Learning from Positive and Unlabeled Data with Arbitrary Positive Shift

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Abstract

Positive-unlabeled (PU) *learning* trains a binary classifier using only positive and unlabeled data. A common simplifying assumption is that the positive data is representative of the target positive class. This assumption rarely holds in practice due to temporal drift, domain shift, and/or adversarial manipulation. This paper shows that PU learning is possible even with arbitrarily non-representative positive data given unlabeled data from the source and target distributions. Our key insight is that only the negative class's distribution need be fixed. We integrate this into two statistically consistent methods to address arbitrary positive bias – one approach combines *negative-unlabeled learning* with *unlabeled-unlabeled learning* while the other uses a novel, recursive risk estimator. Experimental results demonstrate our methods' effectiveness across numerous real-world datasets and forms of positive bias, including disjoint positive class-conditional supports. Additionally, we propose a general, simplified approach to address PU risk estimation overfitting.

1 Introduction

Positive-negative (PN) *learning* (i.e., ordinary supervised classification) trains a binary classifier using positive and negative labeled datasets. In practice, good labeled data are often unavailable for one class. High negative-class diversity may make constructing a representative labeled set prohibitively difficult [1], or negative data may not be systematically recorded in some domains [2].

Positive-unlabeled (PU) *learning* addresses this problem by constructing classifiers using only labeled-positive and unlabeled data. PU learning has been applied to numerous real-world domains including: opinion spam detection [3], disease-gene identification [4], land-cover classification [5], and protein similarity prediction [6]. The related task of *negative-unlabeled* (NU) learning is functionally identical to PU learning but with labeled data drawn from the negative class.

Most PU learning methods assume the labeled set is *selected completely at random* (SCAR) from the target distribution [1, 6, 7, 8, 9, 10, 11]. External factors like temporal drift, domain shift, and adversarial concept drift often cause the labeled-positive and target distributions to diverge.

Biased-positive, unlabeled (bPU) *learning* algorithms relax SCAR by modeling *sample selection bias* for the labeled data [12, 13] or a *covariate shift* between the training and target distributions [14].

This paper generalizes bPU learning to the more challenging *arbitrary-positive, unlabeled* (aPU) learning setting, where the labeled (positive) data may be *arbitrarily different* from the target distribution's positive class. Solving this problem would eliminate the need to spend time and money labeling new data whenever the positive class drifts.

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Devoid of some assumption, aPU learning is impossible [6]. As a first step to address aPU learning, our key insight is that given a labeled-positive set and two unlabeled sets as proposed by Sakai and Shimizu [14], aPU learning is possible when *all negative examples are generated from a single distribution*. The labeled and target-positive distributions' *supports* (sets of examples with non-zero probability) may even be disjoint. Many real-world PU learning tasks feature a shifting positive class but (largely) fixed negative class including:

1. **Land-Cover Classification**: Cross-border land-cover datasets often do not exist due to differing national technological standards or insufficient financial resources by one country [15]. This limits research into natural processes at broad geographic scales. However, cross-border geographic terrains often follow a similar distribution differing primarily in man-made objects (e.g., roads) due to local construction materials and regulations [5].
2. **Adversarial aPU Learning**: Malicious adversaries (email spammers, malware authors) rapidly adapt their attacks to bypass automated detection. The benign class changes much more slowly but may be too diverse to construct a representative labeled set [3, 16, 17, 18].

Our paper's four primary contributions are enumerated below. Note that most experiments and all proofs are in the supplemental materials.

1. We propose abs-PU – a simplified, statistically *consistent* approach to correct general PU risk estimation overfitting. Our aPU methods leverage abs-PU to streamline their optimization.
2. We address our aPU learning task via a two-step formulation; the first step applies standard PU learning and the second uses unlabeled-unlabeled (UU) learning.
3. We separately propose PURR – a novel, recursive, consistent aPU risk estimator.
4. We evaluate our methods on a wide range of benchmarks, demonstrating our algorithms' effectiveness over the state of the art in PU and bPU learning. Our empirical evaluation includes an adversarial aPU learning case study using public spam email datasets.

2 Ordinary Positive-Unlabeled Learning

We begin with an overview of PU learning without distributional shifts, including definitions and notation. Consider two random variables, covariate $X \in \mathbb{R}^d$ and label $Y \in \{\pm 1\}$, with joint distribution $p(x, y)$. Marginal distribution $p_{\mathrm{u}}(x)$ is composed from the positive prior $\pi \coloneqq p(Y{=}{+}1)$, positive class-conditional $p_{\mathrm{p}}(x) \coloneqq p(x|Y{=}{+}1)$, and negative class-conditional $p_{\mathrm{n}}(x) \coloneqq p(x|Y{=}{-}1)$.

Risk Let $g : \mathbb{R}^d \to \mathbb{R}$ be an arbitrary *decision function* parameterized by θ, and let $\ell : \mathbb{R} \to \mathbb{R}_{\geq 0}$ be the *loss function*. Risk $R(g) \coloneqq \mathbb{E}_{(X,Y)\sim p(x,y)}[\ell(Yg(X))]$ quantifies g's expected loss over $p(x, y)$. It decomposes via the product rule to $R(g) = \pi R_{\mathrm{p}}^{+}(g) + (1-\pi)R_{\mathrm{n}}^{-}(g)$, where the *labeled risk* is

$$R_{\mathcal{D}}^{\hat{y}}(g) \coloneqq \mathbb{E}_{X\sim p_{\mathcal{D}}(x)}[\ell(\hat{y}g(X))] \tag{1}$$

for predicted label $\hat{y} \in \{\pm 1\}$ and $\mathcal{D} \in \{\mathrm{p}, \mathrm{n}, \mathrm{u}\}$ denoting the positive class-conditional, negative class-conditional or marginal distribution respectively, as defined above.

Since $p(x, y)$ is unknown, *empirical risk* is used in practice. We consider the *case-control scenario* [19] where each dataset is i.i.d. sampled from its associated distribution. PN learning has two labeled datasets: positive set $\mathcal{X}_{\mathrm{p}} \coloneqq \{x_i^{\mathrm{p}}\}_{i=1}^{n_{\mathrm{p}}} \overset{\text{i.i.d.}}{\sim} p_{\mathrm{p}}(x)$ and negative set $\mathcal{X}_{\mathrm{n}} \coloneqq \{x_i^{\mathrm{n}}\}_{i=1}^{n_{\mathrm{n}}} \overset{\text{i.i.d.}}{\sim} p_{\mathrm{n}}(x)$. These are used to calculate empirical labeled risks $\widehat{R}_{\mathrm{p}}^{+}(g) = \frac{1}{n_{\mathrm{p}}}\sum_{i=1}^{n_{\mathrm{p}}} \ell(g(x_i^{\mathrm{p}}))$ and $\widehat{R}_{\mathrm{n}}^{-}(g) = \frac{1}{n_{\mathrm{n}}}\sum_{i=1}^{n_{\mathrm{n}}} \ell(-g(x_i^{\mathrm{n}}))$. We denote the empirical positive-negative risk

$$\widehat{R}_{\mathrm{PN}}(g) \coloneqq \pi\widehat{R}_{\mathrm{p}}^{+}(g) + (1-\pi)\widehat{R}_{\mathrm{n}}^{-}(g). \tag{2}$$

