcal{Y}^{K}} P(Y|X)
\]

From the above, we can derive the following:

\[
R(f) = \frac{1}{K|S^K|} \int_{\mathcal{X}^{K}} \sum_{Y \in \mathcal{Y}^{K}} \sum_{S \in S^K} P(S,X) \sum_{Y \in \mathcal{Y}^{K}} \frac{P(Y|X)}{P(S|X)} L(f(X), Y) dX
\]

\[
= \frac{1}{K|S^K|} \int_{\mathcal{X}^{K}} \sum_{Y \in \mathcal{Y}^{K}} \sum_{S \in S^K} \Pi_{l=1}^{K} P(Y^{(l)}|X^{(l)}) L(f(X), Y) dX
\]

In the last line, we define \( R_{rc} \) as the risk over \( P(X,S) \).

For \( |S^K| \), the number of classes is \( C \) from the overlapping combinations, i.e.,

\[
|S^K| = \frac{(K + C - 1)!}{K!(C - 1)!}
\]

### 3.2. Risk Analysis

In this section, we discuss the analysis of the estimation error bound. We assume the instance generation is independent and identically distributed within each bag, and \( P(Y|X) \) is the true distribution, which is independent of the hypothesis \( f \in \mathcal{F} \). Let \( \hat{f}_{rc} = \min_{f \in \mathcal{F}} R_{rc}(f) \) be the hypothesis that minimizes the empirical risk, and \( f_{rc} = \min_{f \in \mathcal{F}} R_{rc}(f) \) be the hypothesis that minimizes the true risk. Let the hypothesis space be \( \mathcal{H}_y : \{ h : x \rightarrow f(x) | f \in \mathcal{F} \} \), and let \( \mathcal{R}_{n}(\mathcal{H}_y) \) be the expected Rademacher complexity of \( \mathcal{H}_y \) (Bartlett & Mendelson, 2002). Suppose loss function \( l(f(x), y) \) be \( \rho \)-Lipschitz with respect to \( f(x) \) for all \( y \in \mathcal{Y} \), bounded by \( M \).

**Theorem 3.1.** For any \( \delta > 0 \), we have with probability at least \( 1 - \delta \),

\[
R_{rc}(\hat{f}_{rc}) - R_{rc}(f_{rc}) \leq \frac{4\sqrt{2}\rho C}{|S^K|} \sum_{y=1}^{C} \mathcal{R}_{n}(\mathcal{H}_y) + \frac{2M}{|S^K|} \sqrt{\frac{\log \frac{2}{\delta}}{n}}
\]

In general, \( \mathcal{R}_{n}(\mathcal{H}_y) \) is bounded by some positive constant \( C_n/\sqrt{n} \), which indicates the convergence of \( f_{rc} \) to \( f_{rc}^{*} \), as \( n \to \infty \).

### 3.3. Learning Method

As a learning method, \( P(Y^{(k)}|X^{(k)}) \) is treated as a label weight, which is learned simultaneously as in PRODEN (Lv et al., 2020). Let the class prediction of models with parameter \( \theta \) be \( f_{\theta}(x) \in \mathbb{R}^C \), thus

\[
P(Y^{(k)} = y|X^{(k)}) = \begin{cases} \frac{f_{\theta}(Y^{(k)} = y|X^{(k)})}{\sum_{i=1}^{C} f_{\theta}(Y^{(k)} = i|X^{(k)})} & \text{if } y \in S \\ 0 & \text{otherwise.} \end{cases}
\]

(2)

Therefore, \( R_{rc} \) can be rewritten as follows:

\[
R_{rc}(f) = \frac{1}{K|S^K|} \mathbb{E}_{P(X^K,S^K)} \sum_{Y \in \mathcal{Y}_{s(i)}^{K}} \sum_{Y' \in \mathcal{Y}_{s(i)}^{K}} \frac{\prod_{l=1}^{K} P(Y^{(l)}|X^{(l)})}{\prod_{l=1}^{K} P(Y'^{(l)}|X^{(l)})} L(f(X), Y)
\]

The learning algorithm is shown in Algorithm 1.
In the following, a comparison is performed with existing methods. The main difference from these methods is the use of instance-level constraints. DLLP uses a bag-level loss. Moreover, owing its loss, DLLP is limited to cross-entropy; however, in our method any type of loss can be used. Another policy that has been extensively adopted as a method of MCLLP is assigning pseudo-labels. The proposed loss can also be regarded as a method using pseudo-labels by considering the label weight as a label. However, whereas the OT-based methods for assigning pseudo-labels lack a theoretical background for their assignment, our method is a natural derivation from importance weighting. Finally, the difference in PRODEN used for PLL is that the weights of each instance consider the label weights of the other instances in a bag. For example, for a bag with size 2, if the model has high confidence for one of the instances, the proposed method can assign a label with a large weight to the instance with low confidence.

