Domain Adaptation under Open Set Label Shift

Saurabh Garg, Sivaraman Balakrishnan, Zachary C. Lipton
Machine Learning Department,
Department of Statistics and Data Science,
Carnegie Mellon University
{sgarg2,sbalakri,zlipton}@andrew.cmu.edu

Abstract

We introduce the problem of domain adaptation under Open Set Label Shift (OSLS) where the label distribution can change arbitrarily and a new class may arrive during deployment, but the class-conditional distributions $p(x|y)$ are domain-invariant. OSLS subsumes domain adaptation under label shift and Positive-Unlabeled (PU) learning. The learner's goals here are two-fold: (a) estimate the target label distribution, including the novel class; and (b) learn a target classifier. First, we establish necessary and sufficient conditions for identifying these quantities. Second, motivated by advances in label shift and PU learning, we propose practical methods for both tasks that leverage black-box predictors. Unlike typical open set domain adaptation problems, which tend to be ill-posed and amenable only to heuristics, OSLS offers a well-posed problem amenable to more principled machinery. Experiments across numerous semi-synthetic benchmarks on vision, language, and medical datasets demonstrate that our methods consistently outperform open set domain adaptation baselines, achieving 10–25% improvements in target domain accuracy. Finally, we analyze the proposed methods, establishing finite-sample convergence to the true label marginal and convergence to optimal classifier for linear models in a Gaussian setup[1].

1 Introduction

Suppose that we wished to deploy a machine learning system to recognize diagnoses based on their clinical manifestations. If the distribution of data were static over time, then we could rely on the standard machinery of statistical prediction. However, disease prevalences are constantly changing, violating the assumption of independent and identically distributed (iid) data. In such scenarios, we might reasonably apply the *label shift* assumption, where prevalences can change but clinical manifestations cannot. When only the relative proportion of previously seen diseases can change, principled methods can detect and correcting for label shift on the fly [56, 78, 45, 4, 1, 27]. But what if a new disease, like COVID-19, were to arrive suddenly?

Traditional label shift adaptation techniques break when faced with a previously unseen class. A distinct literature on Open Set Domain Adaptation (OSDA) seeks to handle such cases [51, 5, 14, 70, 43, 73, 58, 59, 25]). Given access to labeled *source* data and unlabeled *target* data, the goal in OSDA is to adapt classifiers in general settings where previous classes can shift in prevalence (and even appearance), and novel classes separated out from those previously seen can appear. Most work on OSDA is driven by the creation of and progress on benchmark datasets (e.g., DomainNet, OfficeHome). Existing OSDA methods are heuristic in nature, addressing settings where the right answers seem intuitive but are not identified mathematically. However, absent assumptions on: (i) the nature of distribution shift among source classes and (ii) the relation between source classes and novel class, standard impossibility results for domain adaptation condemn us to guesswork [8].

[1]Code is available at `https://github.com/acmi-lab/Open-Set-Label-Shift`.

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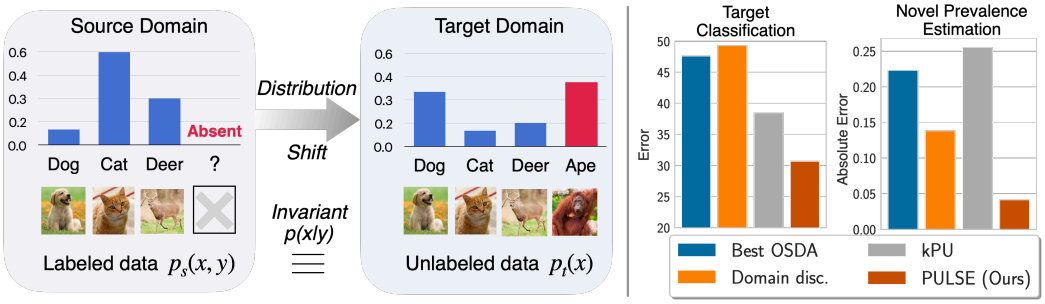

Figure 1: **Left:** *Domain Adaptation under OSLS*. An instantiation of OSDA that applies label shift assumption but allows for a new class to show up in target domain. **Right:** *Aggregated results across seven semi-synthetic benchmark datasets*. For both target classification and novel class prevalence estimation, PULSE significantly outperforms other methods (lower error is better). For brevity, we only include result for the best OSDA method. For detailed comparison, refer Sec. 7.

In this work, we introduce domain adaptation under Open Set Label Shift (OSLS), a coherent instantiation of OSDA that applies the label shift assumption but allows for a new class to show up in the target distribution. Formally, the label distribution may shift between source and target $p_s(y) \neq p_t(y)$, but the class-conditional distributions among previously seen classes may not (i.e., $\forall y \in \{1, 2, \ldots, k\}, p_s(x|y) = p_t(x|y)$). Moreover, a new class $y = k + 1$ may arrive in the target period. Notably, OSLS subsumes label shift [56, 67, 45] (when $p_t(y = k+1) = 0$) and learning from Positive and Unlabeled (PU) data [20, 42, 24] (when $k = 1$). As with label shift and PU learning, our goals are two-fold. Here, we must (i) estimate the target label distribution $p_t(y)$ (including the novel class prevalence); (ii) train a $(k + 1)$-way target-domain classifier.

First, we characterize when the parameters of interest are identified (Sec. 4). Namely, we define a (necessary) *weak positivity* condition, which states that there exists a subset of each label's support that has zero probability mass under the novel class and that the submatrix of $p(x|y)$ consisting only of rows outside the novel class's support is full rank. Moreover, we prove that weak positivity alone is not sufficient. We introduce two sufficient conditions: *strong positivity* and *separability*, either of which (independently) ensures identifiability.

Focusing on cases with strong positivity, we show that OSLS reduces to k PU learning problems (Sec. 5). However, we demonstrate that straightforward applications of this idea fail because (i) bias accumulates across the k mixture proportion estimates leading to grossly underestimating the novel class's prevalence; and (ii) naive combinations of the k PU classifiers are biased and inaccurate.

Thus motivated, we propose the PULSE framework, which combines methods from Positive and Unlabeled learning and Label Shift Estimation, yielding two-stage techniques for both label marginal estimation and classification (Sec. 6). Our methods build on recent advances in label shift [45, 4, 1, 27] and PU learning [38, 35, 29], that leverage appropriately chosen black-box predictors to avoid the curse of dimensionality. PULSE first estimates the label shift among previously seen classes, and then re-samples the source data to formulate a single PU learning problem between (reweighted) source and target data to estimate fraction of novel class and to learn the target classifier. In particular, our procedure builds on the BBE and CVIR techniques proposed in Garg et al. [29]. PULSE is simple to implement and compatible with arbitrary hypothesis classes (including deep networks).

We conduct extensive semi-synthetic experiments adapting seven benchmark datasets spanning vision (CIFAR10, CIFAR100, Entity30), natural language (Newsgroups-20), biology (Tabula Muris), and medicine (DermNet, BreakHis) (Sec. 7). Across numerous data modalities, draws of the label distributions, and model architectures, PULSE consistently outperforms generic OSDA methods, improving by 10–25% in accuracy on target domain. Moreover, PULSE outperforms methods that naively solve k PU problems on both label distribution estimation and classification.

Finally, we analyze our framework (Sec. 8). First, we extend Garg et al. [29]'s analysis of BBE to derive finite-sample error bounds for our estimates of the label marginal. Next, we develop new analyses of the CVIR objective [29] that PULSE relies in the classification stage. Focusing on a Gaussian setup and linear models optimized by gradient descent, we prove that CVIR converges to

a true positive versus negative classifier in population. Addressing the overparameterized setting where parameters exceed dataset size, we conduct an empirical study that helps to elucidate why, on separable data, CVIR outperforms other consistent objectives, including nnPU [38] and uPU [21].

2 Related Work

(Closed Set) Domain Adaptation (DA) Under DA, the goal is to adapt a predictor from a source distribution with labeled data to a target distribution from which we observe only unlabeled examples. DA is classically explored under two distribution shift scenarios [67]: (i) Covariate shift [78, 74, 19, 18, 32] where $p(y|x)$ remains invariant among source and target; and (ii) Label shift [56, 45, 4, 1, 27, 77] where $p(x|y)$ is shared across source and target. In these settings most theoretical analysis requires that the target distribution's support is a subset of the source support [8]. However, recent empirically work in DA [48, 49, 68, 69, 80, 79, 26, 64] focuses on settings motivated by benchmark datasets (e.g., WILDS [57, 39], Office-31 [55] OfficeHome [71], DomainNet [52]) where such overlap assumptions are violated. Instead, they rely on some intuitive notion of semantic equivalence across domains. These problems are not well-specified and in practice, despite careful hyperparameter tuning, these methods often do not improve over standard empirical risk minimization on source data alone for practical, and importantly, previously unseen datasets [57].

Open Set Domain Adaptation (OSDA) OSDA [51, 9, 62] extends DA to settings where along with distribution shift among previously seen classes, we may observe a novel class in the target data. This setting is also known as *universal domain adaptation* [73, 59]. Rather than making precise assumptions about the nature of shift between source and target as in OSLS, the OSDA literature is primarily governed by semi-synthetic problems on benchmark DA datasets (e.g. DomainNet, Office-31 and OfficeHome). Numerous OSDA methods have been proposed [5, 14, 70, 43, 73, 58, 59, 25, 11]. At a high level, most OSDA methods perform two steps: (i) align source and target representation for previously seen classes; and (ii) train a discrimination to reject novel class from previously seen classes. The second step typically uses novelty detection heuristics to identify novel samples.

PU Learning Positive and Unlabeled (PU) learning is the base case of OSLS. Here, we observe labeled data a single source class and unlabeled target data contains data from both the novel class and the source class. In PU learning, our goals are: (i) Mixture Proportion Estimation (MPE), i.e., determining the fraction of previously seen class in target ; and (ii) PU classification, i.e., learning to discriminate between the novel and the positive (source) class. Several classical methods were proposed for both MPE [24, 23, 63, 36, 6, 7] and classification [24, 22, 21]. However, classical MPE methods do not scale to high-dimensional settings [53]. More recent methods alleviate these issues by operating in classifier output space [29, 35]. For classification, traditional methods fail when deployed with models classes with high capacity due to their capacity of fitting random labels [75]. Recent methods [29, 38, 16], avoid over-fitting by employing regularization or self-training techniques.

Other related work A separate line of work looks at the problem of Out-Of-Distribution (OOD) detection [34, 31, 41, 37, 50, 76]. Here, the goal is to identify novel examples, i.e., samples that lie out of the support of training distribution. The main different between OOD detection and OSDA is that in OOD detection we do not have access to unlabeled data containing a novel class. Recently, Cao et al. [13] proposed open-world semi-supervised learning, where the task is to not only identify novel classes in target but also to separate out different novel classes in an unsupervised manner.

Our work takes a step back from the hopelessly general OSDA setup, introducing OSLS, a well-posed OSDA setting where the sought-after parameters can be identified.

3 Open Set Label Shift

Notation For a vector $v \in \mathbb{R}^d$, we use v_j to denote its jth entry, and for an event E, we let $\mathbb{I}[E]$ denote the binary indicator of the event. By $|A|$, we denote the cardinality of set A.

Let $\mathcal{X} \in \mathbb{R}^d$ be the input space and $\mathcal{Y} = \{1, 2, \ldots, k+1\}$ be the output space for multiclass classification. Let P_s and P_t be the source and target distributions and let p_s and p_t denote the corresponding probability density (or mass) functions. By $\mathbb{E}_s$ and $\mathbb{E}_t$, we denote expectations over the source and target distributions. We assume that we are given a loss function $\ell : \Delta^k \times \mathcal{Y} \to \mathbb{R}$, such that $\ell(z, y)$ is the loss incurred by predicting z when the true label is y. Unless specified otherwise, we assume that ℓ

is the cross entropy loss. As in standard unsupervised domain adaptation, we are given independently and identically distributed (iid) samples from labeled source data $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\} \sim \mathrm{P}_s^n$ and iid samples from unlabeled target data $\{x_{n+1}, x_{n+2}, \ldots, x_{n+m}\} \sim \mathrm{P}_t^m$.

Before formally introducing OSLS, we describe label shift and PU learning settings. Under label shift, we observe data from k classes in both source and target where the conditional distribution remain invariant (i.e., $p_s(x|y) = p_t(x|y)$ for all classes $y \in [1, k]$) but the target label marginal may change (i.e., $p_t(y) \neq p_s(y)$). Additionally, for all classes in source have a non-zero support , i.e., for all $y \in [1, k]$, $p_s(y) \geqslant c$, where $c > 0$. Under PU learning, we possess labeled source data from a positive class and unlabeled target data from a mixture of positive and negative class with a goal of learning a positive-versus-negative classifier on target. We now introduce the OSLS setting:

Definition 1 (Open set label shift)**.** *Define $\mathcal{Y}_t = \mathcal{Y}$ and $\mathcal{Y}_s = \mathcal{Y} \backslash \{k+1\}$. Under OSLS, the label distribution among source classes $\mathcal{Y}_s$ may change but the class conditional $p(x|y)$ for those classes remain invariant between source and target, and the target domain may contain a novel class, i.e.,*

$$p_s(x|y = j) = p_t(x|y = j) \quad \forall j \in \mathcal{Y}_s \qquad \textit{and} \qquad p_s(y = k+1) = 0\,. \tag{1}$$

Additionally, we have non-zero support for all k (previously-seen) labels in the source distribution, i.e., for all $y \in \mathcal{Y}_s$, $p_s(y) \geqslant c$ for some $c > 0$.

Note that the label shift and PU learning problems can be obtained as special cases of OSLS. When no novel class is observed in target (i.e., when $p_t(y = k+1) = 0$), we recover the label shift problem, and when we observe only one class in source (i.e., when $k = 1$), the OSLS problem reduces to PU learning. Under OSLS, our goal naturally breaks down into two tasks: (i) estimate the target label marginal $p_t(y)$ for each class $y \in \mathcal{Y}$; (ii) train a classifier $f : \mathcal{X} \to \Delta^k$ to approximate $p_t(y|x)$.

4 Identifiablity of OSLS

We now introduce conditions for OSLS, under which the solution is identifiable. Throughout the section, we will assume access to population distribution for labeled source data and unlabeled target data, i.e., $p_s(x, y)$ and $p_t(x)$ is given. To keep the discussion simple, we assume finite input domain $\mathcal{X}$ which can then be relaxed to continuous inputs. We relegate proofs to App. B.

We first make a connection between target label marginal $p_t(y)$ estimation and learning the target classifier $p_t(y|x)$ showing that recovering $p_t(y)$ is enough to identify $p_t(y|x)$. In population, given access to $p_t(y)$, the class conditional $p_t(x|y = k+1)$ can be obtained in closed form as $\big(p_t(x) - \sum_{j=1}^{k} p_t(y=j) p_s(x|y=j)\big) / p_t(y=k+1)$. We can then apply Bayes rule to obtain $p_t(y|x)$. Henceforth, we will focus our discussion on identifiability of $p_t(y)$ which implies identifiability of $p_t(y|x)$. In following proposition, we present *weak positivity*, a necessary condition for $p_t(y)$ to be identifiable.

Proposition 1 (Necessary conditions)**.** *Assume $p_t(y) > 0$ for all $y \in \mathcal{Y}_t$. Then $p_t(y)$ is identified only if $p_t(x|y = k+1)$ and $p_s(x|y)$ for all $y \in \mathcal{Y}_s$ satisfy weak positivity, i.e., there must exists a subdomain $X_{wp} \subset X$ such that:*

(i) $p_t(X_{wp}|y = k+1) = 0$; and

(ii) the matrix $[p_s(x|y)]_{x \in X_{wp}, y \in \mathcal{Y}_s}$ is full column-rank.

Intuitively, Proposition 1 states that if the target marginal doesn't lie on the vertex of the simplex Δ^k, then their must exist a subdomain X_{wp} where the support of novel class is zero and within X_{wp}, $p_t(y)$ for source classes is identifiable. While it may seem that existence of a subdomain X_{wp} is enough, we show that for the OSLS problem, existence doesn't imply uniqueness. In App. B.1, we construct an example, where the weak positivity condition is not sufficient. In that example, we show that there can exist two subdomains X_{wp} and X'_{wp} satisfying weak positivity, both of which lead to separate solutions for $p_t(y)$. Next, we extend weak positivity to two stronger conditions, either of which (alone) implies identifiability.

Proposition 2 (Sufficient conditions)**.** *The target marginal $p_t(y)$ is identified if for all $y \in \mathcal{Y} \backslash \{k+1\}$, $p_t(x|y = k+1)$ and $p_s(x|y)$ satisfy either:*

(i) Strong positivity, i.e., there exists $X_{sp} \subset \mathcal{X}$ such that $p_t(X_{sp}|y = k+1) = 0$ and the matrix $[p_s(x|y)]_{x \in X_{sp}, y \in \mathcal{Y}_s}$ is full-rank and diagonal; or

(ii) Separability, i.e., there exists $X_{sep} \subset \mathcal{X}$, such that $p_t(X_{sep}|y = k+1) = 0$, $p_s(X_{sep}) = 1$, and the matrix $[p_s(x|y)]_{x \in X_{sep}, y \in \mathcal{Y}_s}$ is full column-rank.

Strong positivity generalizes the irreducibility condition [10], which is sufficient for identifiability under PU learning, to k PU learning problems. Note that while the two conditions in Proposition 2 overlap, they cover independent set of OSLS problems. Informally, strong positivity extends weak positivity by making an additional assumption that the matrix formed by $p(x|y)$ on inputs in X_{wp} is diagonal and the separability assumption extends the weak positivity condition to the full input domain of source classes instead of just X_{wp}. Both of these conditions identify a support region of $\mathcal{X}$ which purely belongs to source classes where we can either individually estimate the proportion of each source classes (i.e., under strong positivity) or jointly estimate the proportion (i.e., under separability).

To extend our identifiability conditions for continuous distributions, the linear independence conditions on the matrix $[p_s(x|y)]_{x \in X_{\text{sep}}, y \in \mathcal{Y}_s}$ has the undesirable property of being sensitive to changes on sets of measure zero. We may introduce stronger notions of linear independence as in Lemma 1 of Garg et al. [27]. We discuss this in App. B.2.