PU learning cannot directly estimate $R_{\mathrm{n}}^{\hat{y}}(g)$ since there is no negative (labeled) data (i.e., $\mathcal{X}_{\mathrm{n}} = \emptyset$). Let $\mathcal{X}_{\mathrm{u}} \coloneqq \{x_i^{\mathrm{u}}\}_{i=1}^{n_{\mathrm{u}}} \overset{\text{i.i.d.}}{\sim} p_{\mathrm{u}}(x)$ be an unlabeled set with empirical labeled risk $\widehat{R}_{\mathrm{u}}^{\hat{y}}(g) = \frac{1}{n_{\mathrm{u}}}\sum_{i=1}^{n_{\mathrm{u}}} \ell(\hat{y}g(x_i^{\mathrm{u}}))$. du Plessis et al. [20] make a foundational contribution that,

$$(1-\pi)R_{\mathrm{n}}^{\hat{y}}(g) = R_{\mathrm{u}}^{\hat{y}}(g) - \pi R_{\mathrm{p}}^{\hat{y}}(g). \tag{3}$$

Their unbiased PU (uPU) risk estimator is therefore $\widehat{R}_{\mathrm{uPU}}(g) \coloneqq \pi\widehat{R}_{\mathrm{p}}^{+}(g) + \widehat{R}_{\mathrm{u}}^{-}(g) - \pi\widehat{R}_{\mathrm{p}}^{-}(g)$. Kiryo et al. [8] observe that highly expressive models (e.g., neural networks) often overfit $\mathcal{X}_{\mathrm{p}}$ causing uPU to estimate that $\widehat{R}_{\mathrm{u}}^{-}(g) - \pi\widehat{R}_{\mathrm{p}}^{-}(g) < 0$.

Since negative-valued risk is impossible, Kiryo et al.'s non-negative PU (nnPU) risk estimator ignores negative estimates of risk via a $\max$ term:

$$\widehat{R}_{\text{nnPU}}(g) \coloneqq \pi \widehat{R}_{\text{p}}^{+}(g) + \max\{0, \widehat{R}_{\text{u}}^{-}(g) - \pi \widehat{R}_{\text{p}}^{-}(g)\}. \tag{4}$$

When Kiryo et al.'s customized empirical risk minimization (ERM) framework detects overfitting (i.e., $\widehat{R}_{\text{u}}^{-}(g) - \pi \widehat{R}_{\text{p}}^{-}(g) < 0$), their framework "defits" g using negated gradient $-\gamma \nabla_\theta (\widehat{R}_{\text{u}}^{-}(g) - \pi \widehat{R}_{\text{p}}^{-}(g))$, where hyperparameter $\gamma \in (0, 1]$ attenuates the learning rate to throttle "defitting." Observe that positive-labeled risk, $\widehat{R}_{\text{p}}^{+}(g)$, is excluded from nnPU's negated gradient.

3 Simplifying Non-Negativity Correction

Rather than enforcing the non-negative risk constraint with two combined techniques (a $\max$ term and "defitting") like Kiryo et al., we propose a simpler approach, inspired by Lagrange multipliers, that directly puts the non-negativity constraint into the risk estimator. Our *absolute-value correction*,

$$(1 - \pi) \ddot{R}_{\text{n}}^{\hat{y}}(g) \coloneqq \left| \widehat{R}_{\text{u}}^{\hat{y}}(g) - \pi \widehat{R}_{\text{p}}^{\hat{y}}(g) \right|, \tag{5}$$

replaces nnPU's $\max$ with absolute value to prevent the optimizer overfitting an implausible risk estimate by explicitly penalizing those risk estimates for being negative. This penalty "defits" the learner automatically, eliminating the need for hyperparameter γ and nnPU's custom ERM algorithm.

Theorem 1. *Let $g : \mathbb{R}^d \to \mathbb{R}$ be an arbitrary decision function and let $\ell : \mathbb{R} \to \mathbb{R}_{\geq 0}$ be a loss function bounded*[1] *w.r.t. g then $\ddot{R}_{\text{n}}^{\hat{y}}(g)$ is a consistent estimator of $\widehat{R}_{\text{n}}^{\hat{y}}(g)$.*

We integrate absolute value correction into our *abs-PU risk estimator*,

$$\widehat{R}_{\text{abs-PU}}(g) \coloneqq \pi \widehat{R}_{\text{p}}^{+}(g) + \left| \widehat{R}_{\text{u}}^{-}(g) - \pi \widehat{R}_{\text{p}}^{-}(g) \right|, \tag{6}$$

which by Theorem 1 is consistent like nnPU. When $\widehat{R}_{\text{u}}^{-}(g) - \pi \widehat{R}_{\text{p}}^{-}(g) < 0$, abs-PU's update gradient, $\nabla_\theta (\pi \widehat{R}_{\text{p}}^{+}(g) - \widehat{R}_{\text{u}}^{-}(g) + \pi \widehat{R}_{\text{p}}^{-}(g))$, includes $\widehat{R}_{\text{p}}^{+}(g)$. Hence, abs-PU spends comparatively more time optimizing the positive-labeled risk than nnPU. Also, by penalizing implausible risk, abs-PU estimates validation performance (i.e., risk) differently than nnPU.

Empirically we observed that abs-PU yields models of similar or slightly better accuracy than nnPU albeit with a simpler, more efficient optimization. The following builds on abs-PU with a full comparison to nnPU in supplemental Section E.6.

4 Arbitrary-Positive, Unlabeled Learning

Arbitrary-positive unlabeled (aPU) learning — the focus of this work — is one of three problem settings proposed by Sakai and Shimizu [14]. We generalize their original definition below.

Consider two joint distributions: train $p_{\text{tr}}(x, y)$ and test $p_{\text{te}}(x, y)$. Notation $p_{\text{tr-}\mathcal{D}}(x)$ where $\mathcal{D} \in \{\text{p}, \text{n}, \text{u}\}$ refers to the training positive class-conditional, negative class-conditional, and marginal distributions respectively. $p_{\text{te-}\mathcal{D}}(x)$ denotes the corresponding test distributions.

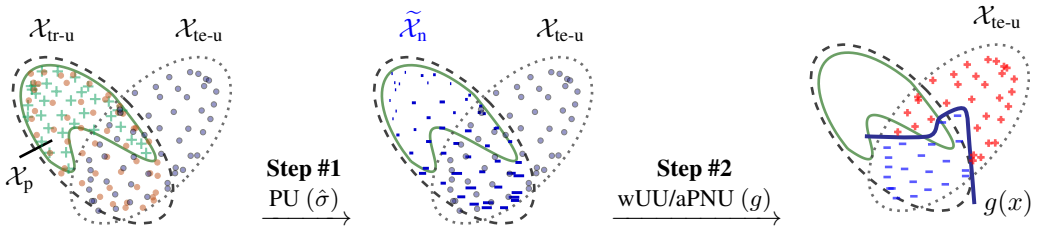
No assumption is made about the label's conditional probability, i.e., $p_{\text{tr}}(y|x)$ and $p_{\text{te}}(y|x)$, nor about positive class-conditionals $p_{\text{tr-p}}(x)$ and $p_{\text{te-p}}(x)$. We only assume a fixed negative class-conditional

$$p_{\text{n}}(x) = p_{\text{tr-n}}(x) = p_{\text{te-n}}(x). \tag{7}$$

Both the train and test positive-class priors, π_{tr} and π_{te} respectively, are treated as known throughout this work. In practice, they may be known *a priori* through domain-specific knowledge. Techniques also exist to estimate them from data [2, 21, 22, 23]. Theorem 4 in the supplemental materials provides an algorithm to estimate π_{te} by training an additional classifier.