### 3.4. Approximation Method

Because the proposed risk estimator is computationally expensive, it is difficult to calculate, when \( K \) becomes large. As a solution to this problem, a proposed method is to approximate \( R_{\text{rec}}(f) \) using the bag-level loss proposed in the existing research. In Equation (3), the expectation of the bag and label set and the loss term are removed, and only the terms related to \( X(1) \) are extracted. Thus, we obtain

\[
P(Y(1)|X(1)) \sum_{Y(1) \in S} \frac{\prod_{l=1}^{K_1} P(Y(l)|X(l))}{Y(1) \in Y_{\sigma(S)}^{K_1} \prod_{l=2}^{K_1} P(Y(l)|X(l))}
\]

In the following, we derive an approximation method of \( K - 1 \) instance weight \( \sum_{Y(1) \in Y_{\sigma(S)}^{K_1} \prod_{l=2}^{K_1} P(Y(l)|X(l))} \).

Note that this term can be rewritten as the \( K - 1 \) size bag weight as

\[
P(S|Y(1) \setminus X(1)) = Y(1) \in Y_{\sigma(S)}^{K_1} \prod_{l=2}^{K_1} P(Y(l)|X(l))
\]

Thus, from Equation (2), the following holds for the label weight of a bag of candidate size \( K - 1 \).

\[
\sum_{Y(1) \in S} P(S|Y(1) \setminus X(1)) = 1
\]

Because the total is fixed, the label weight of a bag is approximated using the likelihood-like score of the candidate bag. In DLLP, for a sample \((X, S)\), the error of the prediction is the cross-entropy of the predicted mean of the instances, \( \bar{p}_X \), and the given class fraction, \( p_s \). It is minimized when \( \bar{p}_X \) and \( p_s \) are equal, and a bag with class proportion \( \bar{p}_X \), is most certain. Therefore, this negative cross-entropy is proposed to be used as a measure of the likelihood of a bag. Specifically, it is proposed to take softmax using the temperature parameter, \( T \), and use it as the label weight. It is approximated as follows:

\[
\hat{P}(S|Y(1) \setminus X(1)) = \frac{\exp(p_{S|Y(1)} \log(\hat{P}_X|X(1))/T)}{\sum_{S' \in (S|Y(1)\setminus Y(1))} \exp(p_{S'|Y(1)} \log(\hat{P}_X|X(1))/T)}
\]

Using this approximation, Equation (3) becomes

\[
R_{\text{rec-approx}}(f) = \frac{1}{K|S^K|} \sum_{Y(1) \in Y_{\sigma(S)}^{K_1}} \sum_{k=1}^{K} P(Y(k)|X(1)) \sum_{Y(1) \in Y_{\sigma(S)}^{K_1}} \sum_{l=1}^{K} P(Y(l)|X(1)) I(f(X(1)), Y(k))
\]

In the following, the approximation in Equation (5) is discussed. To consider the candidates for Equation (4), \( P(S|Y_a(1)|X_{K-1}) \) and \( P(S|Y_b(1)|X_{K-1}) \) are compared, where \( X_{K-1} = X \setminus X(1) \) and \( Y_a(1), Y_b(1) \in S \). Let \( S'_a = S|Y_a(1)|X_{K-1} \) and \( S'_b = S|Y_b(1)|X_{K-1} \). Thus, the estimated and true ratios of these two become

\[
\hat{P}(S'_a|X_{K-1}) = \frac{\exp(p_{S'_a} \log(\hat{P}_X|X_{K-1}))/T)}{\exp(p_{S'_b} \log(\hat{P}_X|X_{K-1}))/T)}
\]

\[
\hat{p}_X|X_{K-1}(Y_a(1)) = \frac{\log \hat{p}_X|X_{K-1}(Y_a(1))}{K - 1} - \log \hat{p}_X|X_{K-1}(Y_b(1))
\]

\[
= \frac{(\hat{p}_X|X_{K-1}(Y_a(1)))^{1/T + x - 1}}{(\hat{p}_X|X_{K-1}(Y_b(1)))^{1/T + x - 1}}
\]

\[
= \frac{(\Sigma_i P(Y(i)|X(1)))^{1/T + x - 1}}{(\Sigma_i P(Y(i)|X(1)))^{1/T + x - 1}}
\]

\[
= \frac{P(S'_a|X_{K-1})}{P(S'_b|X_{K-1})}
\]