5 Reduction of OSLS to k PU Problems

Under the strong positivity condition, the OSLS problem can be broken down into k PU problems as follows: By treating a given source class $y_j \in \mathcal{Y}_s$ as *positive* and grouping all other classes together as *negative* we observe that the unlabeled target data is then a mixture of data from the positive and negative classes. This yields a PU learning problem and the corresponding mixture proportion is the fraction $p_t(y = j)$ (proportion of class y_j) among the target data. By iterating this process for all source classes, we can solve for the entire target label marginal $p_t(y)$. Thus, OSLS reduces to k instances of PU learning problem. Formally, note that $p_t(x)$ can be written as:

$$p_t(x) = p_t(y = j)p_s(x|y = j) + (1 - p_t(y = j)) \left(\sum_{i \in \mathcal{Y} \setminus \{j\}} \frac{p_t(y = i)}{1 - p_t(y = j)} p_s(x|y = i) \right), \quad (2)$$

individually for all $j \in \mathcal{Y}_s$. By repeating this reduction for all classes, we obtain k separate PU learning problems. Hence, a natural choice is to leverage this structure and solve k PU problems to solve the original OSLS problem. In particular, for each class $j \in \mathcal{Y}_s$, we can first estimate its prevalence $\widehat{p}_t(y = j)$ in the unlabeled target. Then the target marginal for the novel class is given by $\widehat{p}_t(y = k+1) = 1 - \sum_{i=1}^{k} \widehat{p}_t(y = i)$. Similarly, for classification, we can train k PU learning classifiers f_i, where f_i is trained to classify a source class i versus others in target. An example is classified as belonging to the class $y = k+1$, if it rejected by all classifiers f_i as other in target. We explain this procedure more formally in App. A.1.

This reduction has been mentioned in past work [60, 72]. However, to the best of our knowledge, no previous work has empirically investigated both classification and target label marginal estimation jointly. Sanderson and Scott [60] focuses only on target marginal estimation for tabular datasets and Xu et al. [72] assumes that the target marginal is known and only trains k separate PU classifiers.

In our work, we perform the first large scale experiments to evaluate efficacy of the reduction of the OSLS problem to k-PU problems. With plugin state-of-the-art PU learning algorithms, we observe that this naive reduction doesn't scale to datasets with large number of classes because of error accumulation in each of the k MPEs and k one-versus-other PU classifiers. To mitigate the error accumulation problem, we propose the PULSE framework in the next section.

6 The PULSE Framework for OSLS

We begin with presenting our framework for OSLS problem under strong positivity condition. First, we explain the structure of OSLS that we leverage in PULSE framework and then elaborate design decisions we make to exploit the identified structure.

Overview of PULSE framework Rather than simply dividing each OSLS instance into k PU problems, we exploit the joint structure of the problem to obtain a *single* PU learning problem. To begin, we note that if only we could apply a *label shift correction* to source, i.e., re-sample source classes according to their relative proportion in the target data, then we could subsequently consider

Algorithm 1 Positive and Unlabeled learning post Label Shift Estimation (PULSE) framework

input : Labeled source data $\{\mathbf{X}^S, \mathbf{y}^S\}$ and unlabeled target samples $\mathbf{X}^T$.

1: Randomly split data into training $\{\mathbf{X}_1^S, \mathbf{y}_1^S\}$, $\mathbf{X}_1^T$ and hold out partition $\{\mathbf{X}_2^S, \mathbf{y}_2^S\}$, $\mathbf{X}_2^T$.

2: Train a source classifier f_s on labeled source data $\{\mathbf{X}_1^S, \mathbf{y}_1^S\}$.

3: Estimate label shift $\widehat{p}'_t(y=j) = \frac{\widehat{p}_t(y=j)}{\sum_{k\in\mathcal{Y}_s}\widehat{p}_t(y=k)}$ using Algorithm 2 and hence importance ratios $\widehat{w}(j)$ among source classes $j \in \mathcal{Y}_s$.

4: Re-sample training source data according to label distribution $\widehat{p}'_t$ to get $\{\widetilde{\mathbf{X}}_1^S, \widetilde{\mathbf{y}}_1^S\}$ and $\{\widetilde{\mathbf{X}}_2^S, \widetilde{\mathbf{y}}_2^S\}$.

5: Using Algorithm 3, train a discriminator f_d and estimate novel class fraction $\widehat{p}_t(y=k+1)$.

6: Assign $[f_t(x)]_j = (f_d(x))\frac{\widehat{w}(j)\cdot[f_s(x)]_j}{\sum_{k\in\mathcal{Y}_s}\widehat{w}(k)\cdot[f_s(x)]_k}$ for all $j \in \mathcal{Y}_s$ and $[f_t(x)]_{k+1} = 1 - f_d(x)$. And for all $j \in \mathcal{Y}_s$, assign $\widehat{p}_t(y=j) = (1-\widehat{p}_t(y=k+1))\cdot\widehat{p}'_t(y=j)$.

output : Target marginal estimate $\widehat{p}_t \in \Delta^k$ and target classifier $f_t(\cdot) \in \Delta^k$.

the unlabeled target data as a mixture of (i) the (reweighted) source distribution; and (ii) the novel class distribution (i.e., $p_t(x|y=k+1)$). Formally, we have

$$p_t(x) = \sum_{j\in\mathcal{Y}_t} p_t(y=j)p_t(x|y=j) = \sum_{j\in\mathcal{Y}_s}\frac{p_t(y=j)}{p_s(y=j)}p_s(x,y=j) + p_t(x|y=k+1)p_t(y=k+1)$$
$$= (1-p_t(y=k+1))p'_s(x) + p_t(y=k+1)p_t(x|y=k+1)\,, \tag{3}$$

where $p'_s(x)$ is the label-shift-corrected source distribution, i.e., $p'_s(x) = \sum_{j\in\mathcal{Y}_s} w(j)p_s(x,y=j)$, where $w(j) = \left(p_t(y=j)/\sum_k p_t(y=k)\right)/p_s(y=j)$ for all $j \in \mathcal{Y}_s$. Intuitively, $p'_t(j) = p_t(y=j)/\sum_k p_t(y=k)$ is re-normalized label distribution in target among source classes and $w(j)$'s are the importance weights. Hence, after applying a label shift correction to the source distribution $p'_s(x)$, we have reduced the OSLS problem to a *single* PU learning problem, where $p'_s(x)$ plays the part of the positive distribution and $p_t(x|y=k+1)$ acts as negative distribution with mixture coefficients $1-p_t(y=k+1)$ and $p_t(y=k+1)$ respectively. We now discuss our methods (i) to estimate the importance ratios $w(y)$; and (ii) to tackle the PU learning instance obtained from OSLS.

Label shift correction: Target marginal estimation among source classes While traditional methods for estimating label shift breakdown in high dimensional settings [78], recent methods exploit black-box classifiers to avoid the curse of dimensionality [45, 4, 1]. However, these recent techniques require overlapping label distributions, and a direct application would require demarcation of samples from $p'_s(x)$ sub-population in target, creating a cyclic dependency. Instead, to estimate the relative proportion of previously seen classes in target, we leverage the k PU reduction described in Sec. 5 with two crucial distinctions. First, we normalize the obtained estimates of fraction previously seen classes to obtain the relative proportions in $p'_s(y)$. In particular, we do not leverage the estimates of previously seen class proportions in target to directly estimate the proportion of novel class which avoids issues due to error accumulation. Second, we exploit a k-way source classifier f_s trained on labeled source data instead of training k one-versus-other PU classifiers. We tailor the recently proposed Best Bin Estimation (BBE) technique from Garg et al. [29]. We describe the modified BBE procedure in App. C (Algorithm 2). After estimating the relative fraction of source classes in target (i.e., $\widehat{p}'_t(j) = \widehat{p}_t(y=j)/\sum_{k\in\mathcal{Y}_s}\widehat{p}_t(y=k)$ for all $j \in \mathcal{Y}_s$), we re-sample the source data according to $\widehat{p}'_t(y)$ to mimic samples from distribution $p'_s(x)$.

PU Learning: Separating the novel class from previously seen classes After obtaining a PU learning problem instance, we resort to PU learning techniques to (i) estimate the fraction of novel class $p_t(y=k+1)$; and (ii) learn a binary classifier $f_d(x)$ to discriminate between label shift corrected source $p'_s(x)$ and novel class $p_t(x|y=k+1)$. With traditional methods for PU learning involving domain discrimination, over-parameterized models can memorize the positive instances in unlabeled, assigning them confidently to the negative class, which can severely hurt generalization on PN data [38, 29]. Rather, we employ Conditional Value Ignoring Risk (CVIR) loss proposed in Garg et al. [29] which was shown to outperform alternative approaches. First, we estimate the proportion of novel class $\widehat{p}_t(y=k+1)$ with BBE. Next, given an estimate $\widehat{p}_t(y=k+1)$, CVIR objective discards the highest loss $(1-\widehat{p}_t(y=k+1))$ fraction of examples on each training epoch, removing the incentive to overfit to the examples from $p'_s(x)$. Consequently, we employ the iterative procedure that alternates

between estimating the prevalence of novel class $\widehat{p}_t(y = k+1)$ (with BBE) and minimizing the CVIR loss with estimated fraction of novel class. We detail this procedure in App. C (Algorithm 3).

Combining PU learning and label shift correction Finally, to obtain a $(k+1)$-way classifier $f_t(x)$ on target we combine discriminator f_d and source classifier f_s with importance-reweighted label shift correction. In particular, for all $j \in \mathcal{Y}_s$, $[f_t(x)]_j = (f_d(x)) \frac{w(j) \cdot [f_s(x)]_j}{\sum_{k \in \mathcal{Y}_s} w(k) \cdot [f_s(x)]_k}$ and $[f_t(x)]_{k+1} = 1 - f_d(x)$. Overall, our approach outlined in Algorithm 1 proceeds as follows: First, we estimate the label shift among previously seen classes. Then we employ importance re-weighting of source data to formulate a single PU learning problem to estimate the fraction of novel class $\widehat{p}_t(y = k+1)$ and to learn a discriminator f_d for the novel class. Combining discriminator and label shift corrected source classifier we get $(k+1)$-way target classifier. We analyse crucial steps in PULSE in Sec. 8.

Our ideas for PULSE framework can be extended to separability condition since (3) continues to hold. However, in our initial experiments, we observe that techniques proposed under strong positivity were empirically stable and outperform methods developed under separability. This is intuitive for many benchmark datasets where it is natural to assume that for each class there exists a subdomain that only belongs to that class. We describe this in more detail in App. C.1.

7 Experiments

Baselines We compare PULSE with several popular methods from OSDA literature. While these methods are not specifically proposed for OSLS, they are introduced for the more general OSDA problem. In particular, we make comparions with DANCE [59], UAN [73], CMU [25], STA [46], Backprop-ODA (or BODA) [58]. We use the open source implementation available at `https://github.com/thuml`. For alternative baselines, we experiment with source classifier directly deployed on the target data which may contain novel class and label shift among source classes (referred to as *source-only*). We also train a domain discriminator classifier for source versus target (referred to as *domain disc.*). This is adaptation of PU learning baseline[24] which assumes no label shift among source classes. Finally, per the reduction presented in Sec. 5, we train k PU classifiers (referred to as *k-PU*). We include detailed description of each method in App. F.1.

Datasets We conduct experiments with seven benchmark classification datasets across vision, natural language, biology and medicine. For each dataset, we simulate an OSLS problem as described in next paragraph. For vision, we use CIFAR10, CIFAR100 [40] and Entity30 [61]. For language, we experiment with Newsgroups-20 (`http://qwone.com/~jason/20Newsgroups/`) dataset. Additionally, inspired by applications of OSLS in biology and medicine, we experiment with Tabula Muris [17] (Gene Ontology prediction), Dermnet (skin disease prediction `https://dermnetnz.org/`), and BreakHis [66] (tumor cell classification). These datasets span language, image and table modalities. We provide interpretation of OSLS problem for each dataset along with other details in App. F.2.

OSLS Setup To simulate an OSLS problem, we experiment with different fraction of novel class prevalence, source label distribution, and target label distribution. We randomly choose classes that constitute the novel target class. After randomly choosing source and novel classes, we first split the training data from each source class randomly into two partitions. This creates a random label distribution for shared classes among source and target. We then club novel classes to assign them a new class (i.e. $k+1$). Finally, we throw away labels for the target data to obtain an unsupervised DA problem. We repeat the same process on iid hold out data to obtain validation data with no target labels.

Training and Evaluation We use Resnet18 [33] for CIFAR10, CIFAR100, and Entity30. For newsgroups, we use a convolutional architecture. For Tabular Muris and MNIST, we use a fully connected MLP. For Dermnet and BreakHis, we use Resnet-50. For all methods, we use the same backbone for discriminator and source classifier. For kPU, we use a separate final layer for each class with the same backbone. We use default hyperparameters for all methods. For OSDA methods, we use default method specific hyperparameters introduced in their works. Since OSDA methods do not estimate the prevalence of novel class explicitly, we use the fraction of examples predicted in class $k+1$ as a surrogate. We train models till the performance on validation source data (labeled) ceases to increase. Unlike OSDA methods, note that we do not use early stopping based on performance on held-out labeled target data. To evaluate classification performance, we report target accuracy on all classes, seen classes and the novel class. For novel class prevalence estimation, we report absolute difference between the true and estimated marginal. We open-source our code and by simply

Table 1: *Comparison of PULSE with other methods*. Across all datasets, PULSE outperforms alternatives for both target classification and novel class prevalence estimation. Acc (All) is target accuracy, Acc (Seen) is target accuracy on examples from previously seen classes, and Acc (Novel) is recall for novel examples. MPE (Novel) is absolute error for novel prevalence estimation. Results reported by averaging across 3 seeds. Detailed results for each dataset with all methods in App. F.4.

Method	CIFAR-10				CIFAR-100			
	Acc (All)	Acc (Seen)	Acc (Novel)	MPE (Novel)	Acc (All)	Acc (Seen)	Acc (Novel)	MPE (Novel)
Source-Only	67.1	87.0	-	-	46.6	66.4	-	-
UAN [73]	15.4	19.7	25.2	0.214	18.1	40.6	14.8	0.133
BODA [58]	63.1	66.2	42.0	0.162	36.1	17.7	81.6	0.41
DANCE [59]	70.4	85.5	14.5	0.174	47.3	66.4	1.2	0.28
STA [46]	57.9	69.6	14.9	0.124	42.6	48.5	34.8	0.14
CMU [25]	62.1	77.9	41.2	0.183	35.4	46.0	15.5	0.161
Domain Disc. [24]	47.4	87.0	30.6	0.331	45.8	66.5	39.1	**0.046**
k-PU	83.6	79.4	**98.9**	0.036	36.3	22.6	**99.1**	0.298
PULSE (Ours)	**86.1**	**91.8**	88.4	**0.008**	**63.4**	**67.2**	63.5	0.078

Method	Entity30		Newsgroups20		Tabula Muris		BreakHis		DermNet	
	Acc (All)	MPE (Novel)	Acc (All)	MPE (Novel)	Acc (All)	MPE (Novel)	Acc (All)	MPE (Novel)	Acc (All)	MPE (Novel)
Source-Only	32.0	-	39.3	-	33.8	-	70.0	-	41.4	-
BODA [58]	42.2	0.189	43.4	0.16	76.5	0.079	71.5	0.077	43.8	0.207
Domain Disc.	43.2	0.135	50.9	0.176	73.0	0.071	56.5	0.091	40.6	0.083
k-PU	50.7	0.394	52.1	0.373	85.9	0.307	75.6	**0.059**	46.0	0.313
PULSE (Ours)	**58.0**	**0.054**	**62.2**	**0.061**	**87.8**	**0.058**	**79.1**	**0.054**	**48.9**	**0.043**

changing a single config file, new OSLS setups can be generated and experimented with. We provide precise details about hyperparameters, OSLS setup for each dataset and code in App. F.3.

Results Across different datasets, we observe that PULSE consistently outperforms other methods for the target classification and novel prevalence estimation (Table 1). For detection of novel classes (Acc (Novel) column), kPU achieves superior performance as compared to alternative approaches because of its bias to default to $(k+1)^{\text{th}}$ class. This is evident by the sharp decrease in performance on previously seen classes. For each dataset, we plot evolution of performance with training in App. F.4. We observe more stability in performance of PULSE as compared to other methods.

We observe that with default hyperparameters, popular OSDA methods significantly under perform as compared to PULSE. We hypothesize that the primary reasons underlying the poor performance of OSDA methods are (i) the heuristics employed to detect novel classes; and (ii) loss functions incorporated to improve alignment between examples from common classes in source and target. To detect novel classes, a standard heuristic employed in popular OSDA methods involves thresholding uncertainty estimates (e.g., prediction entropy, softmax confidence [73, 25, 59]) at a predefined threshold κ. However, a fixed κ, may not for different datasets and different fractions of the novel class. In App. F.5, we ablate by (i) removing loss function terms incorporated with an aim to improve source target alignment; and (ii) vary threshold κ and show improvements in performance of these methods. In contrast, our two-stage method PULSE, first estimates the fraction of novel class which then guides the classification of novel class versus previously seen classes avoiding the need to guess κ.

Ablations Different datasets, in our setup span different fraction of novel class prevalence ranging from 0.22 (in CIFAR10) to 0.64 (in Tabula Muris). For each dataset, we perform more ablations on the novel class proportion in App. F.6. For kPU and PULSE, in the main paper, we include results with BBE and CVIR [29]. In App. F.8, we perform experiments with alternative PU learning approaches

and highlight the superiority of BBE and CVIR over other methods. Moreover, since we have access to unlabeled target data, we experiment with SimCLR [15] pre-training on the mixture of unlabeled source and target dataset. We include setup details and results in App. F.7. While pre-trained backbone architecture improves performance for all methods, PULSE continues to dominate other methods.

8 Analysis of PULSE Framework

In this section, we analyse key steps of our PULSE procedure for target label marginal estimation (Step 3, 5 Algorithm 1) and learning the domain discriminator classifier (Step 5, Algorithm 1). Due to space constraints, we present informal results here and relegate formal statements and proofs to App. D.

Theoretical analysis for target marginal estimation Building on BBE results from Garg et al. [29], we present finite sample results for target label marginal estimation. When the data satisfies strong positivity, we observe that source classifiers often exhibit a threshold c_y on softmax output of each class $y \in \mathcal{Y}_s$ above which the *top bin* (i.e., $[c_y, 1]$) contains mostly examples from that class y. We give empirical evidence to this claim in App. D.1. Then, we show that the existence of (nearly) pure top bin for each class in f_s is sufficient for Step 3 in Algorithm 1 to produce (nearly) consistent estimates:

Theorem 1 (Informal)**.** *Assume that for each class $y \in \mathcal{Y}_s$, there exists a threshold c_y such that for the classifier f_s, if $[f_s(x)]_y > c_y$ for any x then the true label for that sample x is y. Then, we have* $\|\widehat{p}_t - p_t\|_1 \leqslant \mathcal{O}\left(\sqrt{k^3 \log(4k/\delta)/n} + \sqrt{k^2 \log(4k/\delta)/m}\right)$.

