Collective Loss Function for Positive and Unlabeled Learning

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Abstract

People learn to discriminate between classes without explicit exposure to negative examples. On the contrary, traditional machine learning algorithms often rely on negative examples, otherwise the model would be prone to collapse and always-true predictions. Therefore, it is crucial to design the learning objective which leads the model to converge and to perform predictions unbiasedly without explicit negative signals. In this paper, we propose a Collectively loss function to learn from only Positive and Unlabeled data (cPU). We theoretically elicit the loss function from the setting of PU learning. We perform intensive experiments on the benchmark and real-world datasets. The results show that cPU consistently outperforms the current state-of-the-art PU learning methods.

1 Introduction

Positive and unlabeled learning (PU learning) aims at learning from only positive and unlabeled examples, without explicit exposure to negative examples. This setting arises from multiple practical application scenarios: retrieving information with limited feedback given 
\cite{Onoda et al., 2005}, text classification with only positive labels collected \cite{Yu et al., 2003}, and detecting area of interest in images where normal samples are available but the abnormal samples are scarce and diverse \cite{Zuluaga et al., 2011, Li et al., 2011}. It is widely applicable in industrial scenarios such as content censorship \cite{Ren et al., 2014, Li et al., 2014}, disease gene detection \cite{Yang et al., 2012} and drug discovery \cite{Liu et al., 2017}.

Positive labels are considered prefect in most literatures while the unlabeled data are not and thus handled in different ways. The first category tries to identify negative samples from the unlabeled data and convert the problem back to positive-negative classification \cite{Liu et al., 2002, Li and Liu, 2003}. The heuristic strategies in these methods act as external information to recognize negative samples. However, these strategies often heavily rely on subtle design for a single task/dataset and results in low transferability. The second category take the unlabeled data as corrupted negative samples. Early approaches attempt to reweight the unlabeled data \cite{Liu et al., 2003, Lee and Liu, 2003} with a smaller penalty per sample, but their performances are upper bounded due to their intrinsic bias, proved by Du Plessis et al. \cite{Du Plessis et al., 2014, Du Plessis et al., 2015b} who later develop an approach, called uPU, with a non-convex losses to cancel the bias. This work is extended by nnPU \cite{Kiryo et al., 2017} to avoid overfitting by preventing risk estimators from reaching negative values. Hou et al. \cite{Hou et al., 2017} further argue that overfitting is still an issue with flexible deep neural networks. They proposed GenPU, a generative adversarial approach, to address the challenge of limited positive data, whereupon they train two discriminators: one telling fake generated examples from the true and the other assign positive labels to the generated examples that are similar to the positive class.

A similar keypoint behind all the aforementioned solutions is that they all try to recover the true distribution of positive and negative data and thus recover the true risk. However, performing risk rectification at the outcome-of-loss-function level, which is the main cause of the inaccuracy, according to our elaboration in section \ref{42}. In this paper, we propose a novel method called “Collectively loss function to learn from Positive and Unlabeled data” (cPU) to rectify the predictor instead of the total risk. We collectively gather predictions from predictors and rectify them before the calculation of loss function. We design our method with the following principles in mind:

1. Minimum intervention. The only difference between PU learning setting and regular positive/negative learning is that the negative data are not explicitly labeled. Therefore, we also hope minimum feature construction is required. Hence, we only process at prediction level and leave the feature engineering part to the powerful representation of models (especially neural networks) themselves.

2. Robustness. Due to the class uncertainty in the unlabeled data, it is demanding to estimate the class prior accurately in the unlabeled data. As a result, we take the collective prediction to balance the randomness of mini-batch.

Our main contributions are threefold. Firstly, we provide a unbiased approach of estimating the posterior probability in
PU learning setting, which is in harmony with very flexible models and learns on a large scale. Secondly, we propose a general framework of studying the behavior of loss functions via elicitation. Thirdly, we derive the collective loss function to rectify the decision boundary drift and theoretically bounded the generalization error. We conduct comprehensive experiments of in comparison with state-of-the-art approaches.

