ProPaLL: Probabilistic Partial Label Learning

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Abstract

Partial label learning is a type of weakly supervised learning, where each training instance corresponds to a set of candidate labels, among which only one is true. In this paper, we introduce ProPaLL, a novel probabilistic approach to this problem, which has at least three advantages compared to the existing approaches: it simplifies the training process, improves performance, and can be applied to any deep architecture. Experiments conducted on artificial and real-world datasets indicate that ProPaLL outperforms the existing approaches.

1. Introduction

Deep neural networks achieve excellent performance in many real applications. However, they require a large-scale training set with correctly labeled samples. Obtaining such a set is time-consuming, expensive, and, in some domains, impossible due to discrepancies between labeling experts (Armato III et al., 2011). In consequence, many contemporary datasets are weakly labeled, forcing researchers to propose adequate learning strategies within the Weakly Supervised Learning paradigm (Zhou, 2018).

The most common problem setting in supervised learning assumes that the class to which the training data belongs is provided as a label, namely an ordinary label. However, in some cases, each training instance is associated with a set of candidate labels, among which exactly one is true. This setting, known as Partial Label Learning (PLL) (Jin & Ghahramani, 2002), occurs in many real-world tasks, such as image annotation (Chen et al., 2017), web mining (Luo & Orabona, 2010), multimedia content analysis (Zeng et al., 2013; Chen et al., 2017), and ecoinformatics (Liu & Dietterich, 2012; Tang & Zhang, 2017). Moreover, in the special case of PLL, called Complementary Label Learning (CLL) (Ishida et al., 2017), the number of candidate labels is only one less than the number of classes, making this task even more challenging.

The standard approaches to partial and complementary label learning are incompatible with high-efficient stochastic optimization and cannot handle large-scale datasets (Liu & Dietterich, 2012). On the other hand, more contemporary methods use deep networks with stochastic optimizers as a backbone, but they are restricted, e.g. to some specific architectures (Yao et al., 2020). Moreover, they commonly rely on modeling the relationship between the complementary and ground-truth labels for each training instance. For this purpose, they often use the iterative Expectation-Maximization (EM) technique, where M-step learns a predictor while E-step increases weights of more possible labels every few training epochs (Tang & Zhang, 2017; Feng & An, 2019; Lv et al., 2020), resulting in a suboptimal solution. Therefore, partial and complementary label learning still brings many challenges.

In this paper, we introduce ProPaLL (abbr. from Probabilistic Partial Label Learning), a novel probabilistic approach to partial label learning problems to address the abovementioned issues. For this purpose, we modify Binary Cross EntropyLoss as follows:

\[
\text{CE} = -\frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{K} y_{ij} \log p_{ij}
\]

where \( y_{ij} \) is the ground-truth label vector for the \( i \)-th instance and \( p_{ij} \) is the predicted probability of the \( j \)-th label. The total loss is then computed as the sum of CE for all candidate labels.

\[
\text{ProPaLL} = \sum_{i=1}^{N} \text{CE}(y_{i}, \mathbf{p}_i) + \lambda \sum_{i=1}^{N} \frac{1}{K} \sum_{j=1}^{K} \left( p_{ij} - \frac{1}{K} \right)^2
\]

where \( \lambda \) is a hyperparameter controlling the trade-off between classification and smoothness terms.

Figure 1: Accuracy of our ProPaLL and the popular PLL approaches for the MNIST dataset depending on the number of candidate labels. While the performance of baseline PLL methods drops rapidly for more complicated setups, our method maintains 90% accuracy even for 9 candidate labels.

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1Our code with ProPaLL is available on the GitHub repository https://github.com/anonymised.
Figure 2: Detailed analysis of ProPaLL training indicates that it gradually learns consecutive classes instead of progressively increasing sensitivity for all of them. In this image, the middle part presents model accuracy for all classes in time, the bottom part shows the sensitivity of particular classes also in time, while the top part shows confusion matrices in time points corresponding to their location. A model starts with learning classes 1, 3, 4, 6, and 7 (before iteration 1000). Then, around iteration 1500, it learns class 8, while classes 2 and 9 are trained around iteration 2700. Finally, it learns class 5 near iteration 4300.