As shown in Figure 1a, the available datasets are: labeled (positive) set $\mathcal{X}_{\text{p}} \overset{\text{i.i.d.}}{\sim} p_{\text{tr-p}}(x)$ as well as unlabeled sets $\mathcal{X}_{\text{tr-u}} \coloneqq \{x_i\}_{i=1}^{n_{\text{tr-u}}} \overset{\text{i.i.d.}}{\sim} p_{\text{tr-u}}(x)$ and $\mathcal{X}_{\text{te-u}} \coloneqq \{x_i\}_{i=1}^{n_{\text{te-u}}} \overset{\text{i.i.d.}}{\sim} p_{\text{te-u}}(x)$ with their empirical risks defined as before. An optimal classifier minimizes the *test* risk/expected loss: $\mathbb{E}_{(X,Y)\sim p_{\text{te}}(x,y)}[\ell(Yg(X))]$.

[1] Each theorem's definition of "bounded" loss appears in the associated proof. See the supplemental materials.



(a) Example aPU dataset

(b) Weighting $\mathcal{X}_{\text{tr-u}}$ using $\hat{\sigma}(x)$ yields $\widetilde{\mathcal{X}}_{\text{n}}$

(c) Final classifier g

Figure 1: Two-step aPU learning. Fig. 1a shows a toy aPU dataset with (+) representing a labeled positive example, (•) an unlabeled train sample, and (•) an unlabeled test sample. Borders surround each set for clarity. After learning probabilistic classifier $\hat{\sigma}$ in Step #1, Fig. 1b visualizes $\hat{\sigma}$'s predicted negative-posterior probability using marker (–) size. Fig. 1c shows the final decision boundary with (-) and (•) representing $\mathcal{X}_{\text{te-u}}$ examples classified negative and positive respectively.

4.1 Relating aPU Learning and Covariate Shift Adaptation Methods

Covariate shift [24] is a common technique to address differences between $p_{\text{tr}}(x, y)$ and $p_{\text{te}}(x, y)$. Unlike aPU learning, covariate shift restrictively assumes a *consistent input-output relation*, i.e., $p_{\text{tr}}(y|x) = p_{\text{te}}(y|x)$. Define the *importance function* as $w(x) := \frac{p_{\text{te-u}}(x)}{p_{\text{tr-u}}(x)}$. When $p(y|x)$ is fixed, it is easy to show that $w(x)p_{\text{tr}}(x, y) = p_{\text{te}}(x, y)$.

Sakai and Shimizu [14] exploit this relationship in their PUc risk estimator. $w(x)$ is approximated via direct density-ratio estimation [25] – specifically the RuLSIF algorithm [26] over $\mathcal{X}_{\text{tr-u}}$ and $\mathcal{X}_{\text{te-u}}$. Their PUc risk adds importance weighting to uPU, with the labeled risks still estimated from $\mathcal{X}_{\text{p}}$ and $\mathcal{X}_{\text{tr-u}}$. Sakai and Shimizu's formulation specifies linear-in-parameter models to enforce convexity. They improve tractability via a simplified version of du Plessis et al. [1]'s surrogate squared loss for ℓ.

Selection bias bPU methods [12, 13] need the positive-labeled data to meet specific conditions that arbitrary-positive data will not satisfy making a comparison to those methods infeasible. PUc serves as the primary baseline here since as a covariate shift bPU method, it places no requirements on the positive data beyond that the training distribution's support be a superset of the target positive class.

4.2 Comparing Variations of the aPU Learning Problem

Sakai and Shimizu [14] show that PU learning with a fixed positive class and arbitrary negative shift is much simpler than aPU learning. In fact, provided a positive-labeled set and two unlabeled sets as above, they show that arbitrary negative shift is trivially equivalent to ordinary PU learning over $\mathcal{X}_{\text{p}}$ and $\mathcal{X}_{\text{te-u}}$ (since $\mathcal{X}_{\text{p}}$ being drawn from $p_{\text{te-p}}(x)$ renders $\mathcal{X}_{\text{tr-u}}$ unnecessary). When both the positive and negative classes shift arbitrarily, learning is impossible without additional data and/or assumptions. aPU learning's complexity sits between these two extremes.

5 aPU Learning via Unlabeled-Unlabeled Learning

To build an intuition for solving the aPU learning problem, consider the ideal case where a perfect classifier correctly labels $\mathcal{X}_{\text{tr-u}}$. Let $\mathcal{X}_{\text{tr-n}}$ be $\mathcal{X}_{\text{tr-u}}$'s negative examples. $\mathcal{X}_{\text{tr-n}}$ is SCAR w.r.t. $p_{\text{tr-n}}(x)$ and by Eq. (7)'s assumption also $p_{\text{te-n}}(x)$. Multiple options exist to then train the second classifier, g, e.g., NU learning with $\mathcal{X}_{\text{tr-n}}$ and $\mathcal{X}_{\text{te-u}}$.

A perfect classifier is unrealistic. Is there an alternative? Our key insight is that by weighting $\mathcal{X}_{\text{tr-u}}$ (similar to covariate shift's importance function) it can be transformed into a representative negative set. From there, we consider two methods to fit the second classifier g: one a variant of NU learning we call weighted-unlabeled, unlabeled (wUU) learning and the other a semi-supervised method we call arbitrary-positive, negative, unlabeled (aPNU) learning. We refer to the complete algorithms as PU2wUU and PU2aPNU, respectively.

Algorithm 1 Two-step unlabeled-unlabeled aPU learning

Input: Labeled-positive set $\mathcal{X}_{\text{p}}$ and unlabeled sets $\mathcal{X}_{\text{tr-u}}, \mathcal{X}_{\text{te-u}}$
Output: g's model parameters θ

1: Train probabilistic classifier $\hat{\sigma}$ using $\mathcal{X}_{\text{p}}$ and $\mathcal{X}_{\text{tr-u}}$
2: Use $\hat{\sigma}$ to transform $\mathcal{X}_{\text{tr-u}}$ into surrogate negative set $\widetilde{\mathcal{X}}_{\text{n}}$
3: Train final classifier, g, using ERM with $\widehat{R}_{\text{wUU}}(g)$ or $\widehat{R}_{\text{aPNU}}(g)$

Figure 1 visualizes our two-step approach, with a formal presentation in Algorithm 1. Below is a detailed description and theoretical analysis.

Step #1: Create Surrogate Negative Set $\widetilde{\mathcal{X}}_{\text{n}}$ from $\mathcal{X}_{\text{tr-u}}$

This step's goal is to learn the training distribution's negative class-posterior, $p_{\text{tr}}(Y=-1|x)$. We achieve this by training PU probabilistic classifier $\hat{\sigma} : \mathbb{R}^d \to [0,1]$ using $\mathcal{X}_{\text{p}}$ and $\mathcal{X}_{\text{tr-u}}$. In principle, any probabilistic PU method can be used; we focused on ERM-based PU methods so the logistic loss served as surrogate, ℓ. Sigmoid activation is applied to the model's output to bound its range to $(0,1)$.