2 Problem Statement

Consider the input space $\mathcal{X} \subseteq \mathbb{R}^d$ and label space $\mathcal{Y} = \{0, 1\}$, we denote by $P_{XY}$ the joint distribution over $\mathcal{X} \times \mathcal{Y}$. Let $f : \mathcal{X} \mapsto \mathbb{R}$ be a predictor function and $h(X) = \lfloor \sigma(f(X)) \rceil$ be the classifier, where $\lfloor \cdot \rceil$ means rounding to the nearest integer and $\sigma(\cdot) : \mathbb{R} \mapsto (0, 1)$ is a sigmoid function. For example, $\sigma(\cdot) = 1/(1+\exp(\cdot))$. Let $\ell : \mathbb{R} \times \{0, 1\} \mapsto \mathbb{R}^+$ be the loss function for binary classification. According to statistical learning theory [Vapnik, 1999], the risk of $f(x)$ is defined by

$$R(f) := P_{XY}(h(x) \neq Y) = E_{XY}[\ell(f(x), y)], \quad (1)$$

where $E_{XY}[\cdot] = E_{(x,y)} \sim P_{XY} [\cdot]$.

2.1 Conditional Risk for PN Learning

Let $\eta(x) := P_{Y|X}(1|x)$ denote the posterior probability of the positive class. For clarity, we omit the argument $(x)$ in expressions such as $f(x)$ and $\eta(x)$ throughout the paper. The risk decomposes to the conditional form

$$R(\eta, f) = E_X[E_{X|Y}(\ell(f, y)|X = x)]$$

$$= E_X[P_{Y|X}(1|x)\ell(f, 1) + P_{Y|X}(0|x)\ell(f, 0)]$$

$$= E_X[\eta\ell(f, 1)] + E_X[(1-\eta)\ell(f, 0)], \quad (2)$$

where $E_X[\cdot] = E_{x \sim P_X} [\cdot]$. $P(X)$ is the marginal distribution of $X$. We expect Fisher consistency [Lin, 2004] (aka classification-calibration in some literatures) on the predictors, which is a weak condition. To be specific, if the risk $R$ in (2) is minimized, the following equation holds.

$$h^* = \sigma(f^*) = \lfloor \eta \rceil, \quad (3)$$

An example loss function is the zero-one loss:

$$\ell_{0/1} = \begin{cases} 0 & h(x) = y \\ 1 & h(x) \neq y \end{cases} \quad (4)$$

2.2 Risk Estimators for PU Learning

Due to the absence of negative samples in PU learning, risks have to be estimated from only positive and unlabeled samples. In other words, $R_u(\eta, f)$ need to be derived via risks from $P_u$ and $P_n = P(X)$. Formally, a PU learning system receives training samples from $S = P \cup U$, which can be divided into two not-necessarily-independent components. The labeled positive samples: $P = \{x^n_i\} \sim P_p$ and unlabeled samples: $U = \{x^n_u\} \sim P_u$. Underlyingly, the unlabeled set $U$ consists of positive samples $U_p = \{x^{up}_i\} \sim P_p$ and negative samples $U_n = \{x^{un}_i\} \sim P_n$. As a popular practice, negative labels are assigned to the unlabeled samples [du Plessis et al., 2015b] [Kiryo et al., 2017]. Let $R_u(\eta, f, 0) = E_X[\eta\ell(f, 0) + (1-\eta)\ell(f, 0)]$ be the risk of unlabeled samples, which are drawn from the same distribution of $P_X$, with loss function $\ell$ assigning all the labels to negative. **Unbiased PU (aka uPU) learning methods** [du Plessis et al., 2014] [du Plessis et al., 2015b] attempt to estimate the risk for PU learning via subtracting the wrongly included risk

$$R_p(\eta, f, 0) = E_X[\ell(f, 0)]$$

$$R_{upu} := R_p(\eta, f, 1) + R_u(\eta, f, 0) - R_p(\eta, f, 0) \quad (5)$$

Non-negative PU (aka nnPU) [Kiryo et al., 2017] observed that $R_n(\eta, f, 0) = R_u(\eta, f, 0) - R_p(\eta, f, 0)$ should be always non-negative. However, this does not always hold, especially when the model $f$ becomes flexible (i.e., deep neural networks). To mitigate this drawback, they propose a non-negative risk estimator, thus ensuring the risk will not reach negative values:

$$R_{nnpu} := R_p(\eta, f, 1) + \max\{0, R_u(\eta, f, 0) - R_p(\eta, f, 0)\}. \quad (6)$$