Therefore, by taking the temperature parameter as \( T = \frac{1}{K - 1} \), this approximation regards \( P(S'|X_{K-1}\setminus X(1)) \) as a constant independent of \( X(1) \). Alternatively, it can be stated that the approximation method considers a bag with more
instances having a higher likelihood for the added labels, \( Y^{(1)}_a \), to be more confident. This approximation holds exactly for \( K = 2 \). Although it is not necessarily true for a general \( K \), it will be subsequently confirmed in the following section that this approximation can be used to learn for a large \( K \).

4. Experiments

In this section, the analysis of the proposed risk estimator and its approximation method by experiments is discussed. The implementation used PyTorch (Paszke et al., 2019), and the experiments were conducted on a NVIDIA Tesla V100 GPU.

Experimental Settings: Four extensively used datasets are selected: MNIST (LeCun et al., 1998), Fashion-MNIST (Xiao et al., 2017), Kuzushiji-MNIST (Cianuwait et al., 2018), and CIFAR-10 (Krizhevsky, 2009). Each bag is randomly generated from a dataset, and the number of bags is changed as \( K = \{2, 4, 8, 16, 32, 64, 128\} \). Various models are used: linear model, 5-layer perceptron (multilayer perceptron (MLP)), and 12-layer ConvNet (Samuli Laine, 2017). 10% of the training data are used as the validation data, and the learning rate is searched from \( \{10^{-6}, ..., 10^{-1}\} \). The batch size is set as \( \frac{1024}{K} \), and the Adam optimizer is used. A detailed description of the dataset and the experimental setup can be found in Appendix.

Baselines: The proposed method is analyzed by comparing it to some baselines.

- RC updates according to Equation (3).
- RC-approx updates according to Equation (6).
- RC-init, in which the first few epochs are trained according to DLLP, which is subsequently switched to RC-approx.
- RC-const according to Equation (6), where the label weights are estimated as a constant, i.e., \( \tilde{P} = const \).
- PN, a supervised learning method in which instances are given the correct labels.
Table 2. Classification test accuracies (mean±std) on MNIST, Fashion-MNIST (F-MNIST) and Kuzushiji-MNIST (K-MNIST) datasets for MLP model.

|    | $K = 2$ | 4 | 8 | 16 | 32 | 64 | 128 |
|----|--------|---|---|----|----|----|-----|
| MNIST |        |    |   |    |    |    |     |
| PN  | 98.6±0.1% | - | - | - | - | - | - |
| RC  | 98.6±0.1% | 98.5±0.1% | 98.6±0.1% | NA | NA | NA | NA |
| RC-APPROX | 98.6±0.1% | 98.7±0.1% | 98.6±0.1% | 98.6±0.0% | 98.5±0.1% | 98.4±0.1% | 97.8±0.1% |
| RC-INIT | 98.6±0.0% | 98.6±0.1% | 98.6±0.1% | 98.6±0.1% | 98.5±0.1% | 98.5±0.1% | 98.3±0.1% |
| RC-CONST | 98.6±0.1% | 98.2±0.1% | 97.0±0.1% | 94.4±0.2% | 85.6±1.4% | 57.5±2.5% | 34.0±0.5% |
| DLLP | 98.6±0.1% | 98.6±0.1% | 98.5±0.1% | 98.5±0.1% | 98.4±0.1% | 98.4±0.1% | 98.0±0.2% |
| ROT  | 98.7±0.0% | 98.6±0.1% | 98.6±0.1% | 98.3±0.0% | 97.4±0.1% | 95.3±0.2% | 91.4±0.6% |
| PRODEN | 98.6±0.1% | 98.4±0.1% | 98.0±0.1% | 96.7±0.1% | 83.2±1.1% | 43.9±4.0% | 24.6±4.3% |

|    | $K = 2$ | 4 | 8 | 16 | 32 | 64 | 128 |
|----|--------|---|---|----|----|----|-----|
| PRODEN | 98.5±0.1% | 98.5±0.1% | 98.5±0.1% | 98.5±0.1% | 98.5±0.1% | 98.5±0.1% | 98.3±0.1% |

- DLLP (Ardehaly & Culotta, 2017) updates according to bag-wise constraints.
- ROT (Dulac-Arnold et al., 2019) updates according to pseudo-labels based on the OT.
- PRODEN (Lv et al., 2020), a partial label learning that treats the given labels as partial labels.