Theorem 2. *Let $g : \mathbb{R}^d \to \mathbb{R}$ be an arbitrary decision function and $\ell : \mathbb{R} \to \mathbb{R}_{\geq 0}$ be a loss function bounded w.r.t. g. Let $\hat{y} \in \{\pm 1\}$ be a predicted label. Define $\mathcal{X}_{\text{tr-u}} \coloneqq \{x_i\}_{i=1}^{n_{\text{tr-u}}} \overset{\text{i.i.d.}}{\sim} p_{\text{tr-u}}(x)$, and restrict $\pi_{\text{tr}} \in [0,1)$. Define $\widetilde{R}^{\hat{y}}_{\text{n-u}}(g) \coloneqq \frac{1}{n_{\text{tr-u}}} \sum_{x_i \in \mathcal{X}_{\text{tr-u}}} \frac{\hat{\sigma}(x_i)\ell(\hat{y}g(x_i))}{1-\pi_{\text{tr}}}$. Let $\hat{\sigma} : \mathbb{R}^d \to [0,1]$ be in hypothesis set $\widehat{\Sigma}$. When $\hat{\sigma}(x) = p_{\text{tr}}(Y=-1|x)$, $\widetilde{R}^{\hat{y}}_{\text{n-u}}(g)$ is an unbiased estimator of $R^{\hat{y}}_{\text{n}}(g)$. When the concept class of functions that defines $p_{\text{tr}}(Y=-1|x)$ is probably approximately correct (PAC) learnable by some PAC-learning algorithm $\mathcal{A}$ that selects $\hat{\sigma} \in \widehat{\Sigma}$, then $\widetilde{R}^{\hat{y}}_{\text{n-u}}(g)$ is a consistent estimator of $R^{\hat{y}}_{\text{n}}(g)$.*

From Theorem 2, we see that *soft* weighting each unlabeled instance in $\mathcal{X}_{\text{tr-u}}$ by $\hat{\sigma}$ yields a *surrogate negative set* $\widetilde{\mathcal{X}}_{\text{n}}$ that can be used to estimate the train/test negative labeled risk. We form $\widetilde{\mathcal{X}}_{\text{n}}$ transductively, but inductive learning is an option. Since $\mathcal{X}_{\text{tr-u}}$ contains positive examples, $\hat{\sigma}$ may overfit and memorize random positive example variation. This is usually detectable via an implausible validation loss given π_{tr}, n_{p}, and $n_{\text{tr-u}}$. Care should be shown to tune $\hat{\sigma}$'s capacity and regularization.

Supplemental Section E.7 proposes and empirically evaluates two additional methods to construct $\widetilde{\mathcal{X}}_{\text{n}}$. While these other methods are not statistically consistent, they may outperform soft weighting.

What if $\mathcal{X}_{\text{p}}$ is not SCAR? Our aPU learning setting, detailed in Section 4, specifies that $\mathcal{X}_{\text{p}}$ is representative of $\mathcal{X}_{\text{tr-u}}$'s positive examples. In scenarios where $\mathcal{X}_{\text{p}}$ is biased w.r.t. $\mathcal{X}_{\text{tr-u}}$, any bPU method (e.g., [12, 13]) can be used in step #1 to (hard) label $\mathcal{X}_{\text{tr-u}}$ thereby constructing $\widetilde{\mathcal{X}}_{\text{n}}$.

Step #2: Train the Test Distribution Classifier g

Negative-unlabeled (NU) learning is functionally the same as PU learning. Sakai et al. [27] formalize an unbiased NU risk estimator, $\widehat{R}_{\text{NU}}(g) \coloneqq \left|\widehat{R}^{+}_{\text{u}}(g) - (1-\pi)\widehat{R}^{+}_{\text{n}}(g)\right| + (1-\pi)\widehat{R}^{-}_{\text{n}}(g)$ (defined here with our absolute-value correction). Our *weighted-unlabeled, unlabeled*[2] (wUU) estimator,

$$\widehat{R}_{\text{wUU}}(g) \coloneqq \left|\widehat{R}^{+}_{\text{te-u}}(g) - (1-\pi_{\text{te}})\widetilde{R}^{+}_{\text{n-u}}(g)\right| + (1-\pi_{\text{te}})\widetilde{R}^{-}_{\text{n-u}}(g), \tag{8}$$

modifies Sakai et al.'s definition to use $\widetilde{\mathcal{X}}_{\text{n}}$ and $\mathcal{X}_{\text{te-u}}$. Observe that $\widehat{R}_{\text{wUU}}(g)$ uses only data that was originally unlabeled. When $\widetilde{R}^{\hat{y}}_{\text{n-u}}(g)$ is consistent, wUU is also consistent just like nnPU/abs-PU.

Risk Estimation with Positive Data Reuse When $p_{\text{tr-p}}(x)$'s and $p_{\text{te-p}}(x)$'s supports intersect, $\mathcal{X}_{\text{p}}$ may contain useful information about the target distribution given limited data. In such settings, a semi-supervised approach leveraging $\mathcal{X}_{\text{p}}$, surrogate $\widetilde{\mathcal{X}}_{\text{n}}$, and $\mathcal{X}_{\text{te-u}}$ may perform better than wUU.

Sakai et al. [27] propose the PNU risk estimator, $\widehat{R}_{\text{PNU}}(g) \coloneqq (1-\rho)\widehat{R}_{\text{PN}}(g) + \rho\widehat{R}_{\text{NU}}(g)$, where hyperparameter $\rho \in (0,1)$ weights the PN and NU estimators. Our *arbitrary-positive, negative, unlabeled* (aPNU) risk estimator in Eq. (9) modifies PNU to use $\widetilde{\mathcal{X}}_{\text{n}}$ and our absolute-value correction.

$$\widehat{R}_{\text{aPNU}}(g) = (1-\rho)\pi_{\text{te}}\widehat{R}^{+}_{\text{p}}(g) + (1-\pi_{\text{te}})\widetilde{R}^{-}_{\text{n-u}}(g) + \rho\left|\widehat{R}^{+}_{\text{te-u}}(g) - (1-\pi_{\text{te}})\widetilde{R}^{+}_{\text{n-u}}(g)\right| \tag{9}$$

[2] "Unlabeled-unlabeled learning" denotes the two unlabeled sets and is different from UU learning in [28, 29].

If $\rho = 0$, aPNU ignores the test distribution (i.e., $\mathcal{X}_{\text{te-u}}$) entirely. If $\rho = 1$, aPNU is simply wUU. When a large positive shift is expected (e.g., by domain-specific knowledge), $\mathcal{X}_{\text{p}}$ is of limited value so set ρ closer to 1. For small expected positive shifts, set ρ closer to 0. A midpoint value of $\rho = 0.5$ empirically performed well when no knowledge about the positive shift was assumed.

ERM Framework Both $\widehat{R}_{\text{wUU}}(g)$ and $\widehat{R}_{\text{aPNU}}(g)$ integrate into a standard ERM framework since they use our absolute-value correction. For completeness, supplemental materials Section C.1 details their custom ERM algorithm if Kiryo et al. [8]'s non-negativity correction is used instead.

Heterogeneous Classifiers Two-step learners enable different learner architectures in each step (e.g., random forest for step #1 and a neural network for step #2). Our experiments leverage this flexibility where $\hat{\sigma}$'s neural network may have fewer hidden layers or different hyperparameters than g in step #2.

6 Positive-Unlabeled Recursive Risk Estimation

Two-step methods — both ours and PUc — solve a challenging problem by decomposing it into sequential (easier) subproblems. Serial decision making's disadvantage is that earlier errors propagate and can be amplified when subsequent decisions are made on top of those errors.

Can our aPU problem setting be learned in a single *joint* method? Sakai and Shimizu leave it as an open question. We show in this section the answer is yes. To understand why this is possible, it helps to simplify our perspective of unbiased PU and NU learning. When estimating a labeled risk, $\widehat{R}^{\hat{y}}_{\mathcal{D}}(g)$ (where $\mathcal{D} \in \{\text{p}, \text{n}\}$), the ideal case is to use SCAR data from class-conditional distribution $p_{\mathcal{D}}(x)$. When such labeled data is unavailable, the risk *decomposes* via the simple linear transformation,

$$(1-\alpha)\widehat{R}^{\hat{y}}_{A}(g) = \widehat{R}^{\hat{y}}_{\text{u}}(g) - \alpha\widehat{R}^{\hat{y}}_{B}(g) \tag{10}$$

where $A = \text{n}$ and $B = \text{p}$ for PU learning or vice versa for NU learning. α is the positive (negative) prior for PU (NU) learning.