2. Related works

Partial label learning. Existing PLL approaches often aim to fit widely-used learning techniques to disambiguate partial label data. For example, (Jin & Ghahramani, 2002) and (Liu & Dietterich, 2012) maximize the likelihood defined over the candidate label set. (Hüllermeier & Beringer, 2006) and (Zhang & Yu, 2015) determine the class label of an unseen instance via voting among the candidate labels of its k-nearest neighbors. (Nguyen & Caruana, 2008) and (Yu & Zhang, 2016) maximize the classification margins between candidate and non-candidate labels. While boosting techniques (Tang & Zhang, 2017) update the weights and confidence over the candidate labels in each boosting round. Disambiguation strategies ignore considering the generalized label distribution, in contrast to disambiguation-free strategies (Xu et al., 2019; Zhang et al., 2016), which learn a multi-class predictive model by fitting a regularized multi-output regressor with the generalized label distributions (recovered, e.g., by leveraging the topological information of the feature space). The abovementioned methods have low efficiency and cannot handle large-scale datasets. That is why recent approaches move toward deep networks, employing various regularizers (Yao et al., 2020) or risk estimators (Feng et al., 2020; Lv et al., 2020). Moreover, most recent approaches (Xu et al., 2021) consider instance-dependent (feature-dependent) candidate labels.
Complementary label learning. CLL was first proposed in (Ishida et al., 2017), where modified one-versus-all (OVA) and pairwise-comparison (PC) losses are proposed. (Yu et al., 2018) introduce a different formulation for complementary labels by employing the forward loss correction technique (Patrini et al., 2017) but limit the loss function to softmax cross-entropy loss. This limitation is overcome by (Ishida et al., 2019), who propose a new unbiased risk estimator, allowing usage of any loss (convex, non-convex) and any model (parametric, non-parametric). Moreover, one of the most recent approaches generalizes OVA and PC loss functions for more than one complementary label for each training instance (Katsura & Uchida, 2020). (Xu et al., 2020) applies conditional generative adversarial networks (Goodfellow et al., 2014). Finally, (Gao & Zhang, 2021) adopts weighted loss to the empirical risk to maximize the predictive gap between the potential ground-truth and complementary labels. Our method introduces a novel loss function that overpasses the performance of existing approaches in PLL and CLL setups.

3. Probabilistic Partial Label Learning

In this section, we introduce the loss function used by ProPaLL. However, since it bases on Binary Cross Entropy (BCE), we first establish notation and derive the BCE formula in the standard multi-label classification problem.

Notations. Let us consider the classification task for $k$ classes with the product $\{0, 1\}^k$ at the output. Moreover, let $p_i$ denotes the probability of obtaining $1$ at $i$-th output coordinate. Then, the probability of drawing a binary sequence $b = (b_1, \ldots, b_k) \in \{0, 1\}^k$ is defined as

$$P(b) = \prod_{i=1}^{k} p_i^{b_i}(1 - p_i)^{1-b_i}.$$  

Consequently, the probability of predicting class $c$ (i.e. obtaining $1$ at $c$-th coordinate and zero for all other coordinates) is given by

$$P(\text{onehot}(c)) = p_c \cdot \prod_{j \neq c}(1 - p_j).$$  

BCE loss for ordinary labels. In the most common problem setting of supervised learning, each point $x$ from the dataset $X \subset \mathbb{R}^{d}$ is associated with a class $c \in \{1, \ldots, k\}$, and we aim to train a network $F_\theta : \mathbb{R}^{d} \to \mathbb{R}^{k}$

$$F_\theta(x) = (r_1(x), \ldots, r_k(x)) \in \mathbb{R}^{k},$$

where $\theta$ are the network weights and logits $r_i(x)$ denotes the network output before the sigmoid $\sigma(r) = 1/(1+\exp(-r))$. The output after sigmoid corresponds to the probability of predicting class $i$

$$p_i(x) = \sigma(r_i(x)),$$

and the opposite probability, i.e. the probability of predicting class other than $i$ equals

$$1 - \sigma(r_i(x)) = \sigma(-r_i(x)).$$

Thus, by (1) probability for point $x$ and class $c$ is defined as

$$P(\text{onehot}(c)) = p_c(x) \cdot \prod_{j \neq c}(1 - p_j(x)),$$

and consequently the BCE cost is given as the minus log-likelihood:

$$\text{cost}(x) = -\log(p_c(x)) - \sum_{j \neq c} \log(1 - p_j(x)).$$  

Since

$$-\log \sigma(r) = - \log \frac{1}{1+\exp(-r)} = \text{LogSumExp}(0, -r)$$

and

$$-\log(1 - \sigma(r)) = - \log \sigma(-r) = \text{LogSumExp}(0, r),$$

we can rewrite the cost function in terms of the logits by

$$\text{cost}(x) = \text{LogSumExp}(0, -r_c(x)) + \sum_{j \neq c} \text{LogSumExp}(0, r_j(x)).$$

In the evaluation, we associate $x$ with the label obtaining the greatest probability.