For RC-approx, the temperature parameter, $T$, is set as $\frac{1}{n-1}$, as proposed in Section 3.4. For RC-init, the first 40 epochs are trained using DLLP, which is subsequently switched to RC-approx.

**Results**: Tables 1–3 list the means and standard deviations of the test results for five samples for each model and dataset. Considering the results for small bags $K = \{2, 4, 8, 16\}$, our method RC and RC-approx are found to be comparable to or better than the other methods. The accuracy on the test dataset and the update of the label weights measured by the KL-divergence between $n$th and $n + 1$th epoch are shown in Figure 2. The labels are gradually identified as the learning progresses. Some settings perform better than the supervised learning, PN, which is also seen from the PRODEN results.

In contrast, for relatively large bags $K = \{64, 128\}$, DLLP and ROT are more effective than RC-approx in some settings. Because RC-approx learns the label weights simultaneously, the models are probably initially fitted with noisy weights. One possible solution to this problem is to learn the first few epochs using bag-level constraints, such as in DLLP, learn the label weights, and subsequently use RC-approx (RC-init). Although the linear model fits directly the label weights learned by DLLP and its performance is not improved by initializing, the experiments using the deep learning model improve the performance. The test accuracies of DLLP, RC-init, and RC-approx on CIFAR-10 are illustrated in Figure 3. Noticeably, RC-approx is slow in learning and fitting the noisy label weights, whereas RC-init improves the performance by switching the losses after learning the label weights with DLLP.

Finally, the approximation methods are discussed. For small bags with $K = \{2, 4, 8\}$, RC-approx performs as well as
Table 3. Classification test accuracies on CIFAR-10 dataset for ConvNet model.

| CIFAR-10 | K = 2 | 4 | 8 | 16 | 32 | 64 | 128 |
|----------|------|---|---|----|----|----|-----|
| PN       | 86.8±0.4% | - | - | - | - | - | -   |
| RC       | 86.7±0.4% | 86.4±0.3% | 85.3±0.5% | NA | NA | NA | NA   |
| RC-APPROX| 86.5±0.2% | 87.7±0.1% | 86.3±0.3% | 80.2±1.1% | 68.7±2.1% | 59.5±0.8% | 51.3±1.0% |
| RC-INT   | 86.6±0.2% | 87.6±0.3% | 87.1±0.2% | 84.6±0.4% | 77.8±0.6% | 68.6±1.0% | 57.0±0.6% |
| RC-CONST | **87.8±0.4%** | 84.8±0.2% | 78.8±0.7% | 69.1±0.6% | 57.9±1.7% | 46.5±0.7% | 36.9±1.3% |
| DLLP     | 86.1±0.5% | 86.1±0.2% | 85.1±0.4% | 82.4±0.4% | 75.4±0.8% | 65.6±1.0% | 52.9±0.5% |
| ROT      | 87.6±0.4% | 87.3±0.4% | 87.0±0.4% | 79.3±1.5% | 65.9±2.1% | 54.7±0.9% | 47.0±0.6% |
| PRODEN   | 87.4±0.3% | 85.7±0.5% | 81.0±1.0% | 64.6±1.4% | 28.4±3.3% | 13.3±0.6% | 12.2±1.6% |

5. Conclusion

In this paper, an ERM-based learning in instances for MCLLP is proposed. Specifically, risk-consistent losses are derived based on ERM. These losses are typically computationally expensive and difficult to estimate for large bags, and to solve this problem, this calculation is conducted by diverting the constraints for the existing bags. Our proposed method can be applied to any model and any stochastic optimization method. The experimental results show the effectiveness of the proposed method.

