A Boosting Algorithm for Positive-Unlabeled Learning

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Abstract

Positive-unlabeled (PU) learning deals with binary classification problems when only positive (P) and unlabeled (U) data are available. Many recent PU methods are based on neural networks, but little has been done to develop boosting algorithms for PU learning, despite boosting algorithms’ strong performance on many fully supervised classification problems. In this paper, we propose a novel boosting algorithm, AdaPU, for PU learning. Similarly to AdaBoost, AdaPU aims to optimize an empirical exponential loss, but the loss is based on the PU data, rather than on positive-negative (PN) data. As in AdaBoost, we learn a weighted combination of weak classifiers by learning one weak classifier and its weight at a time. However, AdaPU requires a very different algorithm for learning the weak classifiers and determining their weights. This is because AdaPU learns a weak classifier and its weight using a weighted positive-negative (PN) dataset with some negative data weights — the dataset is derived from the original PU data, and the data weights are determined by the current weighted classifier combination, but some data weights are negative. Our experiments showed that AdaPU outperforms neural networks on several benchmark PU datasets, including a large-scale challenging cyber security dataset.

1 Introduction

Positive-unlabeled (PU) learning \cite{5, 4, 6} has recently attracted significant interest as an important machine learning problem. While traditional supervised binary classification considers learning from both positive and negative examples, PU learning considers learning from only positive and unlabeled examples, where an unlabeled example can be either positive (P) or negative (N). PU learning arises naturally in various domains where positive (P) data and unlabeled (U) data are readily available, but obtaining negative examples is costly. For example,
in disease diagnosis, we can easily collect data of confirmed patients provided by the doctors, but not for patients with mild or asymptomatic symptoms that have not been diagnosed yet.

Various approaches have been proposed for PU learning. One common approach is an iterative two-step approach: in each iteration, the current model is used to identify reliable N data from U, then ordinary fully-supervised (PN) learning is performed to update the current model [21, 20]. Another important approach performs supervised learning on a weighted PN dataset derived from the PU dataset [9, 8, 18]. Our work follows this second approach, and is partly motivated by unbiased PU (uPU) [8] and its improved variant, non-negative PU (nnPU) [18].

Recent state-of-the-art (SOTA) PU methods are mostly based on neural networks (NNs) [18, 2, 28], due to the recent successes of NNs in various domains, particularly in computer vision and natural language processing. On the other hand, boosting algorithms are still often used as a preferred method for handling tabular data due to their simplicity and superior performance. Notably, many datasets on Kaggle are tabular, and boosting algorithms are among one of the top choices of Kaggle users. Despite the strong performance of boosting methods in supervised learning, little has been done to develop boosting algorithms for PU learning yet. We thus propose to fill this gap.

In this paper, we propose a novel boosting algorithm, AdaPU, for learning from PU data. Our algorithm is partly motivated by the classical AdaBoost (Adaptive Boosting) [10, 11] algorithm. As in AdaBoost, we learn a number of weak classifiers and their weights sequentially, and use the weighted combination of them as the final model. Each weak classifier is trained to do well on examples that are hard for previous weak classifiers; specifically, the training set of each weak classifier consists of weighted examples, with harder examples having higher weights. However, while AdaBoost minimizes the empirical exponential loss based on PN data, AdaPU minimizes an empirical exponential loss based on PU data. This results in some negative weights in the weighted samples and entails a novel weak learning algorithm: instead of simply training the weak classifiers to minimize weighted classification errors, the training procedure needs to be augmented with a mechanism to prevent overfitting.

The remainder of this paper is organized as follows. Section 2 briefly reviews AdaBoost and PU learning. Section 3 describes our AdaPU algorithm. The experimental results are presented in Section 4, with the conclusion in Section 5.

2 Preliminaries

Our AdaPU algorithm builds on the AdaBoost algorithm and some PU-based risk estimators. We provide a brief description of these important ideas below.

2.1 AdaBoost

Boosting is one of the major types of ensemble methods to “boost” a series of weak classifiers outputted by a weak learner to one strong classifier. Roughly speaking, a weak classifier is one that is only guaranteed to be better than random guessing, while a strong classifier is one that can achieve arbitrarily accurate performance. AdaBoost (Adaptive Boosting) is one of

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1 This is reflected by the 25,973 responses to the 2021 Kaggle Data Science & Machine Learning Survey (https://www.kaggle.com/kaggle-survey-2021).
the most classical boosting algorithms [10, 11], with a lot of successful applications, such as face recognition [29].