The proof technique simply builds on the proof of Theorem 1 in Garg et al. [29]. By assuming that we recover close to ground truth label marginal for source classes, we can also extend the above analysis to Step 5 of Algorithm 1 to show convergence of estimate $\widehat{p}_t(y = k+1)$ to true prevalence $p_t(y = k+1)$. We discuss this further in App. D.3.

Theoretical analysis of CVIR in population While the CVIR loss was proposed in Garg et al. [29], no analysis was provided for convergence of the iterative gradient descent procedure. In our work, we show that in population on a separable Gaussian dataset, CVIR will recover the optimal classifier.

We consider a binary classification problem where we have access to positive distribution (i.e., p_p), unlabeled distribution (i.e., $p_u := \alpha p_p + (1-\alpha)p_n$), and mixture coefficient α. Making a parallel connection to Step 5 of PULSE, positive distribution p_p here refers to the label shift corrected source distribution p'_s and p_u refers to $p_t = p_t(y = k+1)p_t(x|y = k+1) + (1 - p_t(y = k+1))p'_s(x)$. Our goal is to recover the classifier that discriminates p_p versus p_n (parallel p'_s versus $p_t(\cdot|y = k+1)$).

First we introduce some notation. For a classifier f and loss function ℓ (i.e., logistic loss), define $\text{VIR}_\alpha(f) = \inf\{\tau \in \mathbb{R} : \mathrm{P}_{x\sim p_u}(\ell(x, -1; f) \leqslant \tau) \geqslant 1 - \alpha\}$. Intuitively, $\text{VIR}_\alpha(f)$ identifies a threshold τ to capture bottom $1-\alpha$ fraction of the loss $\ell(x, -1)$ for points x sampled from p_u. Additionally, define CVIR loss as $\mathcal{L}(f, w) = \alpha\mathbb{E}_{p_p}[\ell(x, 1; f)] + \mathbb{E}_{p_u}[w(x)\ell(x, -1; f)]$ for classifier f and some weights $w(x) \in \{0, 1\}$. Formally, given a classifier f_t at an iterate t, CVIR procedure proceeds as follows:

$$w_t(x) = \mathbb{I}\left[\ell(x, -1; f_t) \leqslant \text{VIR}_\alpha(f_t)\right] , \tag{4}$$

$$f_{t+1} = f_t - \eta\nabla\mathcal{L}_f(f_t, w_t) . \tag{5}$$

We assume that x are drawn from two half multivariate Gaussian with mean zero and identity covariance, i.e., $x \sim p_p \Leftrightarrow x = \gamma_0\theta_{\text{opt}} + z|\, \theta_{\text{opt}}^T z \geqslant 0$, and $x \sim p_n \Leftrightarrow x = -\gamma_0\theta_{\text{opt}} + z|\, \theta_{\text{opt}}^T z < 0$, where $z \sim \mathcal{N}(0, I_d)$. Here γ_0 is the margin and $\theta_{\text{opt}} \in \mathbb{R}^d$ is the true separator. Here, we have access to distribution p_p, $p_u = \alpha p_p + (1-\alpha)p_n$, and the true proportion α.

Theorem 2 (Informal)**.** *In the data setup detailed above, a linear classifier $f(x; \theta) = \sigma\left(\theta^T x\right)$ trained with CVIR procedure as in* (4)-(5) *will converge to an optimal positive versus negative classifier.*

The proof uses a key idea that for any classifier θ not separating positive and negative data perfectly, the gradient in (5) is non-zero. Hence, convergence of the CVIR procedure (implied by smoothness of CVIR loss) implies converge to an optimal classifier. For separable datasets in general, we can extend the above analysis with some modifications to the CVIR procedure. We discuss this in App. D.4.

Empirical investigation in overparameterized models As noted in our ablation experiments and in Garg et al. [29], domain discriminator trained with CVIR outperforms classifiers trained with other consistent objectives (nnPU [38] and uPU [21]). While the above analysis highlights consistency of CVIR procedure in population, it doesn't capture the observed empirical efficacy of CVIR over alternative methods in overparameterized models. In the Gaussian setup described above, we train overparameterized linear models to compare CVIR with other methods. We discuss precise experiments and results in App. E, but highlight the key takeaway here. First, we observe that when a classifier is trained to distinguish positive and unlabeled data, *early learning* happens [47, 3, 28], i.e., during the initial phase of learning classifier learns to classify positives in unlabeled correctly as positives. Next, we show that post early learning rejection of large fraction of positives from unlabeled training in equation (4) crucially helps CVIR.

9 Conclusion

In this work, we introduce OSLS a well-posed instantiation of OSDA that subsumes label shift and PU learning into a framework for learning adaptive classifiers. We presented identifiability conditions for OSLS and proposed PULSE, a simple and effective approach to tackle the OSLS problem. Moreover, our extensive experiments demonstrate efficacy of PULSE over popular OSDA alternatives when the OSLS assumptions are met. We would like to highlight the brittle nature of benchmark driven progress in OSDA and hope that our work can help to stimulate more solid foundations and enable systematic progress in this area. Finally, we hope that our open source code and benchmarks will foster further progress on OSLS.

9.1 Limitations and Future Work

Here, we discuss limitations of the PULSE framework. First, to estimate the relative label shift among source classes in target, we leverage k-PU reductions with several modifications. While we reduce the issues due to overestimation bias by re-normalizing the label marginal among source classes in target, in future, we may hope to replace this heuristic step to directly estimate the joint target marginal.

Second, since our methods use CVIR and BBE sub-routines, failure of these methods can lead to failure of PULSE. For example, efficacy of BBE relies on the existence of an almost pure top bin in the classifier output space. While this property seems to be satisfied across different datasets spanning different modalities and applications, failure to identify an almost pure top bin can degrade the performance of BBE and hence, our PULSE framework.

In future work, we also hope to bridge the gap between the necessary and sufficient identifiability conditions. While we empirically investigate reasons for CVIR's efficacy in overparameterized models, we aim to extend our theory to overparameterized settings in future. In our work, we strictly operate under the OSLS settings, where we performed semi-synthetic experiments on vision, language and tabular datasets. In future, it will be interesting to experiment with our PULSE procedure in relaxed settings where $p(x|y)$ may shift in some natural-seeming ways from source to target.

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes]
   (c) Did you discuss any potential negative societal impacts of your work? [N/A] We believe that this work, which proposes a novel instantiation of open set domain adaptation problem does not present a significant societal concern. While this could potentially guide practitioners to improve classification and mixture proportion estimation in applications where data from novel classes can arrive during test time, we do not believe that it will fundamentally impact how machine learning is used in a way that could conceivably be socially salient.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] See Sec. 4 and Sec. 8.
   (b) Did you include complete proofs of all theoretical results? [Yes] See Sec. B and Sec. D.
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] We include all the experimental details in App. F. We also open source our code at `https://github.com/acmi-lab/Open-Set-Label-Shift`
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] Yes, see App. F.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] Yes, we run all experiments with three different seeds and include results in with standard deviation in App. F.
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] Yes, see App. F.
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes]
   (b) Did you mention the license of the assets? [Yes]
   (c) Did you include any new assets either in the supplemental material or as a URL? [N/A]
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [Yes]
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A]
5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]

Supplementary Materials for Domain Adaptation under Open Set Label Shift

A Preliminaries

Domain adaptation under label shift Under label shift, we observe data from k classes in both source and target where the conditional distribution remain invariant (i.e., $p_s(x|y) = p_t(x|y)$ for all classes $y \in [1, k]$) but the target label marginal may change (i.e., $p_t(y) \neq p_s(y)$). Additionally, for all classes in source have a non-zero support , i.e., for all $y \in [1, k]$, $p_s(y) \geqslant c$, where $c > 0$. Here, given labeled source data and unlabeled target data our tasks are: (i) estimate the shift in label distribution, i.e., $p_t(y)$ for all $y \in [1, k]$; (ii) train a classifier for the target domain f_t to approximate $p_t(y|x)$.

One common approach to label shift involves estimating the importance ratios $p_t(y)/p_s(y)$ by leveraging a blackbox classifier and then employing re-sampling of source data or importance re-weighted ERM on source to obtain a classifier for the target domain [45, 4, 1].

PU learning Under PU learning, we possess labeled source data from a positive class (p_p) and unlabeled target data from $p_u = \alpha p_p + (1 - \alpha)p_n$ a mixture of positive and negative class (p_n). Our goals naturally break down in to two tasks: (i) MPE, determining the fraction of positives p_p in p_u and (ii) PU classification, learning a positive-versus-negative classifier on target.

Note that given access to population of positives and unlabeled, α can be estimated as $\min_x p_u(x)/p_p(x)$. Next, we briefly discuss recent methods for MPE that operate in the classifier output space to avoid curse of dimensionality:

(i) **EN:** Given a domain discriminator classifier f_d trained to discriminate between positive and unlabeled, Elkan and Noto [24] proposed the following estimator: $\sum_{x_i \in X_p} f_d(x_i)/\sum_{x_i \in X_u} f_d(x_i)$ where X_p is the set of positive examples and X_u is the set of unlabeled examples.

(ii) **DEDPUL:** Given a domain discriminator classifier f_d, Ivanov [35] proposed an estimator that leverages density of the data in the output space of the classifier f_d to directly estimate $\min p_u(f(x))/p_p(f(x))$.

(iii) **BBE:** BBE [29] identifies a threshold on probability scores assigned by the classifier f_d such that by estimating the ratio between the fractions of positive and unlabeled points receiving scores above the threshold, we obtain proportion of positives in unlabeled.

After obtaining an estimate for mixture proportion α, following methods can be employed for PU classification:

(i) **Domain Discriminator:** Given positive and unlabeled data, Elkan and Noto [24] trained a classifier f_d to discriminator between them. To make a prediction on test point from unlabeled data, we can then use Bayes rule to obtain the following transformation on probabilistic output of the domain discriminator: $f = \alpha \left(\frac{m}{n}\right) \left(\frac{f_d(x)}{1-f_d(x)}\right)$, where n and m are the number of positives and unlabeled examples used to train f_d [24].

(ii) **uPU:** Du Plessis et al. [21] proposed an unbiased loss estimator for positive versus negative training. In particular, since $p_u = \alpha p_p + (1 - \alpha)p_n$, the loss on negative examples $\mathbb{E}_{p_n}[\ell(f(x); -1)]$ can be estimated as:

$$\mathbb{E}_{p_n}[\ell(f(x); -1)] = \frac{1}{1-\alpha}\left[\mathbb{E}_{p_u}[\ell(f(x); -1)] - \alpha\mathbb{E}_{p_p}[\ell(f(x); -1)]\right] . \tag{6}$$

Thus, a classifier can be trained with the following uPU loss:

$$\mathcal{L}_{\text{uPU}}(f) = \alpha\mathbb{E}_{p_p}[\ell(f(x); +1)] + \mathbb{E}_{p_u}[\ell(f(x); -1)] - \alpha\mathbb{E}_{p_p}[\ell(f(x); -1)] . \tag{7}$$

(iii) **nnPU:** While unbiased losses exist that estimate the PvN loss given PU data and the mixture proportion α, this unbiasedness only holds before the loss is optimized, and becomes

ineffective with powerful deep learning models capable of memorization. Kiryo et al. [38] proposed the following non-negative regularization for unbiased PU learning:

$$\mathcal{L}_{\text{nnPU}}(f) = \alpha \mathbb{E}_{p_p}\left[\ell(f(x);+1)\right] + \max\left\{\mathbb{E}_{p_u}\left[\ell(f(x);-1)\right] - \alpha \mathbb{E}_{p_p}\left[\ell(f(x);-1)\right], 0\right\} . \tag{8}$$

(iv) **CVIR:** Garg et al. [29] proposed CVIR objective, which discards the highest loss α fraction of unlabeled examples on each training epoch, removing the incentive to overfit to the unlabeled positive examples. CVIR loss is defined as

$$\mathcal{L}_{\text{CVIR}}(f) = \alpha \mathbb{E}_{p_p}\left[\ell(x,1;f)\right] + \mathbb{E}_{p_u}\left[w(x)\ell(x,-1;f)\right] , \tag{9}$$

where weights $w(x) = \mathbb{I}\left[\ell(x,-1;f) \leqslant \text{VIR}_\alpha(f)\right]$ for $\text{VIR}_\alpha(f)$ defined as $\text{VIR}_\alpha(f) = \inf\{\tau \in \mathbb{R} : \mathrm{P}_{x\sim p_u}(\ell(x,-1;f) \leqslant \tau) \geqslant 1-\alpha\}$. Intuitively, $\text{VIR}_\alpha(f)$ identifies a threshold τ to capture bottom $1-\alpha$ fraction of the loss $\ell(x,-1)$ for points x sampled from p_u.

A.1 Reduction of OSLS into k PU problems

Under the strong positivity condition, the OSLS problem can be broken down into k PU problems as follows: By treating a given source class $y_j \in \mathcal{Y}_s$ as *positive* and grouping all other classes together as *negative* we observe that the unlabeled target data is then a mixture of data from the positive and negative classes. This yields a PU learning problem and the corresponding mixture proportion gives the fraction α_j of class y_j among the target data. By iterating this process for all source classes, we can solve for the entire target label marginal $p_t(y)$. Thus, OSLS reduces to k instances of PU learning problem. Formally, note that $p_t(x)$ can be written as:

$$p_t(x) = \underbrace{p_t(y=j)}_{\alpha_j}\underbrace{p_s(x|y=j)}_{p_p} + (1-p_t(y=j))\underbrace{\left(\sum_{i\in\mathcal{Y}\setminus\{j\}} \frac{p_t(y=i)}{1-p_t(y=j)} p_s(x|y=i)\right)}_{p_n}, \tag{10}$$

individually for all $j \in \mathcal{Y}_s$. By repeating this reduction for all classes, we obtain k separate PU learning problems. Hence, a natural choice is to leverage this structure and solve k PU problems to solve the original OSLS problem.

In particular, for each class $j \in \mathcal{Y}_s$, we can first estimate its prevalence $\widehat{\alpha}_j$ in the unlabeled target. Then the target marginal for the novel class is given by $\widehat{\alpha}_{k+1} = 1 - \sum_{i=1}^{k} \widehat{\alpha}_i$. For classification, we can train k PU learning classifiers f_i, where f_i is trained to classify a source class i versus others in target. Assuming that each f_j returns a score between $[0,1]$, during test time, an example x is classified as $f(x)$ given by

$$f(x) = \begin{cases} \arg\max_{j\in\mathcal{Y}_s} f_j(x) & \text{if } \max_{j\in\mathcal{Y}_s} f_j(x) \geqslant 0.5 \\ k+1 & \text{o.w.} \end{cases} \tag{11}$$

That is, if each classifier classifies the example as belonging to other in unlabeled, then we classify the example as belonging to the class $k+1$. In our main experiments, to estimate α_j and to train f_j classifiers for all $j \in \mathcal{Y}_s$, we use BBE and CVIR as described before which was shown to outperform alternative approaches in Garg et al. [29]. We ablate with other methods in App. F.8.

Note that mathematically any OSLS problems can be thought of as k-PU problems as per (10). However, for identifiablity of each of these PU problems, we need the irreduciblity assumption [7]. Put simply, for individual PU problems defined for source classes $j \in \mathcal{Y}_s$, we need existence of a sub-domain X_j such that we only observe example for that class j in X_j. Collectively X_j gives us the X_{sp} defined in the strong positivity condition.

Failure due to error-accumulation While trading off bias with variance, PU learning algorithms tend to over-estimate the mixture proportion [29, 7]. This error incurred due to bias can be mild for a single mixture proportion estimation task but accumulates with increasing number of classes (i.e., k). This error accumulation can significantly under-estimate the proportion of novel class when estimated by subtracting the sum of prevalence of source classes in target from 1.

B Proofs for identifiability of OSLS

For ease, we re-state Proposition 1 and Proposition 2.

Proposition 1 (Necessary conditions)**.** *Assume $p_t(y) > 0$ for all $y \in \mathcal{Y}_t$. Then $p_t(y)$ is identified only if $p_t(x|y = k+1)$ and $p_s(x|y)$ for all $y \in \mathcal{Y}_s$ satisfy weak positivity, i.e., there must exists a subdomain $X_{wp} \subset X$ such that:*

(i) $p_t(X_{wp}|y = k+1) = 0$; and

(ii) the matrix $[p_s(x|y)]_{x \in X_{wp}, y \in \mathcal{Y}_s}$ is full column-rank.

Proof. We prove this by contradiction. Assume that there exists a unique solution $p_t(y)$. We will obtain contradiction when both (i) and (ii) don't hold.

First, assume for no subset $X_{\text{wp}} \subseteq \mathcal{X}$, we have $[p_s(x|y)]_{x \in X_{\text{wp}}, y \in \mathcal{Y}_s}$ as full-rank. Then in that case, we have vectors $[p_s(x|y = j)]_{x \in \mathcal{X}}$ as linearly dependent for $j \in \mathcal{Y}_s$, i.e., there exists $[\alpha_j]_{j \in \mathcal{Y}_s} \in \mathbb{R}^k$ such that $\sum_j \alpha_j p_s(x|y = j) = 0$ for all $x \in \mathcal{X}$. Thus for small enough $\epsilon > 0$, we have infinite solutions of the form $[p_t(y = j) - \epsilon \cdot a_j]_{j \in \mathcal{Y}_s}$.

Hence, there exists $X_{\text{wp}} \subseteq \mathcal{X}$ for which we have $[p_s(x|y)]_{x \in X_{\text{wp}}, y \in \mathcal{Y}_s}$ as full-rank. Without loss of generality, we assume that $|X_{\text{wp}}| = k$. Assume that $p_t(X_{\text{wp}}|y = k+1) > 0$, i.e., $[p_t(x|y = k+1)]_{x \in X_{\text{wp}}}$ has $l < k$ zero entries. We will now construct another solution for the label marginal p_t. For simplicity we denote $A = [p_s(x|y)]_{x \in X_{\text{wp}}, y \in \mathcal{Y}_s}$. Consider the vector $v(\gamma) = [p_t(x) - (p_t(y = k+1) - \gamma) p_t(x|y = k+1)]_{x \in X_{\text{wp}}}$ for some $\gamma > 0$. Intuitively, when $\gamma = 0$, we have $u = A^{-1} v(0)$ where $u = [p_t(y)]_{y \in \mathcal{Y}_s}$, i.e., we recover the true label marginal corresponding to source classes.