BCE adaptation for partial label learning. In the partial label learning setting, each point $x \in X$ is associated with a candidate label set $S \subset \{1, \ldots, k\}$, where exactly one $c \in S$ is true. Therefore, to adapt BCE into this setting, we introduce $S \subset \{0, 1\}^k$, the set with at least one 1 in the set $S$, and 0 outside $S$

$$S = \{b \in \{0, 1\}^k : \sum_{i \in S} b_i \geq 1, \sum_{j \notin S} b_j = 0\},$$

and we aim to maximize the probability of $S$

$$P(S) = (1 - \prod_{i \in S}(1 - p_i(x))) \cdot \prod_{j \notin S}(1 - p_j(x)).$$  

The first part corresponds to the opposite probability of occurring only 0 in $S$ and the second part to the probability of occurring only 0 in labels complementary to $S$. It can seem counterintuitive that we do not penalize the model for predicting more than one label from $S$, but thanks to that, the network can easily switch from one class to another when it learns how to classify a given point.
Table 2: Description of the real-world partial label datasets.

| Datasets         | #Train | #Test | #Feats | #Labels |
|------------------|--------|-------|--------|---------|
| Lost             | 898    | 224   | 108    | 16      | 2.23   |
| Soccer Player    | 13978  | 3494  | 279    | 171     | 2.09   |
| Yahoo! News      | 18393  | 4598  | 163    | 219     | 1.91   |
| MSRCv2           | 1406   | 352   | 48     | 23      | 3.16   |
| BirdSong         | 3998   | 1000  | 38     | 13      | 2.18   |

Table 1: Description of the real-world partial label datasets.

| Methods       | MNIST | Kuzushiji | Fashion | CIFAR-10 |
|---------------|-------|-----------|---------|----------|
| ProPaLL       | 98.73 (0.05) | 93.50 (0.17) | 90.40 (0.06) | 84.32 (0.37) |
| VALEN         | 97.93 (0.05) | 88.76 (0.26) | 88.98 (0.16) | 81.53 (0.53) |
| PRODEN        | 97.97 (0.03) | 88.55 (0.10) | 88.94 (0.12) | 81.61 (1.52) |
| RC            | 97.86 (0.03) | 86.65 (0.10) | 88.59 (0.08) | 81.30 (1.30) |
| CC            | 97.73 (0.02) | 87.99 (0.03) | 88.93 (0.06) | 80.17 (1.09) |
| D^2CNN        | 95.12 (0.16) | 81.03 (0.78) | 80.42 (0.21) | 75.11 (0.11) |
| GA            | 96.29 (0.19) | 82.36 (0.98) | 81.81 (0.99) | 60.14 (1.35) |

Table 2: Test accuracy (mean (std)% ) on artificial datasets corrupted by the uniform generating procedure. The highest accuracy is bolded.

ProPaLL cost function. Based on the previous paragraph, we finally define the cost function of ProPaLL as the minus log-likelihood of probability defined in Equation (3):

\[
\text{cost}(x) = -\log P(S) = -\log \left(1 - \prod_{i \in S} (1 - p_i(x)) \right) - \sum_{j \notin S} \log(1 - p_j(x)),
\]

and in terms of the logits, as

\[
\text{cost}(x) = -\log \left(1 - \exp\left(- \sum_{i \in S} \text{LogSumExp}(0, r_i(x))\right) \right) + \sum_{j \notin S} \text{LogSumExp}(0, r_j(x)).
\]

Please note that when \( S \) is one-element set \( \{c\} \), it reduces to (2). Moreover, in Appendices, we provide details on the implementation of ProPaLL loss function.

4. Experimental Setup

In this section, we describe datasets used in the evaluation and the baseline methods to which we compare our ProPaLL approach.

Datasets. First of all, we consider four artificial datasets, created based on MNIST (LeCun et al., 1998), Fashion-MNIST (Xiao et al., 2017), Kuzushiji-MNIST (Clanuwat et al., 2018), and CIFAR-10 (Krizhevsky et al., 2009). All these datasets contain 60000 images split into 50000 training and 10000 testing sets. The CIFAR-10 has 32 × 32 RGB images, while the remaining datasets have 28 × 28 grayscale images. Moreover, in the original version of those datasets, each point corresponds to one of the 10 classes. Hence, to modify them to a partial label learning setting, we corrupt each training data point by associating it with a candidate label set containing the original label and a few other labels sampled uniformly or using an instance-dependent process (Xu et al., 2021).

In addition, we use five real-world partial label datasets: Lost (Cour et al., 2011), Soccer Player (Zeng et al., 2013) and Yahoo! News (Guillaumin et al., 2010) for automatic face naming from images or videos, MSRCv2 (Liu & Dietterich, 2012) for object classification, and BirdSong (Briggs et al., 2012) for bird song classification. Table 1 shows the statistics on these datasets, including the number of elements in the training and test set, the number of features, the number of classes, and the average number of candidate labels.