Nevertheless, minimizing these risk estimators will lead to insufficient penalty for the negative samples. Maximizing $R_u(\eta, f, 0)$, instead of making $R_u(\eta, f, 0)$ small, will result in the same effect of minimizing the total risk, which is also natural side effect of minimizing $R_p(\eta, f, 1)$ for flexible models and convex surrogate loss functions. Risk estimators are rectification at the outcome-of-loss-function level, which cannot avoid the explosion (i.e., in some worst case an unbounded loss may reach very large value [Kiryo et al., 2017]) of some surrogate losses, such as the popular logarithm loss. In these cases, the flexible model overfits the training data well and sampling may include some easy positive examples which sum up to large $R_p(\eta, f, 0)$ that overwhelms $R_u(\eta, f, 0)$. Thereupon, can we remedy the problem before loss function?

3 Collective Logarithm Loss for PU Learning

In this section, we firstly address the decision boundary drift problem in section 3.1 and provide rectification of the predictor. Then in section 3.2, we introduce the background of elicitation and how it connects to the design of loss function in normal situations. Finally, in section 3.3, we describe the framework of eliciting the loss function under PU learning setting.

3.1 Rectification of Predictor

To satisfy the Fisher consistency, we hope (3) hold during test, while (6) is biased in general [Kiryo et al., 2017], hence leading to biased solutions. A key observation is that the decision boundary is different between training and testing for PU learning problem. Our aim is to rectify the decision boundary so that the classifier for testing also fits the positive and unlabeled train data. We introduce $\tilde{y} \in \hat{Y}$ to denote true labels. $y$ remains the observed labels, where unlabeled samples are regarded as negative $y = 0, \forall x \in U$. Let $\eta_c(x) = P(\tilde{y} = 1|X = x)$ be the posterior probability of testing, namely what we hope to capture by learning. In $U$, the underlying true labels $\tilde{y} = 1$ for $x^{up}_i$ and $\tilde{y} = 0$ for $x^{un}_i$. It
is evident that the data distribution for training and testing is different. Let \( \eta_a \) and \( \eta_t \) be the posterior probability for training and testing. Denote by \( \Omega = |P| + |U_p| + |U_n| \) the total sample space, we can estimate these two expectations by the following equations in empirical estimation.

\[
\mathbb{E}_X[\eta_a] = \mathbb{E}_X[P_{Y|X}(1|x)] = \frac{1}{\Omega} \sum_x \mathbb{I}[x \in P] = \frac{|P|}{\Omega} \tag{7}
\]

\[
\mathbb{E}_X[\eta_t] = \mathbb{E}_X[P_{Y|X}(1|x)] = \frac{1}{\Omega} \sum_x \mathbb{I}[x \in P \cup U_p] = \frac{|P| + |U_p|}{\Omega} \tag{8}
\]

\[
\mathbb{E}[\eta_t] - \mathbb{E}[\eta_a] = \frac{|U_p|}{\Omega} \tag{9}
\]

We denote the value in Eqn. (9) as \( \mu_p \) for the rest of the paper. We hope \( \sum_x \hat{\eta} \stackrel{P}{\sim} \sum_x \eta_t \). However based on PU training data, the model may converge biasedly to \( \eta_a \). Let \( r = \frac{|U_n|}{|P|} \) be the portion of positive data in \( |U| \) compared to the whole P class we can derive:

\[
\mathbb{E}[\eta_t] = (1 + r)\mathbb{E}[\eta_a] \tag{10}
\]

### 3.2 Preliminary for Elicitation

In statistics and economics, elicitation is a practice of designing reward mechanisms that encourage a predictor to make true predictions. Let \( \hat{\eta} \) be the prediction (i.e., an estimator of \( \eta \)), we have \( \hat{\eta} = \sigma(f(x)) \). Savage et al. [1971] defines the total reward \( I \) as a linear function of \( \eta \).