We provide a brief review of AdaBoost based on [14]. Given training data \{(x_1, y_1), \ldots, (x_n, y_n)\}, where \(x_i\) is the \(i\)-th instance and \(y_i \in \{-1, +1\}\) is the label for \(x_i\), AdaBoost aims to find a strong classifier of the form

\[
F_T(x) := \text{sign}(H_T(x)) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right),
\]

(1)

where \(h_t\) is the \(t\)-th weak classifier, and \(\alpha_t > 0\) for all \(t \in \{1, \ldots, T\}\).

Instead of finding \(F_T(x)\) that directly minimizes the classification error based on zero-one loss, AdaBoost uses the exponential loss as the surrogate loss and minimizes

\[
\sum_{i=1}^{n} \exp(-y_i H_{t-1}(x_i))
\]

(2)
in a greedy manner by gradually adding newly learned weak classifiers. Specifically, AdaBoost starts with \(H_0(x) = 0\). At the \(t\)-th iteration, given \(H_{t-1}\), the weak classifier \(h_t\) and its weight \(\alpha_t\) are minimizers of

\[
\sum_{i=1}^{n} e^{-y_i (H_{t-1}(x_i) + \alpha h(x_i))}.
\]

(3)

Let \(w_i^{(t)} = e^{-y_i H_{t-1}(x_i)} / \sum_j e^{-y_j H_{t-1}(x_j)}\), and \(\epsilon_t(h) = \sum_i w_i^{(t)} \mathbb{I}(y_i \neq h(x_i))\) be a weak classifier \(h\)'s weighted classification error, then \(h_t\) and \(\alpha_t\) are given by [14]:

\[
h_t = \arg\min_h \epsilon_t(h),
\]

(4)

\[
\alpha_t = \frac{1}{2} \log \frac{1 - \epsilon_t}{\epsilon_t}.
\]

(5)

At each iteration, we can efficiently calculate the weights \(w_i^{(t)}\) using the recursive formula

\[
w_i^{(t)} = w_i^{(t-1)} e^{-\alpha_t y_i h_{t-1}(x_i)} / Z_{t-1},
\]

(6)

where \(Z_{t-1} = \sum_i w_i^{(t-1)} e^{-\alpha_t y_i h_{t-1}(x_i)}\) is the normalization constant.

2.2 PU learning

The study of PU learning can be traced back to [5, 4, 6]. Early works are usually based on sample selection, which first uses heuristics to select reliable N data from U and then performs PN learning [21, 20, 22]. Various learning algorithms, including boosting, can be used in the supervised learning step. The two-step method’s performance can be sensitive to the selection strategy, and a poor selection strategy may lead to unsatisfactory performance. To the best of our knowledge, the only boosting method for PU data is such a two-step method [30]. Instead of using a PN boosting algorithm as a building block, our AdaPU algorithm is designed as a boosting algorithm that directly learns from PU data.

Besides these two-step methods, another group of methods are based on minimizing loss on a weighted PN dataset constructed using the PU data. The construction of the weighted
PN dataset depends on how PU data is generated. Two data generation mechanisms are often considered in the literature [24]: censored PU learning (e.g., [9]) where data are sampled together and part of P and all of N data become unlabeled, and case-control PU learning (e.g., [19, 7]), where P and U data are sampled separately. This paper considers case-control PU learning. Two recent methods in this category are most closely related to our work: unbiased PU learning (uPU) [8] and non-negative PU learning (nnPU) [18]. uPU allows computing unbiased risk estimates using PU data only. However, uPU suffers from severe overfitting [19, 7], where P and U data are sampled separately. This paper considers case-control PU learning (e.g., [9]), where data are sampled independently.

We describe uPU and nnPU in detail below. Let $X \in \mathbb{R}^d$ and $Y \in \{+1, -1\}$ be the input and output random variables respectively, $p(x) = P(X)$ be the marginal distribution of the input, $p_+(x) = P(x|Y = +1)$ be the distribution of positive examples, $p_-(x) = P(x|Y = -1)$ be the distribution of negative examples, $\pi = \pi_p = P(Y = +1)$ be the probability of positive examples, $\pi_n = 1 - \pi_p$ be the probability of negative examples, and $\ell : \mathbb{R} \times \{+1, -1\} \to \mathbb{R}$ be a loss function with $\ell(y', y)$ being the loss incurred when an example in class $y$ is predicted to have a score $y'$. Following [7, 18, 16, 2], we assume $\pi_p$ is known throughout the paper. As in the fully supervised case, the objective of PU learning is to find a classifier $g : \mathbb{R}^d \to \mathbb{R}$ minimizing the expected risk

$$R(g) = \mathbb{E}(\ell(g(X), Y)).$$ (7)