In standard PU and NU learning, either $\widehat{R}^{\hat{y}}_{A}(g)$ or $\widehat{R}^{\hat{y}}_{B}(g)$ can always be estimated from labeled data. If that were not true, can this decomposition be applied recursively (i.e., nested)? The answer is again yes. Below we apply recursive risk decomposition to our aPU learning task.

Applying Recursive Risk to aPU learning

Our positive-unlabeled recursive risk (PURR) estimator quantifies our aPU setting's empirical risk and integrates into a standard ERM framework. PURR's top-level definition is simply the test risk:

$$\widehat{R}_{\text{PURR}}(g) = \pi_{\text{te}}\widehat{R}^{+}_{\text{te-p}}(g) + (1-\pi_{\text{te}})\widehat{R}^{-}_{\text{te-n}}(g). \tag{11}$$

Since only unlabeled data is drawn from the test distribution, both terms in Eq. (11) require risk decomposition. First, for $\widehat{R}^{-}_{\text{te-n}}(g)$, we consider its more general form $\widehat{R}^{\hat{y}}_{\text{te-n}}(g)$ below since $\widehat{R}^{+}_{\text{te-n}}(g)$ will be needed as well. Using Eq. (7)'s assumption, $\widehat{R}^{\hat{y}}_{\text{te-n}}(g)$ can be estimated directly from the training distribution. Combining Eq. (3) with absolute-value correction, we see that

$$\widehat{R}^{\hat{y}}_{\text{te-n}}(g) = \widehat{R}^{\hat{y}}_{\text{tr-n}}(g) = \frac{1}{1-\pi_{\text{tr}}}\left|\widehat{R}^{\hat{y}}_{\text{tr-u}}(g) - \pi_{\text{tr}}\widehat{R}^{\hat{y}}_{\text{tr-p}}(g)\right|. \tag{12}$$

Next, $\widehat{R}^{+}_{\text{te-p}}(g)$, as a positive risk, undergoes NU decomposition so (with absolute-value correction):

$$\pi_{\text{te}}\widehat{R}^{+}_{\text{te-p}}(g) = \left|\widehat{R}^{+}_{\text{te-u}}(g) - (1-\pi_{\text{te}})\widehat{R}^{+}_{\text{te-n}}(g)\right|. \tag{13}$$

Eq. (12) with $\hat{y} = +1$ substitutes for $\widehat{R}^{+}_{\text{te-n}}(g)$ in Eq. (13) yielding $\widehat{R}_{\text{PURR}}(g)$'s complete definition:

$$\widehat{R}_{\text{PURR}}(g) = \underbrace{\left|\widehat{R}^{+}_{\text{te-u}}(g) - (1-\pi_{\text{te}})\underbrace{\left|\frac{\widehat{R}^{+}_{\text{tr-u}}(g) - \pi_{\text{tr}}\widehat{R}^{+}_{\text{tr-p}}(g)}{1-\pi_{\text{tr}}}\right|}_{\widehat{R}^{+}_{\text{te-n}}(g)}\right|}_{\pi_{\text{te}}\widehat{R}^{+}_{\text{te-p}}(g)} + (1-\pi_{\text{te}})\underbrace{\left|\frac{\widehat{R}^{-}_{\text{tr-u}}(g) - \pi_{\text{tr}}\widehat{R}^{-}_{\text{tr-p}}(g)}{1-\pi_{\text{tr}}}\right|}_{\widehat{R}^{-}_{\text{te-n}}(g)}. \tag{14}$$

Theorem 3. *Fix decision function $g \in \mathcal{G}$. If ℓ is bounded over $g(x)$'s image and $\widehat{R}^{\hat{y}}_{\text{te-n}}(g), \widehat{R}^{+}_{\text{te-p}}(g) > 0$ for $\hat{y} \in \{\pm 1\}$, then $\widehat{R}_{\text{PURR}}(g)$ is a consistent estimator. $\widehat{R}_{\text{PURR}}(g)$ is a biased estimator unless for all $\mathcal{X}_{\text{tr-u}} \overset{\text{i.i.d.}}{\sim} p_{\text{tr-u}}(x)$, $\mathcal{X}_{\text{te-u}} \overset{\text{i.i.d.}}{\sim} p_{\text{te-u}}(x)$, and $\mathcal{X}_{\text{p}} \overset{\text{i.i.d.}}{\sim} p_{\text{tr-p}}(x)$ it holds that $\Pr[\widehat{R}^{\hat{y}}_{\text{tr-u}}(g) - (1-\pi_{\text{te}})\widehat{R}^{\hat{y}}_{\text{tr-p}}(g) < 0] = 0$ and $\Pr[\widehat{R}^{+}_{\text{te-u}}(g) - (1-\pi_{\text{te}})\widehat{R}^{+}_{\text{te-n}}(g) < 0] = 0$.*

Optimization PURR with absolute-value correction integrates into a standard ERM framework. If non-negativity is used instead, PURR's optimization scheme becomes significantly more complicated as it must consider four candidate gradients per update; see suppl. Section C.2 for more details.

7 Experimental Results

We empirically studied the effectiveness of our methods – PURR, PU2wUU, and PU2aPNU – using synthetic and real-world data.[3] Limited space allows us to discuss only two experiment sets here. Suppl. Section E details experiments on: synthetic data, 10 LIBSVM datasets [30] under a totally different positive-bias condition, and a study of our methods' robustness to negative-class shift.

7.1 Experimental Setup

Supplemental Section D enumerates our complete experimental setup with a brief summary below.

Baselines PUc [14] with a linear-in-parameter model and Gaussian kernel basis is the primary baseline.[4] Ordinary nnPU is the performance floor. To ensure the strongest baseline, we separately trained nnPU with unlabeled set $\mathcal{X}_{\text{te-u}}$ as well as with the combined $\mathcal{X}_{\text{tr-u}} \cup \mathcal{X}_{\text{te-u}}$ (using the true, composite prior) and report each experiment's best performing configuration, denoted nnPU*****. PN-test (trained on labeled $\mathcal{X}_{\text{te-u}}$) provides a reference for the performance ceiling. All methods saw identical training/test data splits and where applicable used the same initial weights.

Datasets Section 7.2 considers the MNIST [31], CIFAR10 [32], and 20 Newsgroups [33] datasets with binary classes formed by partitioning each dataset's labels. Section 7.3 uses two different TREC [34] spam email datasets to demonstrate our methods' performance under real-world adversarial concept drift. Further details on all datasets are in the supplemental materials.

Learner Architecture We focus on training neural networks (NNs) via stochastic optimization (i.e., AdamW [35] with AMSGrad [36]). Probabilistic classifier, $\hat{\sigma}$, used our abs-PU risk estimator with logistic loss. All other learners used sigmoid loss for ℓ. Since PUc is limited to linear models with Gaussian kernels, we limited our NNs to at most three fully-connected layers of 300 neurons. For MNIST, our NNs were trained from scratch. Pretrained deep networks encoded the CIFAR10, 20 Newsgroups, and TREC spam datasets into static representations all learners used. Specifically, the 20 Newsgroups documents and TREC emails were encoded into 9,216 dimensional vectors using ELMo [37]. This encoding scheme was used by Hsieh et al. [11] and is based on [38]. DenseNet-121 [39] encoded each CIFAR10 image into a 1,024 dimensional vector.

Hyperparameters Our only individually tuned hyperparameters are learning rate and weight decay. We assume the worst case of no *a priori* knowledge about the positive shift so midpoint value $\rho = 0.5$ was used. PUc's hyperparameters were tuned via importance-weighted cross validation [40]. For the complete hyperparameter details, see supplemental materials Section D.8.

7.2 Partially and Fully Disjoint Positive Class-Conditional Supports

Here we replicate scenarios where positive subclasses exist only in the test distribution (e.g., adversarial zero-day attacks). These experiments are modeled after Hsieh et al. [11]'s experiments for positive, unlabeled, biased-negative (PUbN) learning.