However, since the solution is not at vertex, there exists a small enough $\gamma > 0$ such that $u' = A^{-1} v(\gamma)$ with $\sum_j u'_j \leqslant 1$ and $u'_j \geqslant 0$. Since A is full-rank and $v(\gamma) \neq v(0)$, we have $u' \neq u$. Thus we construct a separate solution with u' as $[p_t(y)]_{y \in \mathcal{Y}_s}$ and $p_t(x) - \sum_{j \in \mathcal{Y}_s} u'_j p_s(x|y = j)$ as $p_t(x|y = k+1)$. Hence, when there exists $X_{\text{wp}} \subseteq \mathcal{X}$ for which we have $[p_s(x|y)]_{x \in X_{\text{wp}}, y \in \mathcal{Y}_s}$ as full-rank, for uniqueness we obtain a contradiction on the assumption $p_t(X_{\text{wp}}|y = k+1) > 0$. □

We now make some comments on the assumption $p_t(y) > 0$ for all $y \in \mathcal{Y}_t$ in Proposition 1. Since, $p_t(y)$ needs to satisfy simplex constraints, if the solution is at a vertex of simplex, then OSLS problem may not require weak positivity. For example, there exists contrived scenarios where $p_s(x|y = j) = p_s(x|y = k)$ for all $j, k \in \mathcal{Y}_s$ and $p_t(x|y = k+1) \neq p_s(x|y = j)$ for all $j \in \mathcal{Y}_s$. Then when $p_t(x) = p_t(x|y = k+1)$, we can uniquely identify the OSLS solution even when weak positivity assumption is not satisfied.

Proposition 2 (Sufficient conditions)**.** *The target marginal $p_t(y)$ is identified if for all $y \in \mathcal{Y} \backslash \{k+1\}$, $p_t(x|y = k+1)$ and $p_s(x|y)$ satisfy either:*

(i) Strong positivity, i.e., there exists $X_{sp} \subset \mathcal{X}$ such that $p_t(X_{sp}|y = k+1) = 0$ and the matrix $[p_s(x|y)]_{x \in X_{sp}, y \in \mathcal{Y}_s}$ is full-rank and diagonal; or

(ii) Separability, i.e., there exists $X_{sep} \subset \mathcal{X}$, such that $p_t(X_{sep}|y = k+1) = 0$, $p_s(X_{sep}) = 1$, and the matrix $[p_s(x|y)]_{x \in X_{sep}, y \in \mathcal{Y}_s}$ is full column-rank.

Proof. For each condition, we will prove identifiability by constructing the unique solution.

Under strong positivity, for all $j \in \mathcal{Y}_s$ there exists $x \in X_{\text{sp}}$ such that $p_t(x|y = k) = 0$ for all $k \in \mathcal{Y}_t \backslash \{j\}$. Set $\alpha_j = \min_{x \in \mathcal{X}, p_s(x|y=j) > 0} \frac{p_t(x)}{p_s(x|y=j)}$, for all $j \in \mathcal{Y}_s$. For $x \in X_{\text{sp}}$ such that $p_t(x|y = k) = 0$ for all $k \in \mathcal{Y}_t \backslash \{j\}$, we get $\frac{p_t(x)}{p_s(x|y=j)} = p_t(y = j)$ and for all $x' \neq x$, we have $\frac{p_t(x)}{p_s(x|y=j)} \geqslant p_t(y = j)$. Thus, we get $\alpha_j = p_t(y = j)$. Finally, we get $\alpha_{k+1} = 1 - \sum_{j \in \mathcal{Y}_s} \alpha_j$. Plugging in values of the label marginal, we can obtain $p_t(x|y = k+1)$ as $p_t(x) - \sum_{y \in \mathcal{Y}_s} p_t(y = j) p_s(x|y = j)$.

Under separability, we can obtain the label marginal p_t for source classes by simply considering the set X_{sep}. Denote $A = [p(x|y)]_{x \in X_{\text{sep}}, y \in \mathcal{Y}_s}$ and $v = [p_t(x)]_{x \in X_{\text{sep}}}$. Then, since A is full column-rank by assumption, we can define $u = (A^T A)^{-1} A^T v$. For all $x \in X_{\text{sep}}$, we have $p_t(x) =$

$\sum_{y\in\mathcal{Y}_s} p_t(y)p_s(x|y)$ and hence, $u = [p_t(y)]_{y\in\mathcal{Y}_s}$. Having obtained $[p_t(y)]_{y\in\mathcal{Y}_s}$, we recover $p_t(y = k+1) = 1 - \sum_{j\in\mathcal{Y}_s} p_t(y = j)$ and $p_t(x|y = k+1) = p_t(x) - \sum_{j\in\mathcal{Y}_s} p_t(y = j)p_s(x|y = j)$. □

B.1 Examples illustrating importance of weak positivity condition

In this section, we present two examples, one, to show that weak positivity isn't sufficient for identifiability. Second, we present another example where we show that conditions in Proposition 2 are not necessary for identifiability.

Example 1 Assume $\mathcal{X} = \{x_1, x_2, x_3, x_4, x_5\}$ and $\mathcal{Y}_t = \{1, 2, 3\}$. Suppose the $p_t(x|y = 1)$, $p_t(x|y = 2)$, and $p_t(x)$ are given as:

	$p_t(x\|y=1)$	$p_t(x\|y=2)$	$p_t(x)$
x_1	0.4	0.56	0.356
x_2	0.3	0.3	0.207
x_3	0.2	0.1	0.09
x_4	0.1	0.04	0.042
x_5	0.0	0.0	0.305

Here, there exists two separate $p_t(x|y = 3)$ and $p_t(y)$ that are consistent with the given $p_t(x|y = 1)$, $p_t(x|y = 2)$, and $p_t(x)$ and both the solutions satisfy weak positivity for two different X_{wp} and X'_{wp}.

In particular, notice that $p_t(x|y = 3) = [0.17, 0.0675, 0.0, 0.0, 0.7625]^T$ and $p_t(y) = [0.3, 0.3, 0.4]$ gives us the first solution. $p_t(x|y = 3) = [0.0, 0.0, 0.0645, 0.0096, 0.9839]^T$ and $p_t(y) = [0.19, 0.5, 0.31]$ gives us another solution. For solution 1, $X_{\text{wp}} = \{x_3, x_4\}$ and for solution 2, $X'_{\text{wp}} = \{x_1, x_2\}$. To check consistency of each solution notice that $\sum_{i\in\mathcal{Y}} p_t(y = i)p_t(x|y = i) = p_t(x)$ for each $x \in \mathcal{X}$. □

In the above example, the key is to show that absent knowledge of which x's constitute the set X_{wp}, we might be able to obtain multiple different solutions, each with different X_{wp} and both $p_t(y)$, $p_t(x|y = k+1)$ satisfying the given information and simplex constraints.

Next, we will show that in certain scenarios weak positivity is enough for identifiability.

Example 2 Assume $\mathcal{X} = \{x_1, x_2, x_3, x_4\}$ and $\mathcal{Y}_t = \{1, 2, 3\}$. Suppose the $p_t(x|y = 1)$, $p_t(x|y = 2)$, and $p_t(x)$ are given as,

	$p_t(x\|y=1)$	$p_t(x\|y=2)$	$p_t(x)$
x_1	0.5	0.2	0.24
x_2	0.3	0.4	0.2
x_3	0.1	0.35	0.35
x_4	0.1	0.05	0.21

Here, out of all ${}^4C_2$ possibilities for X_{wp}, only one possibility yields a solution that satisfies weak positivity and simplex constraints. In particular, the solution is given by $p_t(x|y = 3) = [0.0, 0.0, 0.6, 0.4]^T$ and $p_t(y) = [0.4, 0.2, 0.4]$ with $X_{\text{wp}} = \{x_1, x_2\}$. □

In this example, we show that conditions in Proposition 2 are not necessary to ensure identifiability. For discrete domains, this example also highlights that we can check identifiability in exponential time for any OSLS problem given $p_t(x)$ and $p_s(x|y)$ for all $y \in \mathcal{Y}_s$.

B.2 Extending identifiability conditions to continuous distributions

To extend our identifiability conditions for continuous distributions, the linear independence conditions on the matrix $[p_s(x|y)]_{x\in X_{\text{sep}}, y\in\mathcal{Y}_s}$ has the undesirable property of being sensitive to changes on sets of measure zero. In particular, by changing a collection of linearly dependent distributions on a set of measure zero, we can make them linearly independent. As a consequence, we may impose a *stronger* notion of independence, i.e., the set of distributions $\{p(x|y) : y = 1, ..., k\}$ are such

that there does not exist $v \neq 0$ for which $\int_X |\sum_y p(x|y)v_y|dx = 0$, where $X = X_{\text{wp}}$ for necessary condition and $X = X_{\text{sp}}$ for sufficiency. We refer this condition as *strict linear independence*.

C PULSE Framework

In our PULSE framework, we build on top of BBE and CVIR from Garg et al. [29]. Here, we elaborate on Step 3 and 5 in Algorithm 1.

Extending BBE algorithm to estimate target marginal among previously seen classes We first explain the intuition behind BBE approach. In a PU learning problem, given positive and unlabeled data, BBE estimates the fraction of positives in unlabeled in the push-forward space of the classifier. In particular, instead of operating in the original input space, BBE maps the inputs to one-dimensional outputs (i.e., a score between zero and one) which is the predicted probability of an example being from the positive class. BBE identifies a threshold on probability scores assigned by a domain discriminator classifier such that the ratio between the fractions of positive and unlabeled points receiving scores above the threshold is minimized. Intuitively, if their exists a threshold on probability scores assigned by the classifier such that the examples mapped to a score greater than the threshold are *mostly* positive, BBE aims to identify this threshold. Efficacy of BBE procedure relies on existence of such a threshold. This is referred to as the *top bin property*. We provide empirical evidence to the property in Fig. 2 in App. D.1. We tailor BBE to estimate the relative fraction of previously seen classes in the target distribution by exploiting a k-way source classifier f_s trained on labeled source data. We describe the procedure in Algorithm 2.

We now introduce some notation needed to introduce the tailored BBE proceudre formally. For given probability density function p and a scalar output function f, define a function $q(z) = \int_{A_z} p(x)dx$, where $A_z = \{x \in \mathcal{X} : f(x) \geqslant z\}$ for all $z \in [0, 1]$. Intuitively, $q(z)$ captures the cumulative density of points in a top bin, the proportion of input domain that is assigned a value larger than z by the function f in the transformed space. We define an empirical estimator $\widehat{q}(z)$ given a set $X = \{x_1, x_2, \ldots, x_n\}$ sampled iid from $p(x)$. Let $Z = f(X)$. Define $\widehat{q}(z) = \sum_{i=1}^{n} \mathbb{I}\left[z_i \geqslant z\right]/n$.

Our modified BBE procedure proceeds as follows. Given a held-out dataset of source $\{\mathbf{X}_2^S, \mathbf{y}_2^S\}$ and unlabeled target samples $\mathbf{X}_2^T$, we push all examples through the source classifier f to obtain k dimensional outputs. For all $j \in \mathcal{Y}_s$, we repeat the following: Obtain $Z_s = f_j(\mathbf{X}_2^S[\text{id}_j])$ and $Z_t = f_j(\mathbf{X}_2^T)$. Intuitively, Z_s and Z_t are the push forward mapping of the source classifier. Next, with Z_p and Z_u, we estimate $\widehat{q}_s$ and $\widehat{q}_t$. Finally, we estimate $[\widehat{p}_t]_j$ as the ratio $\widehat{q}_t(\widehat{c})/\widehat{q}_s(\widehat{c})$ at $\widehat{c}$ that minimizes the upper confidence bound at a pre-specified level δ and a fixed parameter $\gamma \in (0, 1)$. Our method is summarized in Algorithm 2. Throughout all the experiments, we fix δ at 0.1 and γ at 0.01.

Algorithm 2 Extending Best Bin Estimation (BBE) for Step 3 in Algorithm 1

input : Validation source $\{\mathbf{X}_2^S, \mathbf{y}_2^S\}$ and unlabeled target samples $\mathbf{X}_2^T$. Source classifier $f : \mathcal{X} \to \Delta^{k-1}$. Hyperparameter $0 < \delta, \gamma < 1$.

1: $\widehat{p}_t \leftarrow \text{zeros}(size = |\mathcal{Y}_s|)$
2: **for** $j \in \mathcal{Y}_s$ **do**
3: $\quad \text{id}_j \leftarrow \text{where}(\mathbf{y}_2^S = j)$.
4: $\quad Z_s, Z_t \leftarrow \left[f(\mathbf{X}_2^S[\text{id}_j])\right]_j, \left[f(\mathbf{X}_2^T)\right]_j$.
5: $\quad \widehat{q}_s(z), \widehat{q}_t(z) \leftarrow \frac{\sum_{z_i \in Z_s} \mathbb{I}[z_i \geqslant z]}{|\text{id}_j|}, \frac{\sum_{z_i \in Z_t} \mathbb{I}[z_i \geqslant z]}{|\mathbf{X}_2^T|}$ for all $z \in [0, 1]$.
6: $\quad \widehat{c}_j \leftarrow \arg\min_{c \in [0,1]} \left(\frac{\widehat{q}_t(c)}{\widehat{q}_s(c)} + \frac{1+\gamma}{\widehat{q}_s(c)} \left(\sqrt{\frac{\log(4/\delta)}{2|\mathbf{X}_2^T|}} + \sqrt{\frac{\log(4/\delta)}{2|\text{id}_j|}} \right) \right)$.
7: $\quad [\widehat{p}_t]_j \leftarrow \frac{\widehat{q}_t(\widehat{c}_j)}{\widehat{q}_s(\widehat{c}_j)}$.
8: **end for**

output : Normalized target marginal among source classes $\widehat{p}'_t \leftarrow \frac{\widehat{p}_t}{\|\widehat{p}_t\|_1}$

Extending CVIR to train discriminator f_d and estimate novel class prevalence After estimating the fraction of source classes in target (i.e., $p'_t(j) = {p_t(y=j)}/{\sum_{k \in \mathcal{Y}_s} p_t(y=k)}$ for all $j \in \mathcal{Y}_s$), we re-sample the source data according to $p'_t(y)$ to mimic samples from distribution $p'_s(x)$. Thus, obtaining

a PU learning problem instance, we resort to PU learning techniques to (i) estimate the fraction of novel class $p_t(y = k+1)$; and (ii) learn a binary classifier $f_d(x)$ to discriminate between label shift corrected source $p'_s(x)$ and novel class $p_t(x|y = k+1)$. Assume that sigmoid output $f_d(x)$ indicates predicted probability of an example x belonging to label shift corrected source $p'_s(x)$. With $\widehat{\mathcal{L}}^+(f_\theta; X)$, we denote the loss incurred by f_θ when classifying examples from X as positive, i.e., $\widehat{\mathcal{L}}^+(f_\theta; X) = \sum_{i=1}^{|X|} \frac{\ell(f_\theta(x_i),+1)}{|X|}$. Similarly, $\widehat{\mathcal{L}}^-(f_\theta; X) = \sum_{i=1}^{|X|} \frac{\ell(f_\theta(x_i),-1)}{|X|}$

Given an estimate of the fraction of novel class $\widehat{p}_t(y = k+1)$, CVIR objective creates a provisional set of novel examples $\mathbf{X}_1^N$ by removing $(1-\widehat{p}_t(y = k+1))$ fraction of examples from $\mathbf{X}_1^T$ that incur highest loss when predicted as novel class on each training epoch. Next, we update our discriminator f_d by minimizing loss on label shift corrected source $\widetilde{\mathbf{X}}_1^S$ and provisional novel examples $\mathbf{X}_1^N$. This step is aimed to remove any incentive to overfit to the examples from $p'_s(x)$. Consequently, we employ the iterative procedure that alternates between estimating the prevalence of novel class $\widehat{p}_t(y = k+1)$ (with BBE) and minimizing the CVIR loss with estimated fraction of novel class. Algorithm 3 summarizes our approach which is used in Step 3 of Algorithm 1.

Note that we need to warm start with simple domain discrimination training, since in the initial stages mixture proportion estimate is often close to 1 rejecting all the unlabeled examples. In Garg et al. [29], it was shown that the procedure is not sensitive to the choice of number of warm start epochs and in a few cases with large datasets, we can even get away without warm start (i.e., $W = 0$) without hurting the performance. In our work, we notice that given an estimate $\widehat{\alpha}$ of prevalence of novel class, we can use unbiased PU error (7) on validation data as a surrogate to identify warm start epochs for domain discriminator training. In particular, we train the domain discriminator classifier for a large number of epochs, say $E(>> W)$, and then choose the discriminator, i.e., warm start epoch W at which f_d achieves minimum unbiased validation loss.

Finally, to obtain a $(k+1)$-way classifier $f_t(x)$ on target we combine discriminator f_d and source classifier f_s with importance-reweighted label shift correction. In particular, for all $j \in \mathcal{Y}_s$, $[f_t(x)]_j = (f_d(x)) \frac{w(j)\cdot[f_s(x)]_j}{\sum_{k\in\mathcal{Y}_s} w(k)\cdot[f_s(x)]_k}$ and $[f_t(x)]_{k+1} = 1 - f_d(x)$. Similarly, to obtain target marginal p_t, we re-scale the label shift estimate among previously seen classes with estimate of prevalence of novel examples, i.e., for all $j \in \mathcal{Y}_s$, assign $\widehat{p}_t(y = j) = (1 - \widehat{p}_t(y = k+1)) \cdot \widehat{p}'_t(y = j)$.

Overall, our approach proceeds as follows (Algorithm 1): First, we estimate the label shift among previously seen classes. Then we employ importance re-weighting of source data to formulate a single PU learning problem between source and target to estimate fraction of novel class $\widehat{p}_t(y = k+1)$ and to learn a discriminator f_d for the novel class. Combining discriminator and label shift corrected source classifier we get $(k+1)$-way target classifier.

C.1 PULSE under separability

Our ideas for PULSE framework can be extended to separability condition since (3) continues to hold. In particular, when OSLS satisfies the separability assumption, we may hope to jointly estimate the label shift among previously seen classes with label shift estimation techniques [45, 1] and learn a domain discriminator classifier. This may be achieved by estimating label shift among examples rejected by domain discriminator classifier as belonging to previously seen classes. However, in our initial experiments, we observe that techniques proposed under strong positivity were empirically stable and outperform methods developed under separability. This is intuitive for many benchmark datasets where it may be more natural to expect that for each class there exists a subdomain that only belongs to that class than assuming separability only between novel class samples and examples from source classes.

D Proofs for analysis of OSLS framework

In this section, we provide missing formal statements and proofs for theorems in Sec. 8. This mainly includes analysing key steps of our PULSE procedure for target label marginal estimation (Step 3, 5 Algorithm 1) and learning the domain discriminator classifier (Step 5, Algorithm 1).