PLL baseline methods. We compare our approach to six state-of-the-art partial label learning methods:

- VALEN (Xu et al., 2021) recovers the label distribution and trains the predictive model iteratively in each epoch.
- PRODEN (Lv et al., 2020) updates the model and identification of true labels in a seamless manner.
- RC (Feng et al., 2020) uses the reweighting strategy to converge the true risk minimizer.
- CC (Feng et al., 2020) uses a transition matrix to form an empirical risk estimator.
- D^2CNN (Yao et al., 2020) uses an entropy-based regularizer to maximize the margin between the potentially correct label and the unlikely ones.
- GA (Ishida et al., 2019) is an unbiased risk estimator approach.

Moreover, in the case of real-world datasets, we additionally compare our method to five classical approaches:

- CLPL (Cour et al., 2011) uses averaging-based disambiguation.
- PL-SVM (Nguyen & Caruana, 2008) uses identification-based disambiguation.
- PL-KNN (Hüllermeier & Beringer, 2006) uses k-nearest neighbor weighted voting.
We compare our method to few state-of-the-art approaches:

Table 3: Test accuracy (mean (std)%) on artificial datasets

| Methods      | MNIST       | Kuzushiji   | Fashion    | CIFAR-10    |
|--------------|-------------|-------------|------------|-------------|
| ProPaLL      | 97.89 (0.08)| 86.26 (0.32)| 85.55 (0.33)| 75.75 (0.63)|
| VALEN        | 97.85 (0.05)| 86.19 (0.14)| 86.17 (0.19)| 80.38 (0.52)|
| PRODEN       | 97.69 (0.04)| 85.71 (0.12)| 85.54 (0.09)| 79.80 (0.28)|
| RC           | 97.60 (0.05)| 84.86 (0.11)| 85.51 (0.10)| 79.46 (0.25)|
| CC           | 97.44 (0.03)| 82.67 (1.82)| 85.19 (0.04)| 78.98 (0.60)|
| D²CNN        | 94.63 (0.16)| 83.03 (0.78)| 82.42 (0.21)| 73.11 (0.11)|
| GA           | 95.25 (0.07)| 82.45 (0.63)| 80.41 (0.24)| 77.57 (0.76)|

Table 3: Test accuracy (mean (std)%) on artificial datasets corrupted by the instance-depending generating procedure (Xu et al., 2021). The highest accuracy is bolded.

Figure 3: Critical difference diagrams comparing results of the considered methods shown in Tables 2 and 3 (smaller is better). ProPaLL performs significantly better than all baseline methods except VALEN and PRODEN.

- IPAL (Zhang et al., 2017) is a non-parametric method that applies the label propagation strategy to iteratively update the confidence of each candidate label.
- PLLE (Xu et al., 2019) estimates the generalized description degree of each class label value via graph Laplacian.

Like in (Lv et al., 2020; Xu et al., 2021), we employ a 5-layer perceptron for MNIST, Fashion-MNIST, Kuzushiji-MNIST datasets, and ResNet-32 (He et al., 2016) for CIFAR-10. Moreover, we train each model for 500 epochs and use the stochastic gradient descent with momentum 0.9 to optimize models. Hyperparameters are the same as in the original papers. Details are provided in Appendices.

CLL baseline methods. In this scenario, we used the typical datasets described in the previous paragraph, namely MNIST, Fashion-MNIST, Kuzushiji-MNIST, CIFAR-10. We compare our method to few state-of-the-art approaches:

- PC and OVA (Katsura & Uchida, 2020) use pairwise classification or one-versus-all in training.
- L-W and L-UW (Gao & Zhang, 2021) are based on the weighted and unweighted losses, respectively.
- Forward (Yu et al., 2018) applies forward loss correction.

We also use GA and PRODEN methods presented in the previous paragraph.

Similarly to (Katsura & Uchida, 2020) and (Gao & Zhang, 2021), we use a 2-layer perceptron for the MNIST, Fashion-MNIST, and Kuzushiji-MNIST datasets, and DenseNet (Huang et al., 2017) for the CIFAR-10. We train each model for 300 epochs and apply the Adam optimizer and stochastic gradient descent for the MLP and DenseNet, respectively. Again, hyperparameters are the same as in the original papers.

**ProPaLL setup.** We run the efficient implementation of the loss function (4) described in the Appendices, with the same number of epochs and optimizers as for the baseline methods. Moreover, we add a Gumbel random noise to the logits ($r$)

$$r_i = r_i + \lambda \cdot (U_i - V_i)$$

where $U_i, V_i$ are drawn independently from the Gumbels distribution, and $\lambda$ is set to 1 for 80\% of training and decreasing linearly to zero afterwards. This way, the model obtains more relevant global minima (Struski et al., 2021; Wang et al., 2021). The derivation of the Equation (5) is provided in the Appendices. All experiments were implemented using PyTorch2 and run on NVIDIA GeForce RTX 3080.

5. Results and Discussion

This section compares our method with the baseline approaches in PLL and CLL settings. Moreover, we present the intriguing behavior of ProPaLL during training and the positive influence of Gumbel noise.