\[
I(\hat{\eta}, \eta) := \eta I_1(\hat{\eta}) + (1 - \eta)I_0(\hat{\eta}), \tag{11}
\]

where \( I_1(\hat{\eta}) \) and \( I_0(\hat{\eta}) \) denote the conditional reward for a certain event obtains or not. In binary classification context, \( I_1(\hat{\eta}) \) and \( I_0(\hat{\eta}) \) refers to the reward for \( y = 1 \) and \( y = 0 \) [Masnadi-Shirazi and Vasconcelos, 2008]. Specifically, \( y = 1 \) is regarded as the event obtains and \( y = 0 \) otherwise. The goal of elicitation is to design the rewards in order that a \( \hat{\eta} \) maximizes \( I(\hat{\eta}, \eta) \) if and only if when \( \hat{\eta} = \eta, \forall \hat{\eta} \). In other words, no larger reward should be given than when prediction is ideal. Lemma 1 finds the sufficient and necessary condition for it.

**Lemma 1** (Savage [1971]). Let \( I(\hat{\eta}, \eta) \) be as defined in (11). Assume that \( J(\hat{\eta}) := I(\hat{\eta}, \eta) \) is differentiable, then

\[
I(\hat{\eta}, \eta) \leq J(\eta), \forall \eta, \tag{12}
\]

holds and if and only if

\[
I_1(\eta) = J(\eta) + (1 - \eta)J'(\eta) \tag{13}
\]

\[
I_0(\eta) = J(\eta) - \eta J'(\eta) \tag{14}
\]

**Remark 1.** The equality in (12) holds if and only if \( \hat{\eta} = \eta \). Eqn. (12) also implies that \( J \) is a strictly convex function of \( \eta \). This is the regular situation where event and prediction are in the same space. The event not observed will never happen, e.g., in PU learning, the event obtains even though it is not observed (i.e., unlabeled).

Masnadi et al. [2008] interpreted loss functions in machine learning as a special form of \( J(\eta) \). We rewrite it in Lemma 2 with \( y \in \mathcal{Y} = \{0, 1\} \) and illustrate the process of deriving the logarithm loss with Example 1.

**Lemma 2** (Masnadi et al. [2008]). If \( J(\eta) = J(1 - \eta) \), then \( I_1 \) and \( I_0 \) from (13) and (14) satisfy the following conditions. Let \( c(\eta) : [0, 1] \rightarrow [0, 1] \) be an invertible function such that \( c^{-1}(v) = 1 - c^{-1}(v) \).

\[
I_1(\hat{\eta}) = -\phi(c(\hat{\eta})) \tag{15}
\]

\[
I_0(\hat{\eta}) = -\phi(c(\hat{\eta})), \tag{16}
\]

**Meanwhile the loss function,**

\[
\phi(v) = J(c^{-1}(v)) + (1 - c^{-1}(v))J'(c^{-1}(v)) \tag{17}
\]

**Remark 2.** Lemma 2 bridges the design of a loss function \( \phi(c) \) with the reward function \( I(\hat{\eta}, \eta) \).

**Example 1** (Eliciting logarithm loss). Let \( c \) be defined as follows,

\[
c(\eta) = \begin{cases} 
\hat{\eta} & \text{if } y = 1 \\
1 - \hat{\eta} & \text{otherwise,} 
\end{cases} \tag{18}
\]

which can be interpreted as the closeness of the prediction to the true label. Intuitively, larger \( c \) should get larger reward (or smaller penalty). Let \( J(\eta) = \eta \ln \hat{\eta}(x) + (1 - \eta) \ln(1 - \hat{\eta}) \) be the convex function. Applying (17), we can derive:

\[
\phi(v) = [v \ln v - (1 - v) \ln(1 - v)] + (1 - v) \ln \left( \frac{v}{1 - v} \right) \tag{19}
\]

\[
= -\ln(v) \]

The loss function is

\[
\ell_{CE} = -\ln(c) \tag{20}
\]