Algorithm 3 Alternating between CVIR and BBE for Step 5 in Algorithm 1

input : Re-sampled training source data $\widetilde{\mathbf{X}}_1^S$, validation source data $\widetilde{\mathbf{X}}_2^S$. Training target data $\mathbf{X}_1^T$ and validation data $\mathbf{X}_2^T$. Hyperparameter W, B, δ, γ.

1: Initialize a training model f_θ and an stochastic optimization algorithm $\mathcal{A}$.
2: $\mathbf{X}_1^N \leftarrow \mathbf{X}_1^T$.
{// Warm start with domain discrimination training}
3: **for** $i \leftarrow 1$ to W **do**
4: Shuffle $(\widetilde{\mathbf{X}}_1^S, \mathbf{X}_1^N)$ into B mini-batches. With $(\widetilde{\mathbf{X}}_1^S[i], \mathbf{X}_1^N[i])$ we denote i^{th} mini-batch.
5: **for** $i \leftarrow 1$ to B **do**
6: Set the gradient $\nabla_\theta \left[\widehat{\mathcal{L}}^+(f_\theta; \widetilde{\mathbf{X}}_1^S[i]) + \widehat{\mathcal{L}}^-(f_\theta; \mathbf{X}_1^N[i])\right]$ and update θ with algorithm $\mathcal{A}$.
7: **end for**
8: **end for**
9: $\widehat{\alpha} \leftarrow$ BBE($\widetilde{\mathbf{X}}_2^S, \mathbf{X}_2^T, f_\theta$) {Algorithm 4}
10: Rank samples $x \in \mathbf{X}_1^T$ according to their loss values $\ell(f_\theta(x), -1)$.
11: $\mathbf{X}_1^N \leftarrow \{\mathbf{X}_1^T\}_{1-\widehat{\alpha}}$ where $\{\mathbf{X}_1^T\}_{1-\widehat{\alpha}}$ denote the lowest ranked $1-\widehat{\alpha}$ fraction of samples.
12: **while** training error $\widehat{\mathcal{E}}^+(f_\theta; \widetilde{\mathbf{X}}_2^S) + \widehat{\mathcal{E}}^-(f_\theta; \mathbf{X}_1^N)$ is not converged **do**
13: Train model f_θ for one epoch on $(\widetilde{\mathbf{X}}_1^S, \mathbf{X}_1^N)$ as in Lines 4-7.
14: $\widehat{\alpha} \leftarrow$ BBE($\widetilde{\mathbf{X}}_2^S, \mathbf{X}_2^T, f_\theta$) {Algorithm 4}
15: Rank samples $x \in \mathbf{X}_1^T$ according to their loss values $\ell(f_\theta(x), -1)$.
16: $\mathbf{X}_1^N \leftarrow \{\mathbf{X}_1^T\}_{1-\widehat{\alpha}}$ where $\{\mathbf{X}_1^T\}_{1-\widehat{\alpha}}$ denote the lowest ranked $1-\widehat{\alpha}$ fraction of samples.
17: **end while**

output : Trained discriminator $f_d \leftarrow f_\theta$ and novel class fraction $\widehat{p}_t(y = k+1) \leftarrow 1 - \widehat{\alpha}$.

Algorithm 4 Best Bin Estimation (BBE)

input : Re-sampled source data $\widetilde{\mathbf{X}}^S$ and target samples $\mathbf{X}^T$. Discriminator classifier $\widehat{f} : \mathcal{X} \to [0,1]$. Hyperparameter $0 < \delta, \gamma < 1$.

1: $Z_s, Z_t \leftarrow f(\widetilde{\mathbf{X}}^S), f(\mathbf{X}^T)$.
2: $\widehat{q}_t(z), \widehat{q}_s(z) \leftarrow \frac{\sum_{z_i \in Z_s} \mathbb{I}[z_i \geqslant z]}{|\widetilde{\mathbf{X}}^S|}, \frac{\sum_{z_i \in Z_t} \mathbb{I}[z_i \geqslant z]}{|\mathbf{X}|^T}$ for all $z \in [0,1]$.
3: Estimate $\widehat{c} \leftarrow \arg\min_{c \in [0,1]} \left(\frac{\widehat{q}_t(c)}{\widehat{q}_s(c)} + \frac{1+\gamma}{\widehat{q}_s(c)} \left(\sqrt{\frac{\log(4/\delta)}{2|\widetilde{\mathbf{X}}^S|}} + \sqrt{\frac{\log(4/\delta)}{2|\mathbf{X}^T|}} \right) \right)$.

output : $\widehat{\alpha} \leftarrow \frac{\widehat{q}_t(\widehat{c})}{\widehat{q}_s(\widehat{c})}$

D.1 Formal statement and proof of Theorem 1

Before introducing the formal statement, we introduce some additional notation. Given probability density function p and a source classifier $f : \mathcal{X} \to \Delta^{k-1}$, define a function $q(z,j) = \int_{A(z,j)} p(x)dx$, where $A(z,j) = \{x \in \mathcal{X} : [f(x)]_j \geqslant z\}$ for all $z \in [0,1]$. Intuitively, $q(z,j)$ captures the cumulative density of points in a top bin for class j, i.e., the proportion of input domain that is assigned a value larger than z by the function f at the index j in the transformed space. We define an empirical estimator $\widehat{q}(z,j)$ given a set $X = \{x_1, x_2, \ldots, x_n\}$ sampled iid from $p(x)$. Let $Z = [f(X)]_j$. Define $\widehat{q}(z,j) = \sum_{i=1}^n \mathbb{I}[z_i \geqslant z]/n$.

For each pdf p_s and p_t, we define q_s and q_t respectively. Moreover, for each class $j \in \mathcal{Y}_s$, we define $q_{t,j}$ corresponding to $p_{t,j} := p_t(x|y=j)$ and $q_{t,-j}$ corresponding to $p_{t,-j} := \frac{\sum_{i \in \mathcal{Y}_t \setminus \{j\}} p_t(y=i) p_t(x|y=i)}{\sum_{i \in \mathcal{Y}_t \setminus \{j\}} p_t(y=j)}$. Assume that we have n source examples and m target examples. Now building on BBE results from Garg et al. [29], we present finite sample results for target label marginal estimation:

Theorem 3 (Formal statement of Theorem 1)**.** *Define* $c_j^* = \arg\min_{c \in [0,1]} (q_{t,-j}(c,j)/q_{t,j}(c,j))$*, for all* $j \in \mathcal{Y}_s$*. Assume* $\min(n,m) \geqslant \max_{j \in \mathcal{Y}_s} \left(\frac{2\log(4k/\delta)}{q_{t,j}^2(c_j^*, j)} \right)$*. Then, for every* $\delta > 0$*,* $\widehat{p}_t$ *(in Algorithm 2*

with δ as δ/k) satisfies with probability at least $1-\delta$, we have:

$$\|\widehat{p}_t - p_t\|_1 \leqslant \sum_{j\in\mathcal{Y}_s} (1 - p_t(y=j)) \left(\frac{q_{t,-j}(c_j^*, j)}{q_{t,j}(c_j^*, j)}\right) + \mathcal{O}\left(\sqrt{\frac{k^3 \log(4k/\delta)}{n}} + \sqrt{\frac{k^2 \log(4k/\delta)}{m}}\right).$$

When the data satisfies strong positivity, we observe that source classifiers often exhibit a threshold c_y on softmax output of each class $y \in \mathcal{Y}_s$ above which the *top bin* (i.e., $[c_y, 1]$) contains mostly examples from that class y. Formally, as long as there exist a threshold $c_j^* \in (0,1)$ such that $q_{t,j}(c_j^*) \geqslant \epsilon$ and $q_{t,-j}(c_j^*) = 0$ for some constant $\epsilon > 0$ for all $j \in \mathcal{Y}_s$, we show that our estimator $\widehat{\alpha}$ converges to the true α with convergence rate $\min(n,m)^{-1/2}$. The proof technique simply builds on the proof of Theorem 1 in Garg et al. [29]. First, we state Lemma 1 from Garg et al. [29]. Next, for completeness we provide the proof for Theorem 3 which extends proof of Theorem 1 [29] for k classes.

Lemma 1. *Assume two distributions q_p and q_u with their empirical estimators denoted by $\widehat{q}_p$ and $\widehat{q}_u$ respectively. Then for every $\delta > 0$, with probability at least $1-\delta$, we have for all $c \in [0,1]$*

$$\left|\frac{\widehat{q}_u(c)}{\widehat{q}_p(c)} - \frac{q_u(c)}{q_p(c)}\right| \leqslant \frac{1}{\widehat{q}_p(c)}\left(\sqrt{\frac{\log(4/\delta)}{2n_u}} + \frac{q_u(c)}{q_p(c)}\sqrt{\frac{\log(4/\delta)}{2n_p}}\right).$$

Proof of Theorem 3. The main idea of the proof is to use the confidence bound derived in Lemma 1 at $\widehat{c}$ and use the fact that $\widehat{c}$ minimizes the upper confidence bound. The proof is split into two parts. First, we derive a lower bound on $\widehat{q}_{t,j}(\widehat{c}_j)$ for all $j \in \mathcal{Y}_s$ and next, we use the obtained lower bound to derive confidence bound on $\widehat{p}_t(y=j)$. With $\widehat{\alpha}_j$, we denote $\widehat{p}_t(y=j)$ for all $j \in \mathcal{Y}_s$. All the statements in the proof simultaneously hold with probability $1-\delta/k$. We derive the bounds for a single $j \in \mathcal{Y}_s$ and then use union bound to combine bound for all $j \in \mathcal{Y}_s$. When it is clearly from context, we denote $q_{t,j}(c,j)$ with $q_{t,j}(c)$ and $q_t(c,j)$ with $q_t(c)$. Recall,

$$\widehat{c}_j := \arg\min_{c\in[0,1]} \frac{\widehat{q}_t(c)}{\widehat{q}_{t,j}(c)} + \frac{1}{\widehat{q}_{t,j}(c)}\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + (1+\gamma)\sqrt{\frac{\log(4k/\delta)}{2np_s(y=j)}}\right) \quad \text{and} \tag{12}$$

$$\widehat{p}_t(y=j) := \frac{\widehat{q}_t(\widehat{c}_j)}{\widehat{q}_{t,j}(\widehat{c}_j)}. \tag{13}$$

Moreover,

$$c_j^* := \arg\min_{c\in[0,1]} \frac{q_t(c)}{q_{t,j}(c)} \quad \text{and} \quad \alpha_j^* := \frac{q_t(c_j^*)}{q_{t,j}(c_j^*)}. \tag{14}$$

Part 1: We establish lower bound on $\widehat{q}_{t,j}(\widehat{c}_j)$. Consider $c_j' \in [0,1]$ such that $\widehat{q}_{t,j}(c_j') = \frac{\gamma}{2+\gamma}\widehat{q}_{t,j}(c_j^*)$. We will now show that Algorithm 2 will select $\widehat{c}_j < c_j'$. For any $c \in [0,1]$, we have with with probability $1-\delta/k$,

$$\widehat{q}_{t,j}(c) - \sqrt{\frac{\log(4k/\delta)}{2n\cdot p_s(y=j)}} \leqslant q_{t,j}(c) \quad \text{and} \quad q_t(c) - \sqrt{\frac{\log(4k/\delta)}{2m}} \leqslant \widehat{q}_t(c). \tag{15}$$

Since $\frac{q_t(c_j^*)}{q_{t,j}(c_j^*)} \leqslant \frac{q_t(c)}{q_{t,j}(c)}$, we have

$$\widehat{q}_t(c) \geqslant q_{t,j}(c)\frac{q_t(c_j^*)}{q_{t,j}(c_j^*)} - \sqrt{\frac{\log(4k/\delta)}{2m}} \geqslant \left(\widehat{q}_{t,j}(c) - \sqrt{\frac{\log(4k/\delta)}{2n\cdot p_s(y=j)}}\right)\frac{q_t(c_j^*)}{q_{t,j}(c_j^*)} - \sqrt{\frac{\log(4k/\delta)}{2m}}. \tag{16}$$

Therefore, at c we have

$$\frac{\widehat{q}_t(c)}{\widehat{q}_{t,j}(c)} \geqslant \alpha_j^* - \frac{1}{\widehat{q}_{t,j}(c)}\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \frac{q_t(c_j^*)}{q_p(c_j^*)}\sqrt{\frac{\log(4k/\delta)}{2n\cdot p_s(y=j)}}\right). \tag{17}$$

Using Lemma 1 at c^*, we have

$$\frac{\widehat{q}_t(c)}{\widehat{q}_{t,j}(c)} \geqslant \frac{\widehat{q}_t(c_j^*)}{\widehat{q}_{t,j}(c_j^*)} - \left(\frac{1}{\widehat{q}_{t,j}(c_j^*)} + \frac{1}{\widehat{q}_{t,j}(c)}\right)\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \frac{q_t(c_j^*)}{q_{t,j}(c_j^*)}\sqrt{\frac{\log(4k/\delta)}{2n \cdot p_s(y=j)}}\right) \tag{18}$$

$$\geqslant \frac{\widehat{q}_t(c_j^*)}{\widehat{q}_{t,j}(c_j^*)} - \left(\frac{1}{\widehat{q}_{t,j}(c_j^*)} + \frac{1}{\widehat{q}_{t,j}(c)}\right)\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \sqrt{\frac{\log(4k/\delta)}{2n \cdot p_s(y=j)}}\right), \tag{19}$$

where the last inequality follows from the fact that $\alpha_j^* = \frac{q_t(c_j^*)}{q_{t,j}(c_j^*)} \leqslant 1$. Furthermore, the upper confidence bound at c is lower bound as follows:

$$\frac{\widehat{q}_t(c)}{\widehat{q}_{t,j}(c)} + \frac{1+\gamma}{\widehat{q}_{t,j}(c)}\left(\sqrt{\frac{\log(4l/\delta)}{2m}} + \sqrt{\frac{\log(4k/\delta)}{2n \cdot p_s(y=j)}}\right) \tag{20}$$

$$\geqslant \frac{\widehat{q}_t(c_j^*)}{\widehat{q}_{t,j}(c_j^*)} + \left(\frac{1+\gamma}{\widehat{q}_{t,j}(c)} - \frac{1}{\widehat{q}_{t,j}(c_j^*)} - \frac{1}{\widehat{q}_{t,j}(c)}\right)\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \sqrt{\frac{\log(4k/\delta)}{2n \cdot p_s(y=j)}}\right) \tag{21}$$

$$= \frac{\widehat{q}_t(c_j^*)}{\widehat{q}_{t,j}(c_j^*)} + \left(\frac{\gamma}{\widehat{q}_{t,j}(c)} - \frac{1}{\widehat{q}_{t,j}(c_j^*)}\right)\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \sqrt{\frac{\log(4k/\delta)}{2n \cdot p_s(y=j)}}\right) \tag{22}$$

Using (22) at $c = c'$, we have the following lower bound on ucb at c':

$$\frac{\widehat{q}_t(c')}{\widehat{q}_{t,j}(c')} + \frac{1+\gamma}{\widehat{q}_{t,j}(c')}\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \sqrt{\frac{\log(4k/\delta)}{2n \cdot p_s(y=j)}}\right) \tag{23}$$

$$\geqslant \frac{\widehat{q}_t(c_j^*)}{\widehat{q}_{t,j}(c_j^*)} + \frac{1+\gamma}{\widehat{q}_{t,j}(c_j^*)}\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \sqrt{\frac{\log(4k/\delta)}{2n \cdot p_s(y=j)}}\right), \tag{24}$$

Moreover from (22), we also have that the lower bound on ucb at $c \geqslant c'$ is strictly greater than the lower bound on ucb at c'. Using definition of $\widehat{c}$, we have

$$\frac{\widehat{q}_t(c_j^*)}{\widehat{q}_{t,j}(c_j^*)} + \frac{1+\gamma}{\widehat{q}_{t,j}(c_j^*)}\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \sqrt{\frac{\log(4k/\delta)}{2n \cdot p_s(y=j)}}\right) \tag{25}$$

$$\geqslant \frac{\widehat{q}_t(\widehat{c})}{\widehat{q}_{t,j}(\widehat{c})} + \frac{1+\gamma}{\widehat{q}_{t,j}(\widehat{c})}\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \sqrt{\frac{\log(4k/\delta)}{2n \cdot p_s(y=j)}}\right), \tag{26}$$

and hence

$$\widehat{c} \leqslant c'. \tag{27}$$

Part 2: We now establish an upper and lower bound on $\widehat{\alpha}_j$. We start with upper confidence bound on $\widehat{\alpha}_j$. By definition of $\widehat{c}_j$, we have

$$\frac{\widehat{q}_t(\widehat{c})}{\widehat{q}_{t,j}(\widehat{c})} + \frac{1+\gamma}{\widehat{q}_{t,j}(\widehat{c})}\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \sqrt{\frac{\log(4k/\delta)}{2n \cdot p_s(y=j)}}\right) \tag{28}$$

$$\leqslant \min_{c\in[0,1]}\left[\frac{\widehat{q}_t(c)}{\widehat{q}_{t,j}(c)} + \frac{1+\gamma}{\widehat{q}_{t,j}(c)}\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \sqrt{\frac{\log(4k/\delta)}{2n \cdot p_s(y=j)}}\right)\right] \tag{29}$$

$$\leqslant \frac{\widehat{q}_t(c_j^*)}{\widehat{q}_{t,j}(c_j^*)} + \frac{1+\gamma}{\widehat{q}_{t,j}(c_j^*)}\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \sqrt{\frac{\log(4k/\delta)}{2n \cdot p_s(y=j)}}\right). \tag{30}$$

Using Lemma 1 at c_j^*, we get

$$\frac{\widehat{q}_t(c_j^*)}{\widehat{q}_{t,j}(c_j^*)} \leqslant \frac{q_t(c_j^*)}{q_{t,j}(c_j^*)} + \frac{1}{\widehat{q}_{t,j}(c_j^*)}\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \frac{q_t(c_j^*)}{q_{t,j}(c_j^*)}\sqrt{\frac{\log(4k/\delta)}{2n\cdot p_s(y=j)}}\right)$$
$$= \alpha_j^* + \frac{1}{\widehat{q}_{t,j}(c_j^*)}\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \alpha_j^*\sqrt{\frac{\log(4k/\delta)}{2n\cdot p_s(y=j)}}\right). \tag{31}$$

Combining (30) and (31), we get

$$\widehat{\alpha}_j = \frac{\widehat{q}_t(\widehat{c})}{\widehat{q}_{t,j}(\widehat{c})} \leqslant \alpha_j^* + \frac{2+\gamma}{\widehat{q}_{t,j}(c_j^*)}\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \sqrt{\frac{\log(4k/\delta)}{2n\cdot p_s(y=j)}}\right). \tag{32}$$