**Results on PLL setting.** In Tables 2 and 3, we report test accuracy for artificial databases corrupted by the uniform distribution.
and instance-dependent generating procedure, respectively. Our method overpasses existing methods for all databases in the case of uniformly corrupted data. Moreover, in the instance-dependent procedure, it is better for MNIST and Kuzushiji-MNIST. The statistical differences are drawn at Critical Difference (CD) diagrams (Demšar, 2006) in Figure 3, generated using all the results shown in Tables 2 and 3. One can observe that ProPaLL, VALEN, and PRODEN are statistically similar with a preference for our approach.

Moreover, in Table 4, we report the results on real-world datasets where our approach achieves the best performance for three out of five databases. Most probably, the weak results for MSRCv2 and BirdSong are caused by shallow architectures and the small scale of those datasets (see Table 1). In this case, the CD diagram (see Figure 4) shows that our method is statistically similar to the best-performing method.

Results on CLL datasets. In Tables 5 and 6, we analyze how models behave if the size of candidate label set increases. For this purpose, we adapted the experiment from (Katsura & Uchida, 2020) with MNIST, Fashion-MNIST, Kuzushiji-MNIST, and CIFAR-10 datasets, for 10 or 5 classes. The results obtained for 3 repetitions of each experiment show that model precision decreases with the increasing number of candidate labels. Moreover, for 9 (or 4) candidate labels (the most challenging setup), our approach returns the highest accuracy for all datasets. The highest gain compared to the second-best method is obtained for the MNIST and Kuzushiji-MNIST databases (14.96% and 11.91%, respectively). However, a similar trend is also observed for the remaining datasets.

We also evaluate considered methods on unbiased complementary labels, as in (Gao & Zhang, 2021). The results presented in Table 7 for 10 repetitions show that our approach achieves the highest accuracy. Moreover, as presented in the critical difference diagram in Figure 5 it is statistically better than all baseline methods except PRODEN.

Behavior of ProPaLL during training. Our cost function from Equation (4) is simple and requires only a few numerical operations, in contrast to the more complex baseline methods. Therefore, it is competitive in terms of numerical efficiency, as observed in Figure 6, where our method finishes 500 learning epochs much faster than VALEN and PRODEN methods. Moreover, it gradually learns consecutive classes instead of progressively increasing sensitivity for all of them. For example, as presented in Figure 2, a model learns most of the classes at the initial training stage and then continues training by considering the remaining classes one after another.

Gumbel noise influence. To provide a convincing argument for using Gumbel noise as a regularization technique, we run an ablation study for real-world databases that test the performance of ProPaLL with and without the noise. As shown in Table 8, the experiment performed on the real-world datasets reveals that adding noise usually slightly increases the accuracy.

6. Conclusions

In this paper, we introduced ProPaLL, a simple and easy-to-implement probabilistic approach to partial label learning. We derived the formula for novel cost function starting from BCE and compared our model with state-of-the-art methods, like PRODEN and VALEN. The extensive experiments
Table 5: Test accuracy (mean (std)%) for 10 classes and the increasing number of candidate labels. The highest accuracy is bolded in ProPaLL. Our ProPaLL overpass baseline methods, especially for a larger number of candidate labels.

| Methods          | Number of candidate labels |
|------------------|-----------------------------|
|                  | 1  | 2     | 3     | 4     | 5     | 6     | 7     | 8     | 9     |
| ProPaLL          | 96.28 (0.08) | 95.99 (0.07) | 95.83 (0.28) | 95.45 (0.22) | 95.10 (0.11) | 94.62 (0.08) | 93.86 (0.22) | 92.56 (0.27) | 90.17 (0.24) |
| MNIST PRODEN      | 96.20 (0.05) | 95.86 (0.30) | 95.51 (0.02) | 94.88 (0.20) | 94.36 (0.33) | 92.82 (0.23) | 90.75 (0.16) | 86.29 (0.15) | 65.25 (0.57) |
| PC                | 95.59 (0.22) | 91.31 (0.19) | 88.88 (0.46) | 88.68 (0.31) | 86.74 (0.87) | 85.89 (1.05) | 82.91 (0.31) | 80.45 (0.47) | 75.21 (0.74) |
| OVA              | 94.15 (0.21) | 93.37 (0.28) | 91.08 (0.33) | 89.07 (1.23) | 86.11 (0.64) | 79.29 (6.48) | 76.82 (5.06) | 70.69 (6.99) | 56.25 (4.13) |

Table 6: Test accuracy (mean (std)%) for 5 classes and the increasing number of candidate labels. The highest accuracy is bolded.