### 3.3 Eliciting Collective Loss Function for PU Learning

In PU learning, the label of a specific sample in \( U \) is unknown. We only possess the statistical information of the samples. Therefore, a reward function that suits this kind of collective information is desired. Lemma 2 indicates the symmetry of the link function \( c(\eta) \), which changes in PU learning setting. Let \( c(x) \) be defined in (18). In PU learning, we must ensure \( \mathbb{E}[c(x)] = 1 \) when \( \ell(c) = 0 \). A straight-forward solution is to encourage making a certain amount of positive predictions when the labels are negative. The amount is such that the expectation of the predictions equals to \( \mu_p \), i.e., the positive prior in unlabeled data, because \( \mathbb{E}[1_{\hat{y}=1}] = P(\hat{y} = 1) = \mu_p \) holds. Under this condition, \( c(x) \):

\[
c(x) = \begin{cases} 
\hat{\eta}(x) & \text{if } y = 1 \\
1 - |\hat{\eta}(x) - \mu_p| & \text{otherwise.} 
\end{cases} \tag{21}
\]

Note that we apply an absolute function because when the prediction \( \hat{\eta} \leq \mu_p \) it is also considered to be a negative event, thus deviates from the correctness. Hence, we derive the rectified reward function as follows. Without loss of generality, we let \( \phi(c) \) be logarithm function \( \ln(c) \).

\[
\ell(\hat{\eta}, \eta) := \eta \ln(\hat{\eta}) + (1 - \eta) \ln(1 - \hat{\eta} - \mu_p). \tag{22}
\]

According to Savage, 1971 section 7, (22) must be upper bounded by a maximum reward. We further detail it in Theorem 1.
Theorem 1 (Maximum reward in PU learning). Let $I(\hat{\eta}, \eta)$ be defined as in (22). There exists convex function:

$$J(\eta) = \begin{cases} \eta \ln(\eta(1+\mu_p) + (1-\eta) \ln((1-\eta)(1+\mu_p)) & \text{if } \eta > \mu_p; \\ \eta \ln(\mu_p) & \text{otherwise}, \end{cases}$$

such that the reward function (22) supports $J(\eta)$ at and only at $\hat{\eta} = \eta(1+\mu_p)$.

Proof. Consider $\eta$ to be fixed at a constant value $k$. At this point,

- if $\hat{\eta} > \mu_p$, $I$ is a concave function of $\hat{\eta}$ that reaches maximum when $\frac{dI}{d\hat{\eta}} = 0$. That is, 
  $$\frac{k}{\hat{\eta}} - \frac{1-k}{1-|\eta - \mu_p|} \hat{\eta} - \mu_p = 0$$
  $$\hat{\eta} = k(1+\mu_p)$$ (24)
- if $\hat{\eta} \leq \mu_p$, $I$ is monotonically increasing and reaches maximum when $\mu_p$ is at maximum
  $$\hat{\eta} = \mu_p$$ (25)

Plugging the value $\hat{\eta}$ in (24) and (25) into (22) will derive (23).

\[ \square \]

3.4 Implementation

We apply stochastic gradient optimization. Instead of traditional one-loss-per-sample paradigm, we collect the model predictions from multiple samples while update the gradient only once. That is equivalent to ask multiple agents to make decisions under condition of (23). The intuition is as follows: It is difficult to ensure the correctness of a single prediction especially under unlabeled data. The underlying label may be either positive or negative. However, when a batch of samples are considered together, the expectation of the prediction converges to $\mu_p$. For all mini-batch $S_b = P_b \cup U_b$, the loss function is as follows.

$$\ell(\hat{\eta}, y) = \begin{cases} -\ln \hat{\eta} & \text{if } y = 1 \\ -\ln(1-1/|U_b|) \sum_{x \in U_b} \hat{\eta} - \mu_p | & \text{if } y = 0. \end{cases}$$ (26)

In practice, we treat the positive class prior $\mu_p$ in $U$ as known during training. Many related works [du Plessis et al., 2015a; Bekker and Davis, 2018] can be applied to estimate it. We further show that our method is insensitive to it in Section 4.2.

3.5 Estimation error bound

We next theoretically upper bound the generalization error. Let $\hat{\eta}_{pu}$ be the empirical risk minimizer corresponding to (26). The learning problem is to find an optimal decision function $\hat{\eta}^*$ in the function class $\mathcal{F} = \{ \eta | \|\eta\|_\infty < C_\eta \}$ where $C_\eta$ is a constant. Formally, $\hat{\eta}^* = \arg \min_{\eta \in \mathcal{F}} R(\eta)$.