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A. Proof of Theorem 3.1

Here we define risk $R_{rc(Q)}$, which is parametrized with fixed distribution $Q$ and a function space of our RC method, $G_{rc}$ as follows:

$$R_{rc(Q)} = \frac{1}{K|S^K|} \mathbb{E}_{p(X^K,S^K)} \left[ \sum_{Y \in Y^K} \frac{1}{Y'^{\ell}} \sum_{Y'^{\ell} \in Y^{\ell}} Q(Y^{\ell}|Y'^{\ell}) \right] L(f(X), Y)$$

Let $G_{rc} = \{(X, S) \mapsto \frac{1}{K|S^K|} \sum_{Y \in Y^K} \frac{1}{Y'^{\ell}} \sum_{Y'^{\ell} \in Y^{\ell}} Q(Y^{\ell}|Y'^{\ell}) \sum_{k=1}^K l(f(X^{(k)}), Y^{(k)}) | f \in F \}$

Note that $R_{rc(Q)}$ coincides with $R$ when $P(Y|X) = Q(Y|X)$ holds.

**Lemma A.1.** Assume $l$ is bounded by constant $M$. ∀δ > 0, at least probability of $1 - δ$,

$$\sup_{f \in F} |R_{rc(Q)}(f) - \hat{R}_{rc(Q)}(f)| \leq 2\mathfrak{R}_n(G_{rc}) + \frac{M}{|S^K|} \sqrt{\frac{\log \frac{2}{\delta}}{2n}}$$

**Proof.** We first consider one direction $\sup_{f \in F} R_{rc(Q)}(f) - \hat{R}_{rc(Q)}(f)$. Since $0 \leq l(x, y) \leq M$ holds, replacing one sample $(X, S)$ to $(X', S')$ will not change $\sup_{f \in F} R_{rc(Q)}(f) - \hat{R}_{rc(Q)}(f)$ larger than $\frac{M}{|S^K|}$. Then by McDiarmid’s inequality, for ∀δ > 0, at least probability of $1 - \frac{\delta}{2}$, the following holds.

$$\sup_{f \in F} R_{rc(Q)}(f) - \hat{R}_{rc(Q)}(f) \leq \mathbb{E} \left[ \sup_{f \in F} R_{rc(Q)}(f) - \hat{R}_{rc(Q)}(f) \right] + \frac{M}{|S^K|} \sqrt{\frac{\log \frac{2}{\delta}}{2n}}$$

By symmetrization trick used in (Vapnik, 1998),

$$\mathbb{E} \left[ \sup_{f \in F} R_{rc(Q)}(f) - \hat{R}_{rc(Q)}(f) \right] \leq 2\mathfrak{R}_n(G_{rc})$$

In the same way, $\sup_{f \in F} \hat{R}_{rc(Q)}(f) - R_{rc(Q)}(f)$ can be bounded with at least probably of $1 - \frac{\delta}{2}$. \hfill \Box

**Lemma A.2.** Assume $l$ is $\rho$-Lipschitz function and the instance generation is independent and identically distributed within each bag, and $Q(Y|X)$ are fixed function independent of hypothesis $f \in F$. Then the following holds.

$$\mathfrak{R}_n(G_{rc}) \leq \sqrt{2\rho} \sum_{y=1}^C \mathfrak{R}_n(H_y)$$

**Proof.** Let $Q(Y|X, S)$ and $\phi_{(X,S)} : \mathbb{R}^C \rightarrow \mathbb{R}_+$, which are fixed function independent of $f \in F$, as

$$Q(Y|X, S) = \frac{\prod_{k=1}^K Q(Y^{(k)}|X^{(k)})}{\sum_{Y'^{\ell} \in Y^{\ell}} \prod_{k=1}^K Q(Y'^{(k)}|X^{(k)})}$$

$$\phi_{(X,S)}(z) = \frac{1}{K|S^K|} \sum_{Y \in Y^K} Q(Y|X, S) l(z, Y^1)$$
Since \( Q_{Y \in Y^K_S} (Y | X, S) = 1 \), \( \phi(X, S) \) is \( \frac{\rho}{K|S^K|} \)-Lipschitz function. Thus,

\[
\mathcal{R}_n(\mathcal{G}_{rc}) = \mathbb{E}_{P(X^K_S, S^K)} \left[ \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \sum_{k=1}^{K} \phi_i \phi_k (f(X^{(i)})) \right] \\
\leq K \mathbb{E}_{P(X^K_S, S^K)} \left[ \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \sum_{k=1}^{K} \phi_i \phi_k (f(X^{(1)})) \right] \\
\leq K \sqrt{2 \rho \log \frac{2}{\delta}} \mathbb{E}_{P(X^K_S, S^K)} \left[ \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{C} \phi_i \phi_j (f(X^{(1)})) \right] \\
= \sqrt{2 \rho \log \frac{2}{\delta}} \sum_{j=1}^{C} \mathcal{R}_n(\mathcal{H}_j)
\]

where we used Rademacher vector contraction inequality (Maurer, 2016) in the second line.