In fully-supervised classification, we have a sample of training data drawn independently from $P(X, Y)$, and this allows us to use the average loss to estimate the expected risk. However, in PU learning, we only have access to positive and unlabeled examples, but not negative examples, thus estimating the expected risk using the available data is non-trivial. To address such a difficulty, the risk is rewritten as the following using PU data [7, 8]

$$R(g) = \pi_p \mathbb{E}_{p_+}(\ell(g(X), +1)) + \left( \mathbb{E}_{p}(\ell(g(X), -1)) - \pi_p \mathbb{E}_{p_+}(\ell(g(X), -1)) \right).$$

If our PU data consists of a set $\mathcal{P} = \{x_1^+, \ldots, x_{n_p}^+\}$ of positive examples sampled independently from $p_+(x)$, and a set $\mathcal{U} = \{x_1^u, \ldots, x_{n_u}^u\}$ of unlabeled examples sampled independently from $p(x)$, we have the following unbiased risk estimator [7, 8]

$$\hat{R}_{pu}(g) = \frac{\pi}{n_p} \sum_{x \in \mathcal{P}} \ell(g(x), +1) + \frac{1}{n_u} \sum_{x \in \mathcal{U}} \ell(g(x), -1) - \frac{\pi}{n_p} \sum_{x \in \mathcal{P}} \ell(g(x), -1).$$ (8)

uPU [8] optimizes the above unbiased risk estimator. It is observed to easily overfit when using highly expressive models such as deep neural networks [18]. This is because the difference of the second and third term in the unbiased risk estimator is an estimate of the non-negative loss $\mathbb{E}_{p}(\ell(g(x), -1))$, but it can be negative. To alleviate overfitting, the nnPU estimator thresholds the estimate to ensure that it is non-negative [18]

$$\hat{R}_{nnpu}(g) = \frac{\pi}{n_p} \sum_{x \in \mathcal{P}} \ell(g(x), +1) + \max \left( 0, \frac{1}{n_u} \sum_{x \in \mathcal{U}} \ell(g(x), -1) - \frac{\pi}{n_p} \sum_{x \in \mathcal{P}} \ell(g(x), -1) \right).$$
Algorithm 1 AdaPU

Input $\pi; P; U; T; \beta; K$

Output $F_T(x)$

1: procedure AdaPU
2: $H_0 \leftarrow 0$, and initialize $w^{(1)}$ according to Eq. (11).
3: for $t = 1, \ldots, T$ do
4: \hspace{1em} $h_t, \alpha_t \leftarrow \text{StumpGenerator}(\pi, w^{(t)}, P, U, K)$.
5: \hspace{1em} $H_t \leftarrow H_{t-1} + \beta \alpha_t h_t$.
6: \hspace{1em} $w^{(t+1)}(x, y) \leftarrow w^{(t)}(x, y)e^{-\beta \alpha_t y h_t(x)}$ for each $(x, y)$.
7: end for
8: $F_T(x) \leftarrow \text{sign}(H_T(x))$.
9: end procedure

3 The AdaPU Algorithm

The overall algorithm of AdaPU is shown in Algorithm 1. Similarly to AdaBoost, AdaPU is designed to minimize an empirical exponential loss. AdaPU has an iterative structure similar to AdaBoost too: at each iteration, it learns a weak classifier $h_t$ and its weight $\alpha_t^{PU}$ on a dataset with weights $\{w^{(t)}\}$ using Algorithm 2. We then compute a new aggregate classifier $H_t = H_{t-1} + \beta \alpha_t^{PU} h_t$, where $\beta \in (0, 1)$ acts as a regularization constant. The weights $w^{(t)}$ are then updated to new weights $w^{(t+1)}$.

While AdaPU and AdaBoost share some similarities at a high level, there is a key difference in their empirical exponential losses that results in important algorithmic differences. Specifically, AdaBoost’s loss relies on a fully labeled dataset, while AdaPU’s loss is based on a weighted PN dataset derived from the PU dataset, where the example weights can be negative. This results in major differences in how a weak classifier and its weight are learned in AdaPU and AdaBoost.

Below, we describe the objective function of AdaPU, provide a derivation of a greedy minimization algorithm for learning a weak classifier and its weight, and then explain the complete pseudo-code for a concrete instantiation of the greedy procedure Algorithm 2.

AdaPU’s empirical exponential loss For any classifier $H : \mathbb{R}^d \rightarrow \mathbb{R}$, AdaPU estimates its expected exponential loss $\mathbb{E}(e^{-y H(x)})$ using the uPU estimator:

$$L_{\text{exp}}(H) = \frac{\pi}{n_p} \sum_{x \in P} e^{-H(x)} + \frac{1}{n_u} \sum_{x \in U} e^{H(x)} - \frac{\pi}{n_p} \sum_{x \in P} e^{H(x)} \tag{9}$$