| Methods          | Number of candidate labels |
|------------------|-----------------------------|
|                  | 1  | 2     | 3     | 4     | 5     | 6     |
| ProPaLL          | 88.73 (0.25) | 88.18 (0.12) | 87.63 (0.25) | 87.04 (0.36) | 86.39 (0.45) | 85.59 (0.47) |
| MNIST PRODEN      | 87.58 (0.26) | 87.92 (0.26) | 87.51 (0.01) | 87.46 (0.05) | 86.98 (0.32) | 85.22 (0.46) |
| PC                | 87.29 (0.18) | 83.38 (0.44) | 81.70 (0.07) | 80.51 (0.37) | 79.31 (0.38) | 77.65 (0.56) |
| OVA              | 83.56 (0.69) | 77.59 (2.11) | 77.86 (1.90) | 73.61 (2.85) | 63.45 (7.17) | 66.08 (3.39) |

Table 7: Test accuracy (mean (std)%) of models trained on data with unbiased complementary labels. The highest accuracy is bolded.

| Methods          | Datasets |
|------------------|----------|
|                  | MNIST    | Fashion | Kuzushiji |
| ProPaLL (our)    | 96.11 (0.19) | 85.50 (0.05) | 76.01 (1.70) |
| PRODEN           | 94.83 (0.09) | 84.53 (0.08) | 75.21 (0.49) |
| PC               | 84.04 (0.55) | 77.55 (0.39) | 59.32 (0.59) |
| L-W              | 92.38 (0.19) | 83.82 (0.29) | 66.86 (1.95) |
| L-UW             | 92.77 (0.21) | 84.01 (0.23) | 67.22 (2.17) |
| Forward          | 91.93 (0.25) | 82.31 (0.24) | 65.59 (0.5) |
| NN               | 89.99 (0.42) | 80.29 (0.47) | 65.44 (0.5) |
| GA               | 92.49 (0.25) | 81.62 (0.19) | 69.56 (0.53) |

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Appendices

A. Efficient Implementation of ProPaLL Loss Function

Recall that the cost function for a point \( x \) is given by

\[
\text{cost}(x) = -\log \left( 1 - \prod_{i \in S} (1 - p_i(x)) \right) - \sum_{j \notin S} \log(1 - p_j(x)),
\]

where \( S \) denotes the candidate label set of \( x \). Moreover, let \( S[i] \) denotes the characteristic function of \( S \). Since

\[
-\log(1 - \sigma(r)) = -\log \left( \frac{1}{1 + \exp(r)} \right) = \text{LogSumExp}(0, r),
\]

part II reduces to

\[
II = \sum_{j \notin S} \text{LogSumExp}(0, r_j(x))
\]

\[
= \sum_j (1 - S[j]) \cdot \text{LogSumExp}(0, r_j(x)),
\]

and \( I \) reduces to

\[
I = -\log \left( 1 - \exp \left( -\sum_i S[i] \cdot \text{LogSumExp}(0, r_i(x)) \right) \right)
\]

To stabilize \( I \), let us observe that for small \( h > 0 \)

\[
-\log(1 - \exp(-h)) = -\log(h - \frac{1}{2!} h^2 + \frac{1}{3!} h^3 + \ldots)
\]

\[
= -\log(h) + \log(1 + \frac{1}{2!} h + \frac{1}{3!} h^2 + \ldots) = -\log(h) + O(h).
\]

Hence, when the sum inside logarithm is close to 1 (i.e., when \( r_i(x) \) are large negative numbers for \( s \in S[i] \)), then

\[
I \approx -\log \left( \sum_i S[i] \cdot \log(1 + \exp(r_i(x))) \right)
\]

\[
\approx -\log \left( \sum_i S[i] \cdot \exp(r_i(x)) \right)
\]

\[
= -\text{LogSumExp}(\log(S[i] \cdot r_i(x) + (1 - S[i]) \cdot \min F)_{i=0..k-1}),
\]

where \( \min F \) denotes the smallest numerical float (with \( \exp(\min F) = 0 \)). Finally, we obtain

\[
I = -\text{LogSumExp} \left( \log(S[i] \cdot r_i(x) + (1 - S[i]) \cdot \min F) \right)
\]

if \( \max_{i=0..k-1} (S[i] \cdot r_i(x) + (1 - S[i]) \cdot \min F) > -10 \) and otherwise

\[
I = -\text{LogSumExp} \left( (S[i] \cdot r_i(x) + (1 - S[i]) \cdot \min F) \right).
\]

B. Derivation of Gumbel Noise

In the standard softmax model, noise from the Gumbel distributions is often added to the logits to widen the space of parameters search. More precisely, logits \( r_1, \ldots, r_n \) are transformed to

\[
r_1 + \lambda U_1, \ldots, r_n + \lambda U_n,
\]
Figure D.1: Detailed analysis of the PRODEN training (presented here) indicates that it differs from ProPaLL training (shown in Figure 2). While PRODEN progressively increases sensitivity for all classes, ProPaLL gradually learns consecutive classes. In this image, the middle part presents model accuracy for all classes in time, the bottom part shows the sensitivity of particular classes also in time, while the top part shows confusion matrices in time points corresponding to their location.