Using DKW inequality on $\widehat{q}_{t,j}(c_j^*)$, we have $\widehat{q}_{t,j}(c_j^*) \geqslant q_{t,j}(c_j^*) - \sqrt{\frac{\log(4k/\delta)}{2n\cdot p_s(y=j)}}$. Assuming $n\cdot p_s(y=j) \geqslant \frac{2\log(4k/\delta)}{q_{t,j}^2(c_j^*)}$, we get $\widehat{q}_{t,j}(c_j^*) \leqslant q_{t,j}(c_j^*)/2$ and hence,

$$\widehat{\alpha}_j \leqslant \alpha_j^* + \frac{4+2\gamma}{q_{t,j}(c_j^*)}\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \sqrt{\frac{\log(4k/\delta)}{2n\cdot p_s(y=j)}}\right). \tag{33}$$

Finally, we now derive a lower bound on $\widehat{\alpha}_j$. From Lemma 1, we have the following inequality at $\widehat{c}$

$$\frac{q_t(\widehat{c})}{q_{t,j}(\widehat{c})} \leqslant \frac{\widehat{q}_t(\widehat{c})}{\widehat{q}_{t,j}(\widehat{c})} + \frac{1}{\widehat{q}_{t,j}(\widehat{c})}\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \frac{q_t(\widehat{c})}{q_{t,j}(\widehat{c})}\sqrt{\frac{\log(4k/\delta)}{2n\cdot p_s(y=j)}}\right). \tag{34}$$

Since $\alpha_j^* \leqslant \frac{q_t(\widehat{c})}{q_{t,j}(\widehat{c})}$, we have

$$\alpha_j^* \leqslant \frac{q_t(\widehat{c})}{q_{t,j}(\widehat{c})} \leqslant \frac{\widehat{q}_t(\widehat{c})}{\widehat{q}_{t,j}(\widehat{c})} + \frac{1}{\widehat{q}_{t,j}(\widehat{c})}\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \frac{q_t(\widehat{c})}{q_{t,j}(\widehat{c})}\sqrt{\frac{\log(4k/\delta)}{2n\cdot p_s(y=j)}}\right). \tag{35}$$

Using (33), we obtain a very loose upper bound on $\frac{\widehat{q}_t(\widehat{c})}{\widehat{q}_{t,j}(\widehat{c})}$. Assuming $\min(n\cdot p_s(y=j), m) \geqslant \frac{2\log(4k/\delta)}{q_{t,j}^2(c_j^*)}$, we have $\frac{\widehat{q}_t(\widehat{c})}{\widehat{q}_{t,j}(\widehat{c})} \leqslant \alpha_j^* + 4 + 2\gamma \leqslant 5 + 2\gamma$. Using this in (35), we have

$$\alpha_j^* \leqslant \frac{\widehat{q}_t(\widehat{c})}{\widehat{q}_{t,j}(\widehat{c})} + \frac{1}{\widehat{q}_{t,j}(\widehat{c})}\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + (5+2\gamma)\sqrt{\frac{\log(4k/\delta)}{2n\cdot p_s(y=j)}}\right). \tag{36}$$

Moreover, as $\widehat{c} \geqslant c'$, we have $\widehat{q}_{t,j}(\widehat{c}) \geqslant \frac{\gamma}{2+\gamma}\widehat{q}_{t,j}(c_j^*)$ and hence,

$$\alpha_j^* - \frac{\gamma+2}{\gamma\widehat{q}_{t,j}(c_j^*)}\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + (5+2\gamma)\sqrt{\frac{\log(4k/\delta)}{2n\cdot p_s(y=j)}}\right) \leqslant \frac{\widehat{q}_t(\widehat{c})}{\widehat{q}_{t,j}(\widehat{c})} = \widehat{\alpha}_j\,. \tag{37}$$

As we assume $n\cdot p_s(y=j) \geqslant \frac{2\log(4k/\delta)}{q_{t,j}^2(c_j^*)}$, we have $\widehat{q}_{t,j}(c_j^*) \leqslant q_{t,j}(c_j^*)/2$, which implies the following lower bound on α:

$$\alpha_j^* - \frac{2\gamma+4}{\gamma q_{t,j}(c_j^*)}\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + (5+2\gamma)\sqrt{\frac{\log(4k/\delta)}{2n\cdot p_s(y=j)}}\right) \leqslant \widehat{\alpha}_j\,. \tag{38}$$

Combining lower bound (38) and upper bound (33), we get

$$\left|\widehat{\alpha}_j - \alpha_j^*\right| \leqslant l_j\left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \sqrt{\frac{\log(4k/\delta)}{2n\cdot p_s(y=j)}}\right), \tag{39}$$

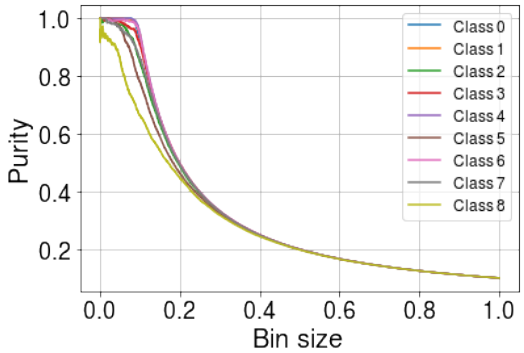


Figure 2: Purity and size (in terms of fraction of unlabeled samples) in the top bin for all classes. Bin size refers to the fraction of examples in the top bin. With purity, we refer to the fraction of examples from a specific class j in the top bin. Results with ResNet-18 on CIFAR10 OSLS setup. Details of the setup in App. F.2. As the bin size increases for all classes the purity decreases.

for some constant l_j. Additionally by our assumption of OSLS problem $p_s(y = j) > c/k$ for some constant $c > 0$, we have

$$\left|\widehat{\alpha}_j - \alpha_j^*\right| \leqslant l'_j \left(\sqrt{\frac{\log(4k/\delta)}{2m}} + \sqrt{\frac{k\log(4k/\delta)}{2n}}\right), \tag{40}$$

for some constant l'_j.

Combining the above obtained bound for all $j \in \mathcal{Y}_s$ with union bound, we get with probability at least $1 - \delta$,

$$\sum_{j\in\mathcal{Y}_s} \left|\widehat{\alpha}_j - \alpha_j^*\right| \leqslant l'_{\max} \left(\sqrt{\frac{k^2\log(4k/\delta)}{2m}} + \sqrt{\frac{k^3\log(4k/\delta)}{2n}}\right), \tag{41}$$

where $l'_{\max} = \max l'_j$. Now, note that for each $j \in \mathcal{Y}_s$, we have $q_t(c) = p_t(y = j)\cdot q_{t,j}(c) + (1 - p_t(y = j)) \cdot q_{t,-j}(c)$. Hence $\alpha_j^* = p_t(y = j) + (1 - p_t(y = j)) \cdot q_{t,-j}(c)/ \cdot q_{t,j}(c)$. Plugging this in, we get the desired bound. □

Intuitively, the guarantees in the previous theorem capture the tradeoff due to the proportion of negative examples in the top bin (bias) versus the proportion of positives in the top bin (variance). As a corollary, we can show convergence to true mixture if there exits c_j^* for all $j \in \mathcal{Y}_s$ such that $q_{t,-j}(c_j^*, j) = 0$ and $q_{t,j}(c_j^*, j) \geqslant \epsilon$ for some $\epsilon > 0$. Put simply, efficacy of BBE relies on existence of a threshold on probability scores assigned by the classifier such that the examples mapped to a score greater than the threshold are *mostly* positive. Using the terminology from Garg et al. [29], we refer to this as the top bin property. Next, we provide empirical evidence of this property while using the source classifier to estimate the relative proportion of target label marginal among source classes.

Empirical evidence of the top bin property We now empirically validate the positive pure top bin property (Fig. 2). We include results with Resnet-18 trained on the CIFAR10 OSLS setup same as our main experiments. We observe that source classifier approximately satisfies the positive pure top bin property for small enough top bin sizes.

D.2 Formal statement and proof of Theorem 2

In this section, we show that in population on a separable Gaussian dataset, CVIR will recover the optimal classifier. Note that here we consider a binary classification problem similar to the one in Step 5 in Algorithm 1. Since we are primarily interested in analysing the iterative procedure for obtaining domain discriminator classifier, we assume that α is known.

In population, we have access to positive distribution (i.e., p_p), unlabeled distribution (i.e., $p_u := \alpha p_p + (1 - \alpha)p_n$), and mixture coefficient α. Our goal is to recover the classifier that discriminates p_p versus p_n.

For ease, we re-introduce some notation. For a classifier f and loss function ℓ, define

$$\text{VIR}_\alpha(f) = \inf\{\tau \in \mathbb{R} : \text{P}_{x\sim p_u}(\ell(x,-1;f) \leqslant \tau) \geqslant 1-\alpha\}\,. \tag{42}$$

Intuitively, $\text{VIR}_\alpha(f)$ identifies a threshold τ to capture bottom $1-\alpha$ fraction of the loss $\ell(x,-1)$ for points x sampled from p_u. Additionally, define CVIR loss as

$$\mathcal{L}(f,w) = \alpha\mathbb{E}_{p_p}\left[\ell(x,1;f)\right] + \mathbb{E}_{p_u}\left[w(x)\ell(x,-1;f)\right]\,, \tag{43}$$

for classifier f and some weights $w(x) \in \{0,1\}$. Recall that given a classifier f_t at an iterate t, CVIR procedure proceeds as follows:

$$w_t(x) = \mathbb{I}\left[\ell(x,-1;f_t) \leqslant \text{VIR}_\alpha(f_t)\right]\,, \tag{44}$$

$$f_{t+1} = f_t - \eta\nabla\mathcal{L}_f(f_t,w_t)\,. \tag{45}$$

We assume a data generating setup with where the support of positive and negative data is completely disjoint. We assume that x are drawn from two half multivariate Gaussian with mean zero and identity covariance, i.e.,

$$x \sim p_p \Leftrightarrow x = \gamma_0\theta_{\text{opt}} + z|\,\theta_{\text{opt}}^T z \geqslant 0,\ \text{where } z \sim \mathcal{N}(0,I_d)$$

$$x \sim p_n \Leftrightarrow x = -\gamma_0\theta_{\text{opt}} + z|\,\theta_{\text{opt}}^T z < 0,\ \text{where } z \sim \mathcal{N}(0,I_d)$$

Here γ_0 is the margin and $\theta_{\text{opt}} \in \mathbb{R}^d$ is the true separator. Here, we have access to distribution p_p and $p_u = \alpha p_p + (1-\alpha)p_n$. Assume ℓ as the logistic loss. For simplicity, we will denote $\mathcal{L}(f_{\theta_t},w_t)$ with $\mathcal{L}(\theta_t,w_t)$.

Theorem 4 (Formal statement of Theorem 2)**.** *In the data setup described above, a linear classifier $f(x;\theta) = \sigma\left(\theta^T x\right)$ initialized at some θ_0 such that $\mathcal{L}(\theta_0,w_0) < \log(2)$, trained with CVIR procedure as in equations* (44)-(45) *will converge to an optimal positive versus negative classifier.*

Proof of Theorem 4. The proof uses two key ideas. One, at convergence of the CVIR procedure, the gradient of CVIR loss in (43) converges to zero. Second, for any classifier θ that is not optimal for positive versus negative classification, we show that the CVIR gradient in (43) is non-zero.

Part 1 We first show that the loss function $\mathcal{L}(\theta,w)$ in (43) is 2-smooth with respect to θ for fixed w. Using gradient descent lemma with the decreasing property of loss in (44)-(45), we show that gradient converges to zero eventually. Considering gradient of $\mathcal{L}$, we have

$$\nabla_\theta\mathcal{L}(\theta,w) = \alpha\mathbb{E}_{p_p}\left[(f(x;\theta)-1)x\right] + \mathbb{E}_{p_u}\left[w(x)(f(x;\theta)-0)x\right]\,. \tag{46}$$

Moreover, $\nabla^2\mathcal{L}$ is given by

$$\nabla_\theta^2\mathcal{L}(\theta,w) = \alpha\mathbb{E}_{p_p}\left[\nabla f(x;\theta)xx^T\right] + \mathbb{E}_{p_u}\left[w(x)\nabla f(x;\theta)xx^T\right]\,. \tag{47}$$

Since $\nabla f(x;\theta) \leqslant 1$, we have $v^T\nabla^2\mathcal{L}v \leqslant 2$ for all unit vector $v \in R^d$. Now, by gradient descent lemma if $\eta \leqslant 1/2$, at any step t we have, $\mathcal{L}(\theta_{t+1},w_t) \leqslant \mathcal{L}(\theta_t,w_t)$. Moreover, by definition of $\text{VIR}_\alpha(\theta)$ in (42) and update (44), we have $\mathcal{L}(\theta_{t+1},w_{t+1}) \leqslant \mathcal{L}(\theta_{t+1},w_t)$. Hence, we have $\mathcal{L}(\theta_{t+1},w_{t+1}) \leqslant \mathcal{L}(\theta_t,w_t)$. Since, the loss is lower bounded from below at 0, for every $\epsilon > 0$, we have for large enough t (depending on ϵ), $\|\nabla_\theta\mathcal{L}(\theta_t,w_t)\|_2 \leqslant \epsilon$, i.e., $\|\nabla_\theta\mathcal{L}(\theta_t,w_t)\|_2 \to 0$ as $t \to \infty$.

Part 2 Consider a general scenario when $\gamma > 0$. Denote the input domain of p_p and p_n as P and N respectively. At any step t, for all points $x \in \mathcal{X}$ such that $p_u(x) > 0$ and $w_t(x) = 0$, we say that x is rejected from p_u. We denote the incorrectly rejected subdomain of p_n from p_u as N_r and the incorrectly accepted subdomain of p_p from p_u as P_a. Formally, $N_r = \{x : p_n(x) > 0 \text{ and } w_t(x) = 0\}$ and $P_a = \{x : p_p(x) > 0 \text{ and } w_t(x) = 1\}$. We will show that $p_p(P_a) \to 0$ as $t \to \infty$, and hence, we will recover the optimal classifier where we reject none of p_u incorrectly.

Observe that at any time t, for fixed w_t and $\theta = \theta_t$, the gradient of CVIR loss in (43), can be expressed as:

$$\nabla_\theta\mathcal{L}(\theta,w_t) = \underbrace{\alpha\int_{x\in P\setminus P_a}(f(x;\theta)-1)x\cdot p_p(x)dx}_{\text{I}} + \underbrace{(1-\alpha)\int_{x\in N\setminus N_r}(f(x;\theta)-0)x\cdot p_n(x)dx}_{\text{II}}$$
$$+\underbrace{\alpha\int_{x\in P_a}(2f(x;\theta)-1)x\cdot p_p(x)dx}_{\text{III}}\,. \tag{48}$$

Note that for any x, θ, $0 \leqslant f(x;\theta) \leqslant 1$. Now consider inner product of individual terms above with θ_{opt}, we get

$$\langle \text{I}, \theta_{\text{opt}} \rangle = \int_{x \in P \setminus P_a} (f(x;\theta) - 1) x^T \theta_{\text{opt}} \cdot p_p(x) dx \leqslant -\gamma_0 \int_{x \in P \setminus P_a} (1 - f(x;\theta)) \cdot p_p(x) dx \,, \quad (49)$$

$$\langle \text{II}, \theta_{\text{opt}} \rangle = \int_{x \in N \setminus N_r} (f(x;\theta) - 0) x^T \theta_{\text{opt}} \cdot p_n(x) dx \leqslant -\gamma_0 \int_{x \in N \setminus N_r} (f(x;\theta) - 0) \cdot p_n(x) dx \,, \quad (50)$$

$$\langle \text{III}, \theta_{\text{opt}} \rangle = \int_{x \in P_a} (2f(x;\theta) - 1) x^T \theta_{\text{opt}} \cdot p_p(x) dx \leqslant -\gamma_0 \int_{x \in P_a} (1 - 2f(x;\theta)) \cdot p_p(x) dx \,. \quad (51)$$

Now, we will argue that individually all the three LHS terms in (49), (50), (51) are negative for all classifiers that do not separate positive versus negative data begining from $\mathcal{L}(\theta_0, w_0) < \log(2)$. And hence, we show that these terms approach zero individually only when the linear classifier approaches an optimal positive versus negative classifier.

First, we consider the term in the LHS of equation (51). When $\alpha = 0.5$, we have $\text{VIR}_\alpha(\theta) = 0.5$ and hence, $(1 - 2f(x;\theta)) \leqslant 0$ for $x \in P_a$. When $\alpha > 0.5$, $\text{VIR}_\alpha(\theta) < 0.5$ because, the proportion $\alpha \cdot p_p(P_a)$ matches with proportion $(1-\alpha) \cdot p_n(N_r)$. Hence, we again have $(1-2f(x;\theta)) \leqslant 0$ for $x \in P_a$.

To handle the case with $\alpha < 0.5$, we use a symmetry of he distribution to because $\text{VIR}_\alpha(\theta) > 0.5$ and $(1-2f(x;\theta))$ can take positive and negative values. However, note that $\text{VIR}_\alpha(\theta)$ will be selected such that the proportion $\alpha \cdot p_p(P_a)$ matches with proportion $(1-\alpha) \cdot P_n(N_r)$. In particular, we can split P_a into three disjoint sets $P_a^{(1)}$, $P_a^{(2)}$, and $P_a^{(3)}$ such that for all $x \in P_a^{(1)}$ we have $f(x;\theta) >= 0.5$, for all $x \in P_a^{(2)} \cup P_a^{(3)}$ we have $f(x;\theta) < 0.5$ and $p_p(P_a^{(3)}) = \frac{\alpha}{1-\alpha} p_p(N_r)$. Additionally, by symmetry of distribution around θ, we have $\int_{x \in P_a^{(1)}} (1-2f(x;\theta)) \cdot p_p(x) dx + \int_{x \in P_a^{(2)}} (1-2f(x;\theta)) \cdot p_p(x) dx = 0$. Hence, we get

$$\langle \text{III}, \theta_{\text{opt}} \rangle \leqslant -\gamma_0 \int_{x \in P_a} (1 - 2f(x;\theta)) \cdot p_p(x) dx = -\gamma_0 \int_{x \in P_a^{(3)}} (1 - 2f(x;\theta)) \cdot p_p(x) dx \,. \quad (52)$$

Combining all three cases, we get $\langle \text{III}, \theta_{\text{opt}} \rangle < 0$ when $p_p(P_a) > 0$.