Let $\mathcal{R}_n$ be the Rademacher complexity defined in [Bartlett and Mendelson, 2001].

Lemma 3 [Ledoux and Talagrand, 1991]. Assuming $\Phi : \mathbb{R} \mapsto \mathbb{R}$ is Lipschitz continuous with constant $L_\Phi$ and $\Phi(0) = 0$, we have

$$\mathcal{R}_n(\Phi \circ \mathcal{F}) \leq L_\Phi \mathcal{R}_n(\mathcal{F}).$$ (27)

Theorem 2 (Generalization error bound). For any $\epsilon > 0$, with probability at least $1 - \epsilon$:

$$R(\hat{\eta}_{pu}) - R(\hat{\eta}^*) \leq 2\mathcal{R}_n(\Phi \circ \mathcal{F}) + \sqrt{\frac{2\log(2/\epsilon)}{n}} + \sqrt{\frac{2\log(2/\epsilon)}{n}},$$ (28)

where $n$ is the total number of i.i.d. samples corresponding to the Rademacher variables.

The Lipschitz constant is $\|X\|_m \leq C_\gamma$ for original cross entropy [Yedida, 2019] where $m = \|\frac{\partial}{\partial x} \|$ and $\|X\|_2 \leq C_x, C_x \in \mathbb{R}^+$ is the input vector norm. This Lipschitz constant also applies for (26), so that the last inequality follows. The penultimate inequality follows from routine proof of generalization bound using Rademacher complexity [Shalev-Shwartz and Ben-David, 2014, Section 26.1].

4 Experiments

We perform experiments on five real-world datasets, including MNIST [LeCun et al., 1998], USPS [Hastie et al., 2005], SVHN [Netzer et al., 2011], CIFAR-10 [Krizhevsky, 2009] and 20ng (twenty news groups) [Lang, 1995]. We choose the positive and negative class in accordance with the previous research [Kiryo et al., 2017]. The specification of datasets are described in Table 1. We still need the actual label for testing the models, hence we use originally labeled data. Specifically, we randomly pick $r = 20\%$, $30\%$, $40\%$, $80\%$ of P class data and mix them with all the N class data to compose the unlabeled set U. The remaining P class data forms the positive set $P$.

We apply neural networks as the predictor function. Specifically, we apply vanilla vgg-16 structure [Simonyan and Zisserman, 2014] to encode the input features. For 20ng, all the details including model structure (a multi-layer perceptron with five layers and the activation functions are Softsign) and pre-trained word embedding (300-dimension GloVe [Pennington et al., 2014] word embeddings) are same with [Kiryo et al., 2017]. For the optimizer, we use Nadam [Dozat, 2016] with learning rate 0.0005 throughout all models. The parameters in nnPU are set equal to the original paper, i.e., $\beta = 0, \gamma = 1$.

We then evaluate the results to show the efficacy of proposed method cPU. We explore the following two common questions in applications: 1) Can it separate the unlabeled positive samples from the negative ones without explicit exposure to negative samples? 2) Is it sensitive to class prior, which may vary and sometimes with uncertainty in real applications?

4.1 Comparison to State of the Art

We first show the overall evaluation results on the real-world datasets. We compare our proposed approach with current state-of-the-art PU learning methods: unbiased PU (uPU) [du Plessis et al., 2015a] and non-negative PU (nnPU) [Kiryo et al., 2017], LDCE [Shi et al., 2018] and PULD [Zhang et al., 2019]. We re-implement uPU and nnPU using the same vgg-16 structure as in our method. We do not compare with
LDCE and PULD, but simply provide the results for reference because: 1) they require additional features construction/engineering process, which is not explicit; 2) these two models deeply involve support vector machine \[\text{Cortes and Vapnik, 1995}\] as their model, and thus can neither be plugged into the data to get better estimation of the class prior \(\pi\). To simulate the scenario, we set \(r = 20\%, 30\%, 40\%\) and misspecify \(\mu_p\). The results are shown in Table 3. We can observe that generally the results are worse if deviation of \(\mu_p\) become big. Another phenomenon is that, the bigger \(r\), the deviation are more influential to the results. This can be avoided by sampling more data to get better estimation of \(\mu_p\), since larger \(r\) indicates more unlabeled data available in real applications. Nevertheless, the fluctuation is acceptable when \(\mu_p\) varies, which means our proposed approach is robust towards wrongly estimated prior probabilities of \(P\) class in unlabeled data.