where $U_i$ are independently sampled from Gumbel distribution, and $\lambda$ is a parameter (usually set to 1 at the beginning of training, which is decreased to 0 during training). Then, for two classes

$$s_0 = r_0 + \lambda U_0, s_1 = r_1 + \lambda U_1,$$

and after applying softmax

$$p_0 = \frac{\exp(s_0)}{\exp(s_0) + \exp(s_1)} = \frac{1}{1 + \exp(s_1 - s_0)},$$

$$p_1 = \frac{1}{1 + \exp(s_0 - s_1)}.$$

Thus

$$p_1 = \sigma(s_1 - s_0) \text{ and } p_0 = \sigma(-(s_1 - s_0)).$$

On the other hand, in the case of binary cross-entropy, where the representation corresponds to one parameter $r = r_1 - r_0$, adding Gumbel noise $\lambda U$ to the softmax logits is equivalent to

$$r = r + \lambda (U - V),$$

where $U$ and $V$ are independent and come from the Gumbel distribution. Since ProPaLL uses binary cross entropy with $k$ outputs, we add this class to the logit of each class.

C. Experimental Setup Details

For PLL setting, we base on experiments and databases described in (Lv et al., 2020; Xu et al., 2021) and the corresponding source codes available at https://github.com/palm-ml/valen and https://github.com/Lvcrezia77/PRODEN. For corrupted MNIST, Fashion-MNIST, and Kuzushiji-MNIST datasets, we use MLP with 5 fully-connected layers (with 300, 301, 302, 303, and 10 neurons), ReLU as the activation function, and batch normalization (Ioffe & Szegedy, 2015) applied before hidden layers. For random corruption, this model is trained with batch size 256, learning rate 0.05, and weight decay $10^{-6}$. For instance-dependent corruption, we use batch size 256, learning rate 0.1 or 0.05, and weight decay 0. For both corruption types of CIFAR-10 database, we use ResNet-32 (He et al., 2016) with batch size 256, learning rate 0.05, and weight decay 0. For the real-world PLL datasets, we use linear model with learning rate 0.01, 0.05, 0.1, 0.5, 0.5 for Lost, MSRCv2, BirdSong, Soccer Player, and Yahoo!News, respectively. Weight decay equals $10^{-4}$ for Lost and MSRCv2, and 0 for the remaining datasets. Mini-batch is set to 100 for Lost, MSRCv2, and BirdSong, and 256 for Soccer Player and Yahoo!News.

For CLL setting, we base on experiments and databases described in (Katsura & Uchida, 2020; Gao & Zhang, 2021) and the corresponding source codes available at https://github.com/YasuhiroKatsura/ord-comp and https://github.com/GaoYi439/complementary-label-learning. We adapted the experiment with MNIST, Fashion-MNIST, Kuzushiji-MNIST, and CIFAR-10 datasets with 10 or 5 classes. For MNIST, Fashion-MNIST, and Kuzushiji-MNIST datasets,
Table D.1: Test accuracy (mean (std)%) of ProPaLL with and without Gumbel noise for 10 classes and the increasing number of candidate labels. The highest accuracy is bolded.

| Number of candidate labels | 1     | 2     | 3     | 4     | 5     | 6     | 7     | 8     | 9     |
|----------------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
|                            | MNIST |       |       |       |       |       |       |       |       |
|                            | ProPaLL (w/o noise) | 96.44(0.09) | 95.99(0.18) | 95.89(0.19) | 95.47(0.10) | 95.19(0.07) | 94.77(0.43) | 93.80(0.21) | 92.33(0.29) | 89.77(0.69) |
|                            | ProPaLL | 96.28 (0.08) | 95.99(0.07) | 95.83(0.28) | 95.45(0.22) | 95.10(0.11) | 94.62(0.08) | 93.86(0.22) | 92.56(0.27) | 90.17(0.24) |
|                            | Fashion (w/o noise) | 88.44(0.35) | 88.12(0.34) | 87.74(0.63) | 87.50(0.42) | 86.59(0.28) | 85.64(0.24) | 84.49(0.11) | 83.10(0.15) | 79.28(0.33) |
|                            | ProPaLL | 88.73(0.25) | 88.18(0.12) | 87.63(0.25) | 87.04(0.36) | 86.39(0.45) | 85.59(0.47) | 84.80(0.33) | 82.93(0.40) | 79.13(0.27) |

Table D.2: Test accuracy (mean (std)%) of ProPaLL with and without Gumbel noise on artificial datasets corrupted by the uniform generating procedure. The highest accuracy is bolded.