Table 1 lists the experiments' positive train/test and negative class definitions. Datasets are sampled u.a.r. from their constituent sublabels. Each dataset has four experimental conditions (ordered by row number): (1) $\text{P}_{\text{train}} = \text{P}_{\text{test}}$, i.e., no bias, (2 & 3 resp.) partially disjoint positive supports without and with prior shift, and (4) disjoint positive class definitions. π_{te} equals P_{test}'s true prior w.r.t. $\text{P}_{\text{test}} \sqcup \text{N}$.

[3] Our implementation is publicly available at: https://github.com/ZaydH/arbitrary_pu.

[4] The PUc implementation was provided by Sakai and Shimizu [14] via personal correspondence.

Table 1: Mean inductive misclassification rate (%) over 100 trials for MNIST, 20 Newsgroups, & CIFAR10 for different positive & negative class definitions. Bold denotes a *shifted task*'s best performing method. For *all* shifted tasks, our three methods – denoted with † – statistically outperformed PUc and nnPU* based on a paired t-test ($p < 0.01$). Each dataset's first three experiments have identical negative (N) & positive-test (P_{test}) class definitions. Positive train (P_{train}) specified as "P_{test}" denotes no bias. Additional shifted tasks (with result standard deviations) are in the supplemental materials.

	N	P_{test}	P_{train}	π_{tr}	π_{te}		Two-Step (PU2)		Baselines		Ref.
						PURR†	aPNU†	wUU†	PUc	nnPU*	PN_{te}
MNIST	0, 2, 4, 6, 8	1, 3, 5, 7, 9	P_{test}	0.5	0.5	10.0	10.0	11.6	8.6	5.5	↑
			7, 9	0.5	0.5	9.4	**7.1**	8.3	26.8	35.1	2.8
				0.29	0.5	6.8	**5.3**	6.0	29.2	36.7	↓
	0, 2	5, 7	1, 3	0.5	0.5	4.0	3.6	**3.1**	17.1	30.9	1.1
20 News.	sci, soc, talk	alt, comp, misc, rec	P_{test}	0.56	0.56	15.4	14.9	16.7	14.9	14.1	↑
			misc, rec	0.56	0.56	17.5	**13.5**	15.1	23.9	28.8	10.5
				0.37	0.56	13.9	**12.8**	14.3	28.9	28.8	↓
	misc, rec	soc, talk	alt, comp	0.55	0.46	5.9	7.1	**5.6**	18.5	35.3	2.1
CIFAR10	Bird, Cat, Deer, Dog, Frog, Horse	Plane, Auto, Ship, Truck	P_{test}	0.4	0.4	14.1	14.2	15.5	13.8	12.3	↑
			Plane	0.4	0.4	**13.8**	14.5	15.1	20.6	27.4	9.8
				0.14	0.4	12.1	**11.9**	12.4	26.7	26.7	↓
	Deer, Horse	Plane, Auto	Cat, Dog	0.5	0.5	14.1	14.9	**11.2**	33.1	47.5	7.7

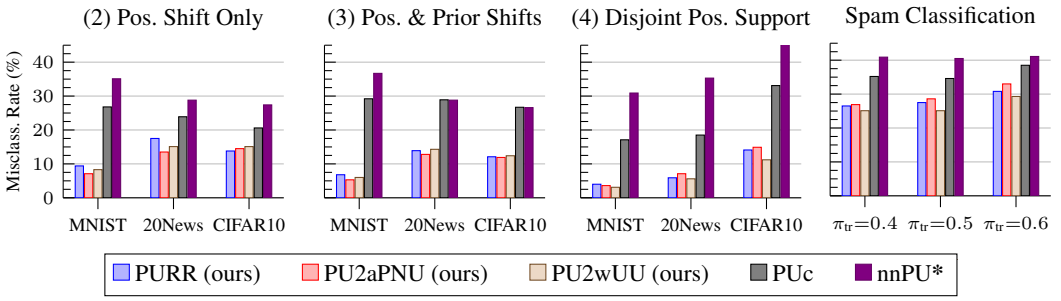


Figure 2: Mean inductive misclassification rate over 100 trials on the MNIST, 20 News., CIFAR10, & TREC spam datasets for our methods & baselines. Each numbered plot (i.e., 2–4) corresponds to one experimental shift task in Table 1. Spam classification experiments are detailed in Section 7.3.

By default $\pi_{tr} = \pi_{te}$; in the prior shift and disjoint support experiments (rows 3 and 4), π_{tr} equals P_{train}'s true prior w.r.t. $P_{train} \sqcup N$.

Analysis Results are shown in Table 1 and Figure 2. On *unshifted* data (row 1 for each dataset), baselines PUc and nnPU* slightly outperformed our methods, which shows that PUc's architecture is sufficiently expressive. In contrast, on *shifted* data (rows 2–4 for each dataset), our methods' performance generally improved while both PUc's and nnPU*'s performance always degraded. This performance divergence demonstrates our methods' algorithmic advantage. In fact for all shifted tasks, our methods always outperformed PUc and nnPU* according to a paired t-test ($p < 0.01$). For partially disjoint positive supports (rows 2 and 3 for each dataset), PU2aPNU was the top performer for five of six setups (PURR was top on the other). This pattern reversed for fully disjoint supports (row 4) where PU2aPNU always lagged PU2wUU; this is expected as explained in Section 5.

Reducing π_{tr} always improved our algorithms' performance and degraded PUc's. A smaller prior enables easier identification of $\mathcal{X}_{\text{tr-u}}$'s negative examples and in turn a more accurate estimation of $\mathcal{X}_{\text{te-u}}$'s negative risk. In contrast, importance weighting is most accurate in the absence of bias (see row 1 for each dataset). Any shift increases density estimation's (and by extension PUc's) inaccuracy.

Table 2: Mean inductive misclassification rate (%) over 100 trials for spam adversarial drift. Our methods – PURR, PU2wUU, and PU2aPNU – outperformed PUc & nnPU* based on a 1% paired t-test. Each result's standard deviation appears in supplemental Table 14.

Train Set		Test Set		π_{tr}	π_{te}		Two-Step (PU2)		Baselines		Ref.
Pos.	Neg.	Pos.	Neg.			PURR	aPNU	wUU	PUc	nnPU*	PN_{te}
2005 Spam	2005 Ham	2007 Spam	2007 Ham	0.4	0.5	26.5	26.9	**25.1**	35.2	40.9	↑
				0.5	0.5	27.5	28.6	**25.1**	34.6	40.5	0.6
				0.6	0.5	30.8	33.0	**29.3**	38.5	41.1	↓

nnPU* outperformed both PUc and our methods when there was no bias. This is expected. If an algorithm searches for non-existent phenomena, any additional patterns found will not generalize.

7.3 Case Study: Arbitrary Adversarial Concept Drift

PU learning has been applied to multiple adversarial domains including opinion spam [3, 16, 17, 18]. We use spam classification as a vehicle to test our methods in an adversarial setting by considering two different TREC email spam datasets – training on TREC05 and evaluating on TREC07. Spam – the positive class – evolves quickly over time, but the two datasets' ham emails are also quite different: TREC05 relies on Enron emails while TREC07 contains mostly emails from a university server. Thus, this represents a more challenging, realistic setting where Eq. (7)'s assumption does not hold.

Table 2 and Figure 2 show that our methods outperformed PUc and nnPU* according to a 1% paired t-test across three training priors (π_{tr}). PU2wUU was the top-performer as $\hat{\sigma}$ accurately labeled $\mathcal{X}_{\text{tr-u}}$, yielding a strong surrogate negative set. PU2aPNU performed slightly worse than PU2wUU as the significant adversarial concept drift greatly limited $\mathcal{X}_{\text{p}}$'s value. Overall, these experiments show that our aPU setting arises in real-world domains. All of our methods handled large positive shifts better than prior work, even in realistic cases where the negative class also shifts.