### 4.2 Robustness

In this section, we study a common scenario of PU-learning in which the class prior is not accurately estimated. This usually happens in real applications, where a small sample can be achieved to approximate the class prior \(\pi\). To simulate the scenario, we set \(r = 20\%, 30\%, 40\%\) and misspecify \(\mu_p\). The results are shown in Table 3. We can observe that generally the results are worse if deviation of \(\mu_p\) become big. Another phenomenon is that, the bigger \(r\), the deviation are more influential to the results. This can be avoided by sampling more data to get better estimation of \(\mu_p\), since larger \(r\) indicates more unlabeled data available in real applications. Nevertheless, the fluctuation is acceptable when \(\mu_p\) varies, which means our proposed approach is robust towards wrongly estimated prior probabilities of \(P\) class in unlabeled data.

### 4.3 Training Process Analysis and Case Study

In order to get a deeper insight on how loss function take effect, we project the layer before last onto a 2D fully connected
Figure 1: Training process visualization. The feature space contains data points from the 1st, 4th and 7th epoch. Some interesting examples (e.g., photograph with human) in data are shown from sample 1 to 5 (denoted S1...S5 for short). S1 is a labeled dog. S2 is a cat (unlabeled). The rest are dogs (unlabeled). Note that, cat and unlabeled dogs are unlabeled in the view of model.

| Dataset | \( r \) | \( \Delta \mu_p \) |
|---------|--------|----------------|
|        | -10%   | -5%   | +5%   | +10%  |
| MNIST  | 0.2    | 0.9925| 0.9924| 0.9927| 0.9842|
|        | 0.3    | 0.9905| 0.9912| 0.9911| 0.9878|
|        | 0.4    | 0.9908| 0.9907| 0.9907| 0.9881|
|        | 0.8    | 0.9832| 0.9842| 0.9855| 0.9609|
|        | 0.2    | 0.9651| 0.9616| 0.9621| 0.9542|
|        | 0.3    | 0.9641| 0.9581| 0.9656| 0.9517|
|        | 0.4    | 0.9631| 0.9631| 0.9606| 0.9527|
|        | 0.8    | 0.9601| 0.9562| 0.9283| 0.9128|
| USPS   | 0.2    | 0.9136| 0.9078| 0.9124| 0.9022|
|        | 0.3    | 0.9106| 0.9159| 0.9097| 0.8921|
|        | 0.4    | 0.9085| 0.9096| 0.8989| 0.8888|
|        | 0.8    | 0.8763| 0.8755| 0.8402| 0.8283|
|        | 0.2    | 0.8597| 0.8607| 0.8609| 0.8543|
|        | 0.3    | 0.8542| 0.8527| 0.8519| 0.8549|
|        | 0.4    | 0.8343| 0.8401| 0.8435| 0.8311|
|        | 0.8    | 0.7778| 0.7854| 0.7854| 0.7797|
| SVHN   | 0.2    | 0.8593| 0.8594| 0.8606| 0.8598|
|        | 0.3    | 0.8589| 0.8598| 0.8602| 0.8596|
|        | 0.4    | 0.8590| 0.8605| 0.8578| 0.8563|
|        | 0.8    | 0.8417| 0.8421| 0.8426| 0.8352|

Table 3: Demonstrating the robustness of our method. \( \mu_p \) is adjusted slightly lower/higher for in each column to test whether the accuracy result is sensitive to some imprecise \( \mu_p \).

In this paper, we identify the bias caused by class uncertainty in the unlabeled as the major difficulty for current risk estimators. We propose a novel approach towards PU learning dubbed “cPU” that collectively process the predictions. We design the loss function through theoretical elicitation PU learning setting and rectification of the predictor. It outperforms the state-of-the-art methods on PU learning and shows robustness against wrongly estimated class prior on the unlabeled data.

5 Conclusion

References

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\[\text{We uniformly sample 500 examples from the training set for clarity of plot.} \]

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