Now we consider LHS terms in (49) and (50). Note that for all $x \in P \cup N$, we have $0 \leqslant f(x) \leqslant 1$. Thus with $p_p(P \setminus P_a) > 0$, $\langle \text{I}, \theta_{\text{opt}} \rangle \to 0$ when $f(x,\theta) \to 1$ for all $x \in P \setminus P_a$. Similarly with $p_n(N \setminus N_r) > 0$, $\langle \text{II}, \theta_{\text{opt}} \rangle \to 0$ when $f(x,\theta) \to 0$ for all $x \in N \setminus N_r$.

From part 1, for gradient $\|\nabla_\theta \mathcal{L}(\theta_t, w_t)\|_2$ to converge to zero as $t \to \infty$, we must have that LHS in equations (49), (50), and (51) converges to zero individually. Since CVIR loss decreases continuously and $\mathcal{L}(\theta_0, w_0) < \log(2)$, we have that $p_p(P_a) \to 0$ and hence, $f(x,\theta) \to 1$ for all $x \in P$ and $f(x,\theta) \to 0$ for all $x \in N$.

□

The above analysis can be extended to show convergence to max-margin classifier by using arguments from Soudry et al. [65]. In particular, as $p_p(P_a) \to 0$, we can show that $\theta_t / \|\theta_t\|_2$ will converge to the max-margin classifier for p_p versus p_n, i.e., θ_{opt} if $p_p(P_a) \to 0$ in finite number of steps. Note that we need an assumption that the initialized model θ_0 is strictly better than a model that randomly guesses or initialized at all zeros. This is to avoid convergence to the local minima of $\theta = \mathbf{0}$ with CVIR training. This assumption is satisfied when the classifier is initialized in a way such that $\langle \theta_0, \theta_{\text{opt}} \rangle > 0$. In general, we need a weaker assumption that during training with any randomly initialized classifier, there exists an iterate t during CVIR training such that $\langle \theta_t, \theta_{\text{opt}} \rangle > 0$.

D.3 Extension of Theorem 1

We also extend the analysis in the proof of Theorem 3 to Step 5 of Algorithm 1 to show convergence of estimate $\widehat{p}_t(y = k+1)$ to true prevalence $p_t(y = k+1)$. In particular, we show that the estimation error for prevalence of the novel class will primarily depend on sum of two terms: (i) error in

approximating the label shift corrected source distribution, i.e., $p'_s(x)$; and (ii) purity of the top bin of the domain discriminator classifier.

Before formally introducing the result, we introduce some notation. Similar to before, given probability density function p and a domain discriminator classifier $f : \mathcal{X} \to \Delta$, define a function $q = \int_{A(z)} p(x)dx$, where $A(z) = \{x \in \mathcal{X} : f(x) \geqslant z\}$ for all $z \in [0, 1]$. Intuitively, $q(z)$ captures the cumulative density of points in a top bin, i.e., the proportion of input domain that is assigned a value larger than z by the function f in the transformed space. We denote $p_t(x|y = k + 1)$ with $p_{t,k+1}$. For each pdf p_t, $p_{t,k+1}$, and p'_s, we define q_t, $q_{t,k+1}$, and q'_s respectively. Note that since We define an empirical estimator $\widehat{q}(z)$ given a set $X = \{x_1, x_2, \ldots, x_n\}$ sampled iid from $p(x)$. Let $Z = f(X)$. Define $\widehat{q}(z) = \sum_{i=1}^{n} \mathbb{I}\left[z_i \geqslant z\right]/n$.

Recall that in Step 5 of Algorithm 1, to estimate the proportion of novel class, we have access to re-sampled data from approximate label shift corrected source distribution $\widehat{q}'_s(x)$. Assume that we the size of re-sampled dataset is n.

Theorem 5. *Define* $c^* = \arg\min_{c\in[0,1]} \left(q_{t,k+1}(c)/\widehat{q}'_s(c)\right)$. *Assume* $\min(n, m) \geqslant \left(\frac{2\log(4/\delta)}{(\widehat{q}'_s(c^*))^2}\right)$. *Then, for every* $\delta > 0$, $[\widehat{p}_t]_{k+1} := \widehat{p}_t(y = k + 1)$ *in Step 5 of Algorithm 1 satisfies with probability at least* $1 - \delta$, *we have:*

$$|[\widehat{p}_t]_{k+1} - [p_t]_{k+1}| \leqslant (1 - [p_t]_{k+1}) \underbrace{\frac{|q'_s(c^*) - \widehat{q}'_s(c^*)|}{\widehat{q}'_s(c^*)}}_{\substack{\textit{Error in estimating} \\ \textit{label shift corrected source}}} + [p_t]_{k+1} \underbrace{\left(\frac{q_{t,k+1}(c^*)}{\widehat{q}'_s(c^*)}\right)}_{\substack{\textit{Impurity in} \\ \textit{top bin}}}$$
$$+ \mathcal{O}\left(\sqrt{\frac{\log(4/\delta)}{n}} + \sqrt{\frac{\log(4/\delta)}{m}}\right).$$

Proof. We can simply prove this theorem as Corollary of Theorem 1 from Garg et al. [29]. Note that $q_t(c^*) = (1 - p_t(y = k + 1)) \cdot q'_s(c^*) + p_t(y = k + 1) \cdot q_{t,k+1}(c^*)$. Adding and subtracting $(1-p_t(y = k+1))\cdot\widehat{q}'_s(c^*)$ and dividing by $\widehat{q}'_s$, we get $\frac{q_t(c^*)}{\widehat{q}'_s(c^*)} = (1-p_t(y = k+1))\cdot\frac{|q'_s(c^*)-\widehat{q}'_s(c^*)|}{\widehat{q}'_s(c^*)} + (1 - p_t(y = k + 1)) + p_t(y = k + 1) \cdot \frac{q_{t,k+1}(c^*)}{\widehat{q}'_s(c^*)}$. Plugging in bound for LHS from Theorem 1 in Garg et al. [29], we get the desired result. □

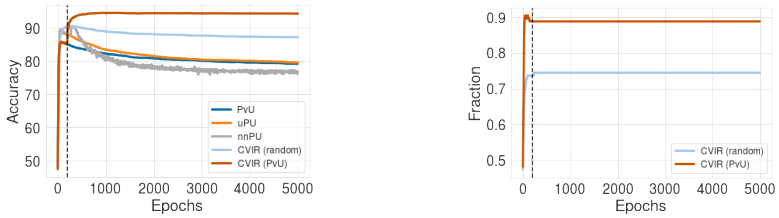
D.4 Extensions of Theorem 2 to general separable datasets

For general separable datasets, CVIR has undesirable property of getting stuck at local optima where gradient in (51) can be zero by maximizing entropy on the subset P_a which is (incorrectly) not-rejected from p_u in CVIR iterations. Intuitively, if the classifier can perfectly separate $P\backslash P_a$ and $N\backslash N_r$ and at the same time maximize the entropy of the region P_a, then the classifier trained with CVIR can get stuck in this local minima.

However, we can extend the above analysis with some modifications to the CVIR procedure. Note that when the CVIR classifier maximizes the entropy on P_a. it makes an error on points in P_a. Since, we have access to the distribution p_p, we can add an additional regularization penalty to the CVIR loss that ensures that the converged classifier with CVIR correctly classifies all the points in p_p. With a large enough regularization constant for the supervised loss on p_p, we can dominate the gradient term in (51) which pushes CVIR classifier to correct decision boundary even on P_a (instead of maximizing entropy). We leave formal analysis of this conjecture for future work. Since we warm start CVIR training with a positive versus unlabeled classifier, if we obtain an initialization close enough to the true positive versus negative decision boundary, by monotonicity property of CVIR iterations, we may never get stuck in such a local minima even without modifications to loss.

E Empirical investigation of CVIR in toy setup

As noted in our ablation experiments and in Garg et al. [29], domain discriminator trained with CVIR outperforms classifiers trained with other consistent objectives (nnPU [38] and uPU [21]). While the analysis in Sec. 8 highlights consistency of CVIR procedure in population, it doesn't capture the



(a) Accuracy on validation positive versus negative data

(b) Fraction of correctly rejected examples with CVIR

Figure 3: **Comparison of different methods in overparameterized toy setup.** CVIR (random) denotes CVIR with random initialization and CVIR (PvU) denotes warm start with a positive versus negative classifier. Vertical line denotes the epoch at which we switch from PvU to CVIR in CVIR (PvU) training. (a) We observe that CVIR (PvU) improves significantly even over the best early stopped PvU model. As training proceeds, we observe that accuracy of nnPU, uPU and PvU training drops whereas CVIR (random) and CVIR (PvU) maintains superior and stable performance. (b) We observe that warm start training helps CVIR over randomly initialized model to correctly identity positives among unlabeled for rejection.

observed empirical efficacy of CVIR over alternative methods in overparameterized models. In the Gaussian setup described in Sec. D.2, we train overparameterized linear models to compare CVIR with other methods (Fig. 3). We fix $d = 1000$ and use $n = 250$ positive and $m = 250$ unlabeled points for training with $\alpha = 0.5$. We set the margin γ at 0.05. We compare CVIR with unbiased losses uPU and nnPU. We also make comparison with a naive positive versus unlabeled classifier (referred to as PvU). For CVIR, we experiment with a randomly initialized classifier and initialized with a PvU classifier trained for 200 epochs.

First, we observe that when a classifier is trained to distinguish positive and unlabeled data, *early learning* happens [47, 3, 28], i.e., during the initial phase of learning classifier learns to classify positives in unlabeled correctly as positives achieving high accuracy on validation positive versus negative data. While the early learning happens with all methods, soon in the later phases of training PvU starts overfitting to the unlabeled data as negative hurting its validation performance. For uPU and nnPU, while they improve over PvU training during the initial epochs, the loss soon becomes biased hurting the performance of classifiers trained with uPU and nnPU on validation data.

For CVIR trained from a randomly initialized classifier, we observe that it improves slightly over the best PvU or the best nnPU model. Moreover, it maintains a relatively stable performance throughout the training. CVIR initialized with a PvU classifier significantly improves the performance. In Fig. 3 (b), we show that CVIR initialized with a PvU correctly rejects significantly more fraction of positives from unlabeled than CVIR trained from scratch. Thus, post early learning rejection of large fraction of positives from unlabeled training in equation (4) crucially helps CVIR.

F Experimental Details

F.1 Baselines

We compare PULSE with several popular methods from OSDA literature. While these methods are not specifically proposed for OSLS, they are introduced for the more general OSDA problem. In particular, we make comparions with DANCE [59], UAN [73], CMU [25], STA [46], Backprop-ODA (or BODA) [58]. We use the open source implementation available at `https://github.com/thuml` and `https://github.com/VisionLearningGroup/DANCE/`. Since OSDA methods do not estimate the prevalence of novel class explicitly, we use the fraction of examples predicted in class $k + 1$ as a surrogate. We next briefly describe the main idea for each method:

Backprob-ODA Saito et al. [58] proposed backprob ODA to train a $(k + 1)$-way classifier. In particular, the network is trained to correctly classify source samples and for target samples, the classifier (specifically the last layer) is trained to output 0.5 for the probability of the unknown class.

The feature extractor is trained adversarially to move the probability of unknown class away from 0.5 on target examples by utilizing the gradient reversal layer.

Separate-To-Adapt (STA) Liu et al. [46] trained a network that learns jointly from source and target by learning to separate negative (novel) examples from target. The training is divided into two parts. The first part consists of training a multi-binary $G_c|_{c=1}^{|\mathcal{Y}_s|}$ classifier on labeled source data for each class and a binary classifier G_b which generates the weights w for rejecting target samples in the novel class. The second part consists of feature extractor G_f, a classifier G_y and domain discriminator G_d to perform adversarial domain adaptation between source and target data in the source label space. G_y and G_d are trained with incorporating weights w predicted by G_b in the first stage.

Calibrated Multiple Uncertainties (CMU) Fu et al. [25] trained a source classifier and a domain discriminator to discriminate the novel class from previously seen classes in target. To train the discriminator network, CMU uses a weighted binary cross entropy loss where $w(x)$ for each example x in target which is the average of uncertainty estimates, e.g. prediction confidence of source classifier. During test time, target data x with $w(x) \geqslant w_0$ (for some pre-defined threshold w_0) is classified as an example from previously seen classes and is given a class prediction with source classifier. Otherwise, the target example is classified as belonging to the novel class.

DANCE Saito et al. [59] proposed DANCE which combines a self-supervised clustering loss to cluster neighboring target examples and an entropy separation loss to consider alignment with source. Similar to CMU, during test time, DANCE uses thresholded prediction entropy of the source classifier to classifier a target example as belonging to the novel class.

Universal Adaptation Networks (UAN) You et al. [73] proposed UAN which also trains a source classifier and a domain discriminator to discriminate the novel class from previously seen classes in target. The objective is similar to CMU where instead of using uncertainty estimates from multiple classifiers, UAN uses prediction confidence of domain discriminator classifier. Similar to CMU, at test time, target data x with $w(x) \leqslant w_0$ (for some pre-defined threshold w_0) is classified as an example from previously seen classes and is given a class prediction with source classifier. Otherwise, the target example is classified as belonging to the novel class.

For alternative baselines, we experiment with source classifier directly deployed on the target data which may contain novel class and label shift among source classes (referred to as *source-only*). This naive comparison is included to quantify benefits of label shift correction and identifying novel class over a typical k-way classifiers.

We also train a domain discriminator classifier for source versus target (referred to as *domain disc.*). This is an adaptation of PU learning baseline[24] which assumes no label shift among source classes. We use simple domain discriminator training to distinguish source versus target. To estimate the fraction of novel examples, we use the EN estimator proposed in Elkan and Noto [24]. For any target input, we make a prediction with the domain discriminator classifier (after re-scaling the sigmoid output with the estimate proportion of novel examples). Any example that is classified as target, we assign it the class $k+1$. For examples classified as source, we make a prediction for them using the k-way source classifier.

Finally, per the reduction presented in Sec. 5, we train k PU classifiers (referred to as *k-PU*). To train each PU learning classifier, we can plugin any method discussed in Sec. A. In the main paper, we included results obtained with plugin state-of-the-art PU learning algorithms. In App. F.8, we present ablations with other PU learning methods.

F.2 Dataset and OSLS Setup Details

We conduct experiments with seven benchmark classification datasets across vision, natural language, biology and medicine. Our datasets span language, image and table modalities. For each dataset, we simulate an OSLS problem. We experiment with different fraction of novel class prevalence, source label distribution, and target label distribution. We randomly choose classes that constitute the novel target class. After randomly choosing source and novel classes, we first split the training data from each source class randomly into two partitions. This creates a random label distribution for shared classes among source and target. We then club novel classes to assign them a new class (i.e. $k+1$). Finally, we throw away labels for the target data to obtain an unsupervised DA problem. We repeat the same process on iid hold out data to obtain validation data with no target labels. For main

experiments in the paper, we next describe important details for the OSLS setup simulated. All the other details can be found in the code repository.

For vision, we use CIFAR10, CIFAR100 [40] and Entity30 [61]. For language, we experiment with Newsgroups-20 dataset. Additionally, inspired by applications of OSLS in biology and medicine, we experiment with Tabula Muris [17] (Gene Ontology prediction), Dermnet (skin disease prediction), and BreakHis [66] (tumor cell classification).

CIFAR10 For CIFAR10, we randomly select 9 classes as the source classes and a novel class formed by the remaining class. After randomly sampling the label marginal for source and target randomly, we get the prevalence for novel class as 0.2152.

CIFAR100 For CIFAR100, we randomly select 85 classes as the source classes and a novel class formed by aggregating the data from 15 remaining classes. After randomly sampling the label marginal for source and target randomly, we get the prevalence for novel class as 0.2976.

Entity30 Entity30 is a subset of ImageNet [54] with 30 super classes. For Entity30, we randomly select 24 classes as the source classes and a novel class formed by aggregating the data from 6 remaining classes. After randomly sampling the label marginal for source and target randomly, we get the prevalence for novel class as 0.3942.

Newgroups-20 For Newsgroups20[2], we randomly select 16 classes as the source classes and a novel class formed by aggregating the data from 4 remaining classes. After randomly sampling the label marginal for source and target randomly, we get the prevalence for novel class as 0.3733. This dataset is motivated by scenarios where novel news categories can appear over time but the distribution of articles given a news category might stay relatively unchanged.

BreakHis BreakHis[3] contains 8 categories of cell types, 4 types of benign breast tumor and 4 types malignant tumors (breast cancer). Here, we simulate OSLS problem specifically where 6 cell types are observed in the source (3 from each) and a novel class appears in the target with 1 cell type from each category. After randomly sampling the label marginal for source and target randomly, we get the prevalence for novel class as 0.2708.

Dermnet Dermnet data contains images of 23 types of skin diseases taken from Dermnet NZ[4]. We simulate OSLS problem specifically where 18 diseases are observed in the source and a novel class appears in the target with the rest of the 5 diseases. After randomly sampling the label marginal for source and target randomly, we get the prevalence for novel class as 0.3133.

Tabula Muris Tabula Muris dataset [17] comprises of different cell types collected across 23 organs of the mouse model organism. We use the data pre-processing scripts provided in [12][5]. We just use the training set comprising of 57 classes for our experiments. We simulate OSLS problem specifically where 28 cell types are observed in the source and a novel class appears in the target with the rest of the 29 cell types. After randomly sampling the label marginal for source and target randomly, we get the prevalence for novel class as 0.6366.

F.3 Details on the Experimental Setup

We use Resnet18 [33] for CIFAR10, CIFAR100, and Entity30. For all three datasets, in our main experiments, we train Resnet-18 from scratch. We use SGD training with momentum of 0.9 for 200 epochs. We start with learning rate 0.1 and decay it by multiplying it with 0.1 every 70 epochs. We use a weight decay of 5×10^{-4}. For CIFAR100 and CIFAR10, we use batch size of 200. For Entity30, we use a batch size of 32. In App. F.7, we experiment with contrastive pre-training instead of random initialization.

For newsgroups, we use a convolutional architecture[6]. We use glove embeddings to initialize the embedding layer. We use Adam optimizer with a learning rate of 0.0001 and no weight decay. We use a batch size of 200. We train with constant learning rate for 120 epochs.

[2] `http://qwone.com/~jason/20Newsgroups/`

[3] `https://web.inf.ufpr.br/vri/databases/breast-cancer-histopathological-database-breakhis/`

[4] `http://www.dermnet.com/dermatology-pictures-skin-disease-pictures`

[5] `https://github.com/snap-stanford/comet`

[6] `https://github.com/mireshghallah/20Newsgroups-Pytorch`

For Tabular Muris, we use the fully connected MLP used in Cao et al. [12]. We use the hyperparameters used in Cao et al. [12]. We use Adam optimizer with a learning rate of 0.0001 and no weight decay. We train with constant learning rate for 40 epochs. We use a batch size of 200.