7.4 Discussion

Our two-step methods assume asymptotic consistency for $\widetilde{\mathcal{X}}_{\text{n}}$ in step #1, but finite training data ensures a non-consistent evaluation setting. Nonetheless, either PU2aPNU or PU2wUU was the top performer in all but one experiment in this section.[5] Supplemental Section E.7 includes additional experiments where we further stress our two-step methods by forcing $\hat{\sigma}$ away from our posterior estimate. Even under those deleterious step #1 conditions, our two-step learners are robust.

Conventional wisdom suggests that joint method PURR should outperform pipeline approaches. This intuition breaks down in our case because PURR, with its three risk decompositions, is strictly harder to optimize than wUU, aPNU, abs-PU, and nnPU – all of which have a single decomposition. This harder optimization can lead to worse accuracy compared to the two-step methods, especially on easier problems (e.g., MNIST), where each step can be solved accurately on its own.

For completeness, suppl. Section E.5 compares our methods to bPU selection bias method PUSB [13]. Our algorithms generally outperformed PUSB on data specifically tuned for their method even after accounting for the differing unlabeled sets. Those experiments indicate that PUSB's underlying assumption entails only a small data shift and further point to potential PUSB learning brittleness.

8 Conclusions

We examined arbitrary-positive, unlabeled (aPU) learning, where the labeled-positive and target-positive distributions may be arbitrarily different. A (nearly) fixed negative class-distribution allows us to train accurate classifiers without any labeled data from the target distribution (i.e., disjoint positive supports). Empirical results on real-world data above and in the supplementals show that our methods are still robust in the realistic case of some negative shift. Future work seeks a less restrictive yet statistically-sound replacement assumption of a fixed negative class-conditional distribution.

[5] Supplemental Sections E.2 and E.4 enumerate multiple empirical setups where PURR is the top performer.

9 Broader Impact

The algorithms proposed in this work are general and could be applied to many different applications. Forecasting the broader impact of work like this is challenging and generally inaccurate. With that caveat, we discuss potential impacts based on possible applications.

The case study on email spam suggests that our methods may be useful in adversarial domains, such as the detection of fraud, malware, network intrusion, distributed denial of service (DDoS) attacks, and many types of spam. In these settings, one class (e.g., spam) evolves quickly as attackers try to evade detection. For many of these domains, improved classifiers would benefit society by reducing spam and fraud. However, for domains such as facial recognition, improved robustness could lead to reduced privacy and other societal harms. See Albert et al. [41] for an extensive discussion of the politics of adversarial machine learning.

In other domains, such as epidemiological analysis and land-cover classification, our work may lead to new or better models by reducing the need for labeled data and relaxing the SCAR assumption. As detailed in Section 1, only recently has the PU SCAR barrier been broken [12, 13, 14]. aPU learning pushes PU learning's positive-shift boundary to a new extreme. We hope this paper will enable PU learning to be applied in domains where existing bPU\PU methods are impractical. This could also benefit society if used responsibly, with experts performing proper model validation and vetting risks. Careful model validation is especially important when labeled data is limited and biased.

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References

[1] Marthinus du Plessis, Gang Niu, and Masashi Sugiyama. Convex formulation for learning from positive and unlabeled data. In *Proceedings of the 32nd International Conference on Machine Learning*, ICML'15, 2015.

[2] Jessa Bekker and Jesse Davis. Estimating the class prior in positive and unlabeled data through decision tree induction. In *Proceedings of the 32nd AAAI Conference on Artificial Intelligence*, AAAI'18, 2018.

[3] Donato Hernández Fusilier, Rafael Guzmán Cabrera, Manuel Montes-y Gómez, and Paolo Rosso. Using PU-learning to detect deceptive opinion spam. In *Proceedings of the 4th Workshop on Computational Approaches to Subjectivity, Sentiment and Social Media Analysis*, pages 38–45, 6 2013.

[4] Peng Yang, Xiao-Li Li, Jian-Ping Mei, Chee-Keong Kwoh, and See-Kiong Ng. Positive-unlabeled learning for disease gene identification. *Bioinformatics*, 28(20):2640–2647, 08 2012.

[5] Wenkai Li, Qinghua Guo, and Charles Elkan. A positive and unlabeled learning algorithm for one-class classification of remote-sensing data. *IEEE Transactions on Geoscience and Remote Sensing*, 49:717 – 725, 2011.

[6] Charles Elkan and Keith Noto. Learning classifiers from only positive and unlabeled data. In *Proceedings of the 14th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, KDD'08, pages 213–220, 2008.

[7] Ming Hou, Brahim Chaib-Draa, Chao Li, and Qibin Zhao. Generative adversarial positive-unlabeled learning. In *Proceedings of the 27th International Joint Conference on Artificial Intelligence*, IJCAI'18, page 2255–2261, 2018.

[8] Ryuichi Kiryo, Gang Niu, Marthinus C. du Plessis, and Masashi Sugiyama. Positive-unlabeled learning with non-negative risk estimator. In *Proceedings of the 30th Conference on Neural Information Processing Systems*, NeurIPS'17, pages 1674–1684, 2017.

[9] Tieliang Gong, Guangtao Wang, Jieping Ye, Zongben Xu, and Ming Lin. Margin based PU learning. In *Proceedings of the 32nd AAAI Conference on Artificial Intelligence*, AAAI'18, 2018.

[10] Chuang Zhang, Dexin Ren, Tongliang Liu, Jian Yang, and Chen Gong. Positive and unlabeled learning with label disambiguation. In *Proceedings of the 28th International Joint Conference on Artificial Intelligence*, IJCAI'19, pages 4250–4256, 2019.

[11] Yu-Guan Hsieh, Gang Niu, and Masashi Sugiyama. Classification from positive, unlabeled and biased negative data. In *Proceedings of the 36th International Conference on Machine Learning*, ICML'19, pages 2820–2829, 2019.

[12] Jessa Bekker, Pieter Robberechts, and Jesse Davis. Beyond the selected completely at random assumption for learning from positive and unlabeled data. In *Proceedings of the 2019 European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases*, ECML-PKDD'19, 2019.

[13] Masahiro Kato, Takeshi Teshima, and Junya Honda. Learning from positive and unlabeled data with a selection bias. In *Proceedings of the 7th International Conference on Learning Representations*, ICLR'19, 2019.

[14] Tomoya Sakai and Nobuyuki Shimizu. Covariate shift adaptation on learning from positive and unlabeled data. In *Proceedings of the 33rd AAAI Conference on Artificial Intelligence*, AAAI'19, pages 4838–4845, 2019.

[15] Galen Maclaurin and Stefan Leyk. Extending the geographic extent of existing land cover data using active machine learning and covariate shift corrective sampling. *International Journal of Remote Sensing*, 37: 5213–5233, 11 2016.

[16] Huayi Li, Zhiyuan Chen, Bing Liu, Xiaokai Wei, and Jidong Shao. Spotting fake reviews via collective positive-unlabeled learning. In *Proceedings of the 14th IEEE International Conference on Data Mining*, ICDM'14, page 899–904, 2014.

[17] Ya-Lin Zhang, Longfei Li, Jun Zhou, Xiaolong Li, Yujiang Liu, Yuanchao Zhang, and Zhi-Hua Zhou. POSTER: A PU learning based system for potential malicious URL detection. In *Proceedings of the 2017 ACM SIGSAC Conference on Computer and Communications Security*, CCS'17, page 2599–2601, 2017.