| Datasets      | Methods                      | Number of candidate labels | ProPaLL (w/o noise) | ProPaLL |
|---------------|------------------------------|----------------------------|---------------------|---------|
| MNIST         | ProPaLL                      | 98.68 (0.03)               | 98.73 (0.05)        |         |
| Kuzushiji     | ProPaLL                      | 93.30 (0.21)               | 93.50 (0.17)        |         |
| Fashion       | ProPaLL                      | 90.40 (0.23)               | 90.40 (0.06)        |         |
| CIFAR-10      | ProPaLL                      | 83.90 (0.22)               | 84.32 (0.37)        |         |

Table D.3: Test accuracy (mean (std)%) of ProPaLL with and without Gumbel noise on artificial datasets corrupted by the instance-dependent generating procedure (Xu et al., 2021). The highest accuracy is bolded.

| Datasets      | Methods                      | Number of candidate labels | ProPaLL (w/o noise) | ProPaLL |
|---------------|------------------------------|----------------------------|---------------------|---------|
| MNIST         | ProPaLL                      | 97.85 (0.10)               | 97.89 (0.08)        |         |
| Kuzushiji     | ProPaLL                      | 86.14 (0.37)               | 86.26 (0.32)        |         |
| Fashion       | ProPaLL                      | 85.63 (0.09)               | 85.55 (0.33)        |         |
| CIFAR-10      | ProPaLL                      | 74.13 (1.33)               | 75.75 (0.63)        |         |

we use MLP with 2 fully-connected layers (with 500 and 10 neurons), ReLU as the activation function, batch size 64, weight decay $10^{-4}$, and learning rate $5 \cdot 10^{-4}$. For CIFAR-10, we apply DenseNet (Huang et al., 2017) with weight decay $5 \cdot 10^{-4}$, learning rate 0.01, and momentum 0.9. For unbiased complementary labels, as in (Gao & Zhang, 2021), we use the same MLP model, Adam optimization, number of epoch 300, and mini-batch 256. Moreover, for the MNIST and Kuzushiji-MNIST datasets, we use learning rate $10^{-3}$ and weight decay $10^{-5}$. For Fashion-MNIST, we used learning rate 0.001 and weight decay 0.

D. Additional Results

Behavior of PRODEN during training. To highlight the difference in ProPaLL training (shown in Figure 2) compared to existing methods, we provide similar details on PRODEN training in Figure D.1. One can observe that, while ProPaLL gradually learns consecutive classes, PRODEN progressively increases sensitivity for all of them. It can be caused by EM (Jin & Ghahramani, 2002) inspirations of PRODEN and the fact that “frequent patterns” are remembered for all classes already from the initial training iterations thanks to the memorization effects (Arpit et al., 2017; Han et al., 2018).

Gumbel noise influence. Finally, we provide test accuracy of our approach without and with Gumbel noise regularization for the remaining settings and datasets (complementary to Table 8). In Tables D.2 and D.3, we report results for artificial databases corrupted by the uniform and instance-dependent generating procedure, respectively. In Tables D.1 and D.5, we analyze how ProPaLL with and without noise behave if the size of candidate label set increases. Finally, in Table D.4, we provide results for unbiased complementary labels. We conclude that adding noise to the logits of the model usually improves the results.
Table D.4: Test accuracy (mean (std)% ) of ProPaLL with and without Gumbel noise trained on data with unbiased complementary labels. The highest accuracy is bolded.

| Datasets | ProPaLL (w/o noise) | ProPaLL |
|----------|---------------------|---------|
| MNIST    | 98.80 (0.06)        | 98.83 (0.13) |
| Fashion  | 90.45 (0.79)        | 89.79 (0.27) |
| Kuzushiji| 87.84 (0.49)        | 88.15 (0.59) |
| CIFAR-10 | 78.39 (0.66)        | 78.98 (1.06) |

Table D.5: Test accuracy (mean (std)%) of ProPaLL with and without Gumbel noise for 5 classes and the increasing number of candidate labels. The highest accuracy is bolded.

| Datasets | ProPaLL (w/o noise) | ProPaLL |
|----------|---------------------|---------|
| MNIST    | 98.24 (0.19)        | 98.27 (0.11) |
| Fashion  | 88.30 (0.20)        | 88.02 (0.25) |
| Kuzushiji| 83.13 (1.42)        | 83.68 (0.84) |
| CIFAR-10 | 69.51 (1.80)        | 70.94 (0.66) |

| Datasets | ProPaLL (w/o noise) | ProPaLL |
|----------|---------------------|---------|
| MNIST    | 97.83 (0.34)        | 97.47 (0.18) |
| Fashion  | 86.18 (0.45)        | 86.31 (1.13) |
| Kuzushiji| 78.16 (1.43)        | 78.82 (1.91) |
| CIFAR-10 | 62.45 (0.48)        | 62.25 (0.20) |

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