For Dermnet and BreakHis, we use Resnet-50 pre-trained on Imagenet. We use an initial learning rate of 0.0001 and decay it by 0.96 every epoch. We use SGD training with momentum of 0.9 and weight decay of 5×10^{-4}. We use a batch size of 32. These are the default hyperparameters used in Alom et al. [2] and Liao [44].

For all methods, we use the same backbone for discriminator and source classifier. Additionally, for PULSE and domain disc., we use the exact same set of hyperparameters to train the domain discriminator and source classifier. For kPU, we use a separate final layer for each class with the same backbone. We use the same hyperparameters described above for all three methods. For OSDA methods, we use default method specific hyperparameters introduced in their works. Since we do not have access to labels from the target data, we do not perform hyperparameter tuning but instead use the standard hyperparameters used for training on labeled source data. In future, we may hope to leverage heuristics proposed for accuracy estimation without access to labeled target data [30].

We train models till the performance on validation source data (labeled) ceases to increase. Unlike OSDA methods, note that we do not use early stopping based on performance on held-out labeled target data. To evaluate classification performance, we report target accuracy on all classes, seen classes and the novel class. For target marginal, we separately report estimation error for previously seen classes and for the novel class. For the novel class, we report absolute difference between true and estimated marginal. For seen classes, we report average absolute estimation error. We open-source our code at `https://github.com/Neurips2022Anon`. By simply changing a single config file, new OSLS setups can be generated and experimented with.

Note that for our main experiments, for vision datasets (i.e., CIFAR10, CIFAR100, and Entity30) and for language dataset, we do not initialize with a (supervised) pre-trained model to avoid overlap of novel classes with the classes in the dataset used for pre-training. For example, labeled Imagenet-1k is typically used for pre-training. However, Imagenet classes overlaps with all three vision datasets employed and hence, we avoid pre-trained initialization. In App. F.7, we experiment with contrastive pre-training on Entity30 and CIFAR100. In contrast, for medical datasets, we leverage Imagenet pre-trained models as there is no overlap between classes in BreakHis and Dermnet with Imagenet.

F.4 Detailed results from main paper

For completeness, we next include results for all datasets. In particular, for each dataset we tabulate (i) overall accuracy on target; (ii) accuracy on seen classes in target; (iii) accuracy on the novel class; (iv) sum of absolute error in estimating target marginal among previously seen classes, i.e., $\sum_{y \in \mathcal{Y}_s} |\widehat{p}_t(y) - p_t(y)|$; and (v) absolute error for novel fraction estimation, i.e., $|\widehat{p}_t(y = k+1| - p_t(y = k+1)$. Table 5 presents results on all the datasets. Fig. 4 and Fig. 5 presents epoch-wise results.

F.5 Investigation into OSDA approaches

We observe that with default hyperparameters, popular OSDA methods significantly under perform as compared to PULSE. We hypothesize that the primary reasons underlying the poor performance of OSDA methods are (i) the heuristics employed to detect novel classes; and (ii) loss functions incorporated to improve alignment between examples from common classes in source and target. To detect novel classes, a standard heuristic employed popular OSDA methods involves thresholding uncertainty estimates (e.g., prediction entropy, softmax confidence [73, 25, 59]) at a predefined threshold κ. However, a fixed κ, may not for different datasets and different fractions of the novel class. Here, we ablate by (i) removing loss function terms incorporated with an aim to improve source target alignment; and (ii) vary threshold κ and show improvements in performance of these methods.

For our investigations, we experiment with CIFAR10, with UAN and DANCE methods. For DANCE, we remove the entropy separation loss employed to encourage align target examples with source examples. For UAN, we remove the adversarial domain discriminator training employed to align target examples with source examples. For both the methods, we observe that by removing the corresponding loss function terms we obtain a marginal improvement. For DANCE on CIFAR10, the

performance goes up from 70.4 to 72.5 (with the same hyperparameters as the default run). FOR UAN, we observe similar minor improvements, where the performance goes up from 15.4 to 19.6.

Next, we vary the threshold used for detecting the novel examples. By optimally tuning the threshold for CIFAR10 with UAN, we obtain a substantial increase. In particular, the overall target accuracy increases from 19.6 to 33.1. With DANCE on CIFAR10, optimal threshold achieves 75.6 as compared to the default accuracy 70.4. In contrast, our two-stage method PULSE avoids the need to guess κ, by first estimating the fraction of novel class which then guides the classification of novel class versus previously seen classes.

F.6 Ablation with novel class fraction

In this section, we ablate on novel class proportion on CIFAR10, CIFAR100 and Newsgroups20. For each dataset we experiment with three settings, each obtained by varying the number of classes from the original data that constitutes the novel classes. We tabulate our results in Table 4.

F.7 Contrastive pre-training on unlabeled data

Here, we experiment with contrastive pre-training to pre-train the backbone networks used for feature extraction. In particular, we initialize the backbone architectures with SimCLR pre-trained weights. We experiment with CIFAR100 and Entity30 datasets. Instead of pre-training on mixture of source and target unlabeled data, we leverage the publicly available pre-trained weights[7]. Table 2 summarizes our results. We observe that pre-training improves over random initialization for all the methods with PULSE continuing to outperform other approaches.

Table 2: Comparison with different OSLS approaches with pre-trained feature extractor. We use SimCLR pre-training to initialize the feature extractor for all the methods. All methods improve over random initialization (in Table 1). Note that PULSE continues to outperform other approaches.

Method	CIFAR100		Entity30	
	Acc (All)	MPE (Novel)	Acc (All)	MPE (Novel)
BODA [58]	37.1	0.34	52.1	0.376
Domain Disc.	49.4	0.041	57.4	0.024
kPU	37.5	0.297	70.1	0.32
PULSE (Ours)	67.3	0.052	72.4	0.002

F.8 Ablation with different PU learning methods

In this section, we experiment with alternative PU learning approaches for PULSE and kPU. In particular, we experiment with the next best alternatives, i.e., nnPU instead of CVIR for classification and DEDPUL instead of BBE for target marginal estimation. We refer to these as kPU (alternative) and PULSE (alternative) in Table 3. We present results on three datasets: CIFAR10, CIFAR100 and Newsgroups20 in the same setting as described in Sec. F.2. We make two key observations: (i) PULSE continues to dominate kPU with alternative choices; (ii) CVIR and BBE significantly outperform alternative choices.

F.9 Age Prediction Task

We consider an experiment on UTK Face dataset[8]. We create an 8-way class classification problem where we split the age in the following 8 groups: 0–10, 11–20, $\cdots$, 60–70 and > 70. We consider the first 7 age groups in source and introduce age group > 70 into the target data. OSLS continues to

[7]For CIFAR100: `https://drive.google.com/file/d/1huW-ChBVvKcx7t8HyDaWTQB5Li1Fht9x/view` and for Entity30, we use Imagenet pre-trained weights from here: `https://github.com/AndrewAtanov/simclr-pytorch`.

[8]`https://susanqq.github.io/UTKFace/`

Table 3: Comparison with different PU learning approaches. 'Alternative' denotes results with employing nnPU for classification and DEDPUL for target marginal estimation instead of 'default' which uses CVIR and BBE.

Method	**CIFAR10**		**CIFAR100**		**Newsgroups20**	
	Acc (All)	MPE (Novel)	Acc (All)	MPE (Novel)	Acc (All)	MPE (Novel)
k-PU (alternative)	53.4	0.215	12.1	0.298	14.1	0.373
k-PU (default)	83.6	0.036	36.3	0.298	52.1	0.307
PULSE (alternative)	80.5	0.05	30.1	0.231	39.8	0.223
PULSE (default)	86.1	0.008	63.4	0.078	62.2	0.061

Table 4: Comparison with different OSLS approaches for different novel class prevalence. We observe that for on CIFAR100 and Newsgroups20, PULSE maintains superior performance as compared to other approaches. On CIFAR10, as the proportion of novel class increases, the performance of of kPU improves slightly over PULSE for target accuracy.

	CIFAR10 ($p_t(k+1) = 0.215$)		**CIFAR10** ($p_t(k+1) = 0.406$)		**CIFAR10** ($p_t(k+1) = 0.583$)	
Method	Acc (All)	MPE (Novel)	Acc (All)	MPE (Novel)	Acc (All)	MPE (Novel)
BODA [58]	63.1	0.162	65.5	0.166	48.6	0.265
Domain Disc.	47.4	0.331	57.5	0.232	68.7	0.144
kPU	83.6	0.036	87.8	0.010	89.9	0.036
PULSE (Ours)	86.1	0.008	87.4	0.009	83.7	0.006

	CIFAR100 ($p_t(k+1) = 0.2976$)		**CIFAR100** ($p_t(k+1) = 0.4477$)		**CIFAR100** ($p_t(k+1) = 0.5676$)	
Method	Acc (All)	MPE (Novel)	Acc (All)	MPE (Novel)	Acc (All)	MPE (Novel)
BODA [58]	36.1	0.41	41.6	0.075	50.2	0.03
Domain Disc.	45.8	0.046	52.3	0.092	58.7	0.187
kPU	36.3	0.298	52.2	0.448	63.9	0.568
PULSE (Ours)	63.4	0.078	66.6	0.052	68.2	0.088

	Newsgroups20 ($p_t(k+1) = 0.3733$)		**Newsgroups20** ($p_t(k+1) = 0.6452$)		**Newsgroups20** ($p_t(k+1) = 0.7688$)	
Method	Acc (All)	MPE (Novel)	Acc (All)	MPE (Novel)	Acc (All)	MPE (Novel)
BODA [58]	43.4	0.16	25.5	0.645	17.7	0.769
Domain Disc.	50.9	0.176	44.8	0.085	47.8	0.064
kPU	52.1	0.373	50.2	0.645	35.5	0.769
PULSE (Ours)	62.2	0.061	71.7	0.044	75.73	0.179

outperform the kPU baseline for novel prevalence estimation. Additionally, for target classification performance of OSLS is similar to kPU baseline (ref. Table 6).

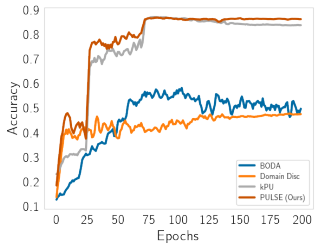
Table 5: *Comparison of PULSE with other methods*. Across all datasets, PULSE outperforms alternatives for both target classification and novel class prevalence estimation. Acc (All) is target accuracy, Acc (Seen) is target accuracy on examples from previously seen classes, and Acc (Novel) is recall for novel examples. MPE (Seen) is sum of absolute error for estimating target marginal among previously seen classes and MPE (Novel) is absolute error for novel prevalence estimation. Results reported by averaging across 3 seeds.

Method	CIFAR-10					CIFAR-100				
	Acc (All)	Acc (Seen)	Acc (Novel)	MPE (Seen)	MPE (Novel)	Acc (All)	Acc (Seen)	Acc (Novel)	MPE (Seen)	MPE (Novel)
Source-Only	67.1	87.0	-	-	-	46.6	66.4	-	-	-
UAN [73]	15.4	19.7	25.2	1.44	0.214	18.1	40.6	14.8	1.48	0.133
BODA [58]	63.1	66.2	42.0	0.541	0.162	36.1	17.7	81.6	0.564	0.41
DANCE [59]	70.4	85.5	14.5	0.784	0.174	47.3	66.4	1.2	0.702	0.28
STA [46]	57.9	69.6	14.9	0.409	0.124	42.6	48.5	34.8	0.798	0.14
CMU [25]	62.1	77.9	41.2	0.443	0.183	35.4	46.0	15.5	0.695	0.161
Domain Disc.	47.4	87.0	30.6	-	0.331	45.8	66.5	39.1	-	**0.046**
k-PU	83.6	79.4	**98.9**	**0.062**	0.036	36.3	22.6	**99.1**	6.31	0.298
PULSE (Ours)	**86.1**	**91.8**	88.4	0.091	**0.008**	**63.4**	**67.2**	63.5	**0.365**	0.078

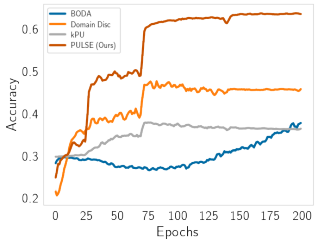
Method	Entity30					Newsgroup20				
	Acc (All)	Acc (Seen)	Acc (Novel)	MPE (Seen)	MPE (Novel)	Acc (All)	Acc (Seen)	Acc (Novel)	MPE (Seen)	MPE (Novel)
Source-Only	32.0	53.5	-	-	-	39.3	64.4	-	-	-
BODA [58]	42.22	25.9	67.2	0.367	0.189	43.4	38.0	34.1	0.550	0.167
Domain Disc.	43.2	53.5	68.0	-	0.135	50.9	64.4	**93.2**	-	0.176
k-PU	50.7	22.3	**94.4**	0.99	0.394	52.1	57.8	42.7	0.776	0.373
PULSE (Ours)	**58.0**	**54.3**	72.2	**0.215**	**0.054**	**62.2**	**65.0**	83.6	**0.232**	**0.061**

Method	Tabula Muris					BreakHis				
	Acc (All)	Acc (Seen)	Acc (Novel)	MPE (Seen)	MPE (Novel)	Acc (All)	Acc (Seen)	Acc (Novel)	MPE (Seen)	MPE (Novel)
Source-Only	33.8	93.3	-	-	-	70.0	95.8	-	-	-
BODA [58]	76.5	59.8	87.0	0.200	0.079	71.5	81.8	44.0	0.163	0.077
Domain Disc.	73.0	93.3	**94.7**	-	0.071	56.5	95.8	**90.4**	-	0.09
k-PU	85.9	91.6	83.3	**0.279**	0.307	75.6	71.7	86.1	0.094	0.058
PULSE (Ours)	**87.8**	**94.6**	88.8	0.388	**0.058**	**79.1**	**96.1**	76.3	**0.090**	**0.054**

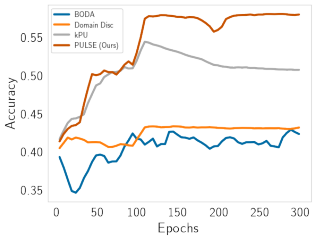
Method	Dermnet				
	Acc (All)	Acc (Seen)	Acc (Novel)	MPE (Seen)	MPE (Novel)
Source-Only	41.4	53.6	-	-	-
BODA [58]	43.8	31.4	58.4	**0.401**	0.207
Domain Disc.	40.6	53.6	82.7	-	0.083
k-PU	46.0	26.0	**89.9**	1.44	0.313
PULSE (Ours)	**48.9**	**53.7**	57.7	**0.41**	**0.043**



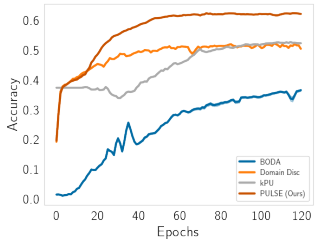
(a) CIFAR10



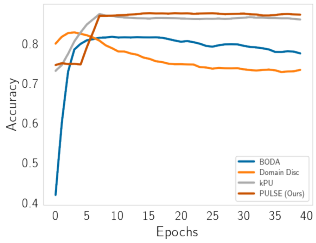
(b) CIFAR100



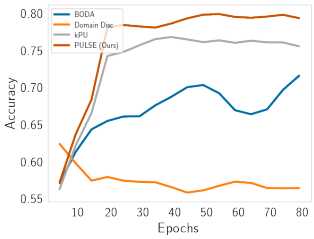
(c) Entity30



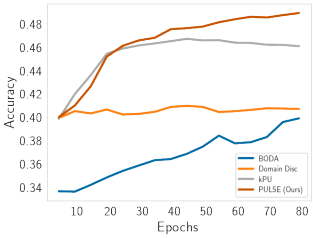
(d) Newsgroups20



(e) Tabula Muris



(f) BreakHis

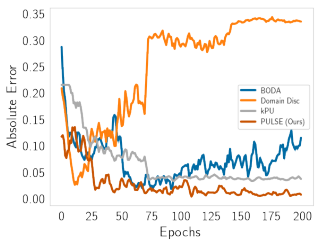


(g) Dermnet

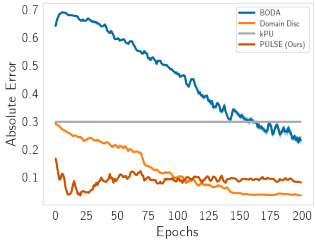
Figure 4: **Epoch wise results for target accuracy.** Results aggregated over 3 seeds. PULSE maintains stable and superior performance when compared to alternative methods.

Table 6: Results on age prediction dataset. We observe that the prevalence of the novel class as estimated with our PULSE framework is significantly closer to the true estimate. Additionally target classification performance of OSLS is similar to that of kPU both of which significantly improve over domain discriminator and source only baselines.

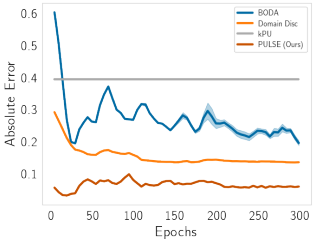
Method	**UTK Face**	
	Acc (All)	MPE (Novel)
Source Only	50.1	0.11
Domain Disc.	52.4	0.08
kPU	56.7	0.11
PULSE (Ours)	56.8	0.01



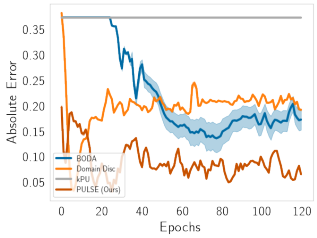
(a) CIFAR10



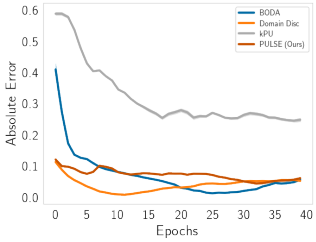
(b) CIFAR100



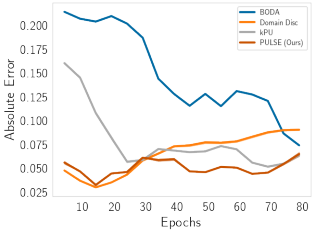
(c) Entity30



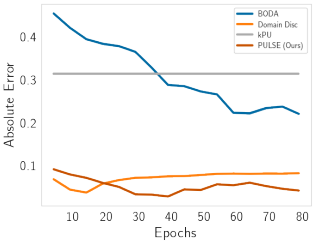
(d) Newsgroups20



(e) Tabula Muris



(f) BreakHis



(g) Dermnet

Figure 5: **Epoch wise results for novel prevalence estimation.** Results aggregated over 3 seeds. PULSE maintains stable and superior performance when compared to alternative methods.