[18] J. Zhang, M. F. Khan, X. Lin, and Z. Qin. An optimized positive-unlabeled learning method for detecting a large scale of malware variants. In *Proceedings of the 2019 IEEE Conference on Dependable and Secure Computing*, DSC'19, 2019.

[19] Gang Niu, Marthinus C. du Plessis, Tomoya Sakai, Yao Ma, and Masashi Sugiyama. Theoretical comparisons of positive-unlabeled learning against positive-negative learning. In *Proceedings of the 29th Conference on Neural Information Processing Systems*, NeurIPS'16, page 1207–1215, 2016.

[20] Marthinus C du Plessis, Gang Niu, and Masashi Sugiyama. Analysis of learning from positive and unlabeled data. In *Proceedings of the 27th Conference on Neural Information Processing Systems*, NeurIPS'14, 2014.

[21] Harish G. Ramaswamy, Clayton Scott, and Ambuj Tewari. Mixture proportion estimation via kernel embedding of distributions. In *Proceedings of the 33rd International Conference on Machine Learning*, ICML'16, page 2052–2060, 2016.

[22] Marthinus C. du Plessis, Gang Niu, and Masashi Sugiyama. Class-prior estimation for learning from positive and unlabeled data. *Machine Learning*, 106(4):463–492, 2017.

[23] Daniel Zeiberg, Shantanu Jain, and Predrag Radivojac. Fast nonparametric estimation of class proportions in the positive-unlabeled classification setting. In *Proceedings of the 34th AAAI Conference on Artificial Intelligence*, AAAI'20, 2020.

[24] Hidetoshi Shimodaira. Improving predictive inference under covariate shift by weighting the log-likelihood function. *Journal of Statistical Planning and Inference*, 90:227–244, Oct 2000.

[25] Masashi Sugiyama, Taiji Suzuki, and Takafumi Kanamori. *Density Ratio Estimation in Machine Learning*. Cambridge University Press, USA, 1st edition, 2012.

[26] M. Yamada, T. Suzuki, T. Kanamori, H. Hachiya, and M. Sugiyama. Relative density-ratio estimation for robust distribution comparison. *Neural Computation*, 25(5):1324–1370, May 2013.

[27] Tomoya Sakai, Marthinus Christoffel du Plessis, Gang Niu, and Masashi Sugiyama. Semi-supervised classification based on classification from positive and unlabeled data. In *Proceedings of the 34th International Conference on Machine Learning*, ICML'17, pages 2998–3006, 2017.

[28] Aditya Menon, Brendan Van Rooyen, Cheng Soon Ong, and Bob Williamson. Learning from corrupted binary labels via class-probability estimation. In *Proceedings of the 32nd International Conference on Machine Learning*, ICML'15, pages 125–134, 2015.

[29] Nan Lu, Gang Niu, Aditya Krishna Menon, and Masashi Sugiyama. On the minimal supervision for training any binary classifier from only unlabeled data. In *Proceedings of the 7th International Conference on Learning Representations*, ICLR'19, 2019.

[30] Chih-Chung Chang and Chih-Jen Lin. LIBSVM: A library for support vector machines. *ACM Transactions on Intelligent Systems and Technology*, 2:27:1–27:27, 2011.

[31] Yann LeCun, Léon Bottou, Yoshua Bengio, and Patrick Haffner. Gradient-based learning applied to document recognition. In *Proceedings of the IEEE*, volume 86, pages 2278–2324, 1998.

[32] Alex Krizhevsky, Vinod Nair, and Geoffrey Hinton. The CIFAR-10 dataset, 2014.

[33] Ken Lang. Newsweeder: Learning to filter netnews. In *Proceedings of the 12th International Conference on Machine Learning*, ICML'95, pages 331–339, 1995.

[34] TREC. Text REtrieval Conference (TREC) overview. `https://trec.nist.gov/overview.html`, 2019 (accessed May 19, 2020).

[35] Ilya Loshchilov and Frank Hutter. Fixing weight decay regularization in Adam. *CoRR*, abs/1711.05101, 2017. URL `http://arxiv.org/abs/1711.05101`.

[36] Sashank J. Reddi, Satyen Kale, and Sanjiv Kumar. On the convergence of Adam and beyond. In *Proceedings of the 6th International Conference on Learning Representations*, ICLR'18, 2018.

[37] Matthew E. Peters, Mark Neumann, Mohit Iyyer, Matt Gardner, Christopher Clark, Kenton Lee, and Luke Zettlemoyer. Deep contextualized word representations. In *Proceedings of the 16th Annual Conference of the North American Chapter of the Association for Computational Linguistics*, NAACL'18, 2018.

[38] Andreas Rücklé, Steffen Eger, Maxime Peyrard, and Iryna Gurevych. Concatenated power mean embeddings as universal cross-lingual sentence representations. *CoRR*, abs/1803.01400, 2018. URL `http://arxiv.org/abs/1803.01400`.

[39] Gao Huang, Zhuang Liu, and Kilian Q. Weinberger. Densely connected convolutional networks. In *Proceedings of the 2017 IEEE Conference on Computer Vision and Pattern Recognition*, CVPR'17, pages 2261–2269, 2017.

[40] Masashi Sugiyama, Matthias Krauledat, and Klaus-Robert Müller. Covariate shift adaptation by importance weighted cross validation. *Journal of Machine Learning Research*, 8:985–1005, Dec. 2007.

[41] Kendra Albert, Jonathon Penney, Bruce Schneier, and Ram Shankar Siva Kumar. Politics of adversarial machine learning. In *ICLR Workshop Towards Trustworthy ML: Rethinking Security and Privacy for ML*, 2020.

[42] Mehryar Mohri, Afshin Rostamizadeh, and Ameet Talwalkar. *Foundations of Machine Learning*. The MIT Press, 2012.

[43] Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, Alban Desmaison, Andreas Kopf, Edward Yang, Zachary DeVito, Martin Raison, Alykhan Tejani, Sasank Chilamkurthy, Benoit Steiner, Lu Fang, Junjie Bai, and Soumith Chintala. PyTorch: An imperative style, high-performance deep learning library. In *Proceedings of the 33rd Conference on Neural Information Processing Systems*, NeurIPS'19, 2019.

[44] Han Xiao, Kashif Rasul, and Roland Vollgraf. Fashion-MNIST: A novel image dataset for benchmarking machine learning algorithms. *arXiv*, 2017.

[45] Tarin Clanuwat, Mikel Bober-Irizar, Asanobu Kitamoto, Alex Lamb, Kazuaki Yamamoto, and David Ha. Deep learning for classical Japanese literature. *NeurIPS'18 Workshop on Machine Learning for Creativity and Design*, 2018.

[46] Jason Rennie. 20 newsgroups. `http://qwone.com/~jason/20Newsgroups/`, 2001.

[47] Sergey Ioffe and Christian Szegedy. Batch normalization: Accelerating deep network training by reducing internal covariate shift. In *Proceedings of the 32nd International Conference on Machine Learning*, ICML'15, pages 448–456, 2015.

[48] Seiya Tokui, Kenta Oono, Shohei Hido, and Justin Clayton. Chainer: a next-generation open source framework for deep learning. In *Proceedings of the 29th Conference on Neural Information Processing Systems*, 2015.

[49] Diederik P. Kingma and Jimmy Ba. Adam: A method for stochastic optimization. In *Proceedings of the 3rd International Conference on Learning Representations*, ICLR'15, 2015.

[50] Chuan Guo, Geoff Pleiss, Yu Sun, and Kilian Q Weinberger. On calibration of modern neural networks. In *Proceedings of the 34th International Conference on Machine Learning*, ICML'17, 2017.