From above lemmas, we can derive,

\[
R_{rc(Q)}(\hat{f}) - R_{rc(Q)}(f^*) \leq R_{rc(Q)}(\hat{f}) - \hat{R}_{rc(Q)}(\hat{f}) + \hat{R}_{rc(Q)}(\hat{f}) - R_{rc(Q)}(f^*) \\
\leq R_{rc(Q)}(\hat{f}) - \hat{R}_{rc(Q)}(\hat{f}) + R_{rc(Q)}(\hat{f}) - R_{rc(Q)}(f^*) \\
\leq 2 \sup_{f \in \mathcal{F}} |\hat{R}_{rc(Q)}(f) - R_{rc(Q)}(f)| \\
\leq 4 \mathcal{R}_n(\mathcal{G}_{rc}) + \frac{2M}{|S^K|} \sqrt{\frac{\log \frac{2}{\delta}}{2n}} \\
\leq 4 \sqrt{2 \rho \log \frac{2}{\delta}} \sum_{j=1}^{C} \mathcal{R}_n(\mathcal{H}_j) + \frac{2M}{|S^K|} \sqrt{\frac{\log \frac{2}{\delta}}{2n}}
\]

In Theorem 3.1, we assume \( P(Y | X) \) is the true distribution, which concludes the proof. However, although we derived the estimation error bound of \( R_{rc(Q)} \), what we really want to minimize is \( R \). Here we bound the difference between \( R \) and \( R_{rc(Q)} \).

**Lemma A.3.** Let \( \epsilon = \mathbb{E}_{P(X^K_S, S^K)} \left[ \sum_{Y \in Y^K_S} |P(Y | X, S) - Q(Y | X, S)| \right] \). For all \( f \in \mathcal{F} \), it holds that

\[
|R(f) - R_{rc(Q)}(f)| \leq \frac{M \epsilon}{|S^K|}
\]

**Proof.**

\[
|R(f) - R_{rc(Q)}(f)| \leq \mathbb{E}_{P(X^K_S, S^K)} \left[ \sum_{i=1}^{K} \frac{1}{K|S^K|} \sum_{Y \in Y^K_S} |P(Y | X, S) - Q(Y | X, S)| \right] \\
\leq \frac{M}{|S^K|} \mathbb{E}_{P(X^K_S, S^K)} \left[ \sum_{Y \in Y^K_S} |P(Y | X, S) - Q(Y | X, S)| \right] \\
= \frac{M \epsilon}{|S^K|}
\]

\[\square\]
B. Experiment Settings

In this section, we describe detail information of the experiments.

B.1. Datasets

We used four extensively used datasets:

- MNIST (LeCun et al., 1998): 10-class datasets of handwritten digits. Each image is grayscale and has $28 \times 28$ size.
- Fashion-MNIST (Xiao et al., 2017): 10-class datasets of fashion-items. Each image is grayscale and has $28 \times 28$ size.
- Kuzushiji-MNIST (Clanuwat et al., 2018): 10-class datasets of japanese handwritten kuzushiji, a cursive writing style letter. Each image is grayscale and has $28 \times 28$ size.
- CIFAR-10 (Krizhevsky, 2009): 10-class datasets of vehicles and animals datasets. Each image has RGB channel and has $32 \times 32$ size.

B.2. Models

We used linear and MLP models for MNIST, Fashion-MNIST and Kuzushiji-MNIST datasets, ConvNet model for CIFAR-10 dataset. The linear model refers to a $d$-$10$ linear function, where $d$ is input size. MLP is 5-layer perceptron $d$-$300$-$300$-$300$-$300$-$10$ model with ReLU activation. Each dense layers are followed by Batch normalization. ConvNet architecute is discribed in Table 5. We add $1e-5$ weight decay to each model.

| Input $3\times32\times32$ image | $3\times3$ conv. 128 followed by LeakyReLU $\times 3$ |
|--------------------------------|--------------------------------------------------|
|                                 | max-pooling, dropout with $p = 0.25$            |
|                                 | $3\times3$ conv. 256 followed by LeakyReLU $\times 3$ |
|                                 | max-pooling, dropout with $p = 0.25$            |
|                                 | $3\times3$ conv. 512 followed by LeakyReLU $\times 3$ |
|                                 | global mean pooling, Dense 10                   |

*Table 5. ConvNet model for CIFAR-10.*