This can be written down as the exponential loss of $H$ on a weighted PN dataset $D$ derived from the PU data:

$$L_{\text{exp}}(H) = \sum_{(x, y) \in D} w^{(1)}(x, y)e^{-y H(x)}, \tag{10}$$
where $\mathcal{D} = \mathcal{P}^+ \cup \mathcal{P}^- \cup \mathcal{U}^-$ is the union of three fully labeled datasets $\mathcal{P}^+ = \{(x, +1) : x \in \mathcal{P}\}$, $\mathcal{P}^- = \{(x, -1) : x \in \mathcal{P}\}$, and $\mathcal{U}^- = \{(x, -1) : x \in \mathcal{U}\}$. The weights $w^{(1)}$ are defined by

$$w^{(1)}(x, y) = \begin{cases} \frac{1}{n_p}, & (x, y) \in \mathcal{P}^+ \\ \frac{1}{n_u}, & (x, y) \in \mathcal{U}^- \\ -\frac{1}{n_p}, & (x, y) \in \mathcal{P}^- . \end{cases}$$

(Note that for $(x, y) \in \mathcal{P}^-$, the weight $w^{(1)}(x, y)$ is negative.)

**Derivation of a greedy minimization algorithm**  
AdaPU uses an iterative greedy algorithm to construct a classifier $H_T(x) = \sum_{t=1}^{T} \alpha_t h_t(x)$, where each $h_t$ is a weak classifier and each $\alpha_t > 0$. It starts with an initial classifier $H_0 = 0$. At iteration $t$, given $H_{t-1}$, AdaPU aims to choose $h_t$ and $\alpha_t$ to further reduce the exponential loss

$$L_t(h, \alpha) = \sum_{(x,y) \in \mathcal{D}} w^{(1)}(x, y) e^{-y[H_{t-1}(x) + \alpha h(x)]} .$$

Let $w^{(t)}(x, y) = w^{(1)}(x, y) e^{-y(h_{t-1}(x))}$, and $Z_t = \sum_{(x,y) \in \mathcal{D}} w^{(t)}(x, y)$ be the total weight. By grouping examples based on whether they are correctly classified by $h$, we can rewrite $L_t(h, \alpha)$ as

$$L_t(h, \alpha) = (Z_t - E_t(h)) e^{-\alpha} + E_t(h) e^{\alpha},$$

where $E_t(h)$ is the total weight of examples misclassified by $h$:

$$E_t(h) = \sum_{(x,y) \in \mathcal{D}, h(x) \neq y} w^{(t)}(x, y).$$

Naively, we can choose $h_t$ and $\alpha_t$ as the minimizers of $L_t(h, \alpha)$, but this can easily lead to overfitting. To see this, first note that if $E_t(h) > 0$ for any $h$, then the minimizer of $L_t(h, \alpha)$ can be found by taking $h$ as the minimizer of $E_t$, and then setting $\alpha = \ln \frac{Z_t - E_t(h)}{E_t(h)}$. However, $E_t(h)$ may be negative, because the weight $w^{(t)}(x, y)$ for $(x, y) \in \mathcal{P}^-$ is negative — in fact, the weight becomes a large negative number if previous weak classifiers correctly classify the positive example $x$ and classify the unlabeled examples as negative. When $E_t(h)$ is negative, the loss takes a minimum value of $-\infty$ when $\alpha = \infty$, and the ensemble is thus dominated by $h$ alone. This easily leads to overfitting as even the best weak classifier may have low accuracy.

We introduced a regularization mechanism motivated by mPU by requiring the estimated error of the weak classifier $h$ on negative examples to be non-negative. Specifically, consider the weighted classification error $e_t(h) = E_t(h)/Z_t$ and $e_t^{\text{nn}}(h) = \sum_{(x,y) \in \mathcal{P}^- \cup \mathcal{U}^-, h(x) \neq y} w^{(t)}(x, y)/Z_t$. We interpret $e_t^{\text{nn}}(h)$ as an estimate for the expected error of $h$ on the negative examples. Then we choose $h_t$ by minimizing $E_t(h)$ under the constraints that $e_t(h) \in [0, 0.5]$ and $e_t^{\text{nn}}(h) \geq 0$. The $\alpha$ value is chosen to minimize $L(h_t, \alpha)$, giving us $\alpha_t = \frac{1}{2} \ln \frac{1 - e_t(h_t)}{e_t(h_t)}$. In summary, we have

$$h_t = \arg \min_{h : e_t(h) \in [0,0.5], e_t^{\text{nn}}(h) \geq 0} E_t(h),$$

$$\alpha_t = \frac{1}{2} \ln \frac{1 - e_t(h_t)}{e_t(h_t)} .$$


The condition \( e_t(h) \in [0, 0.5] \) can be interpreted as requiring \( h \) to be better than random guessing, and it ensures that the weight \( \alpha_t \) is positive. The condition \( e_t^{nn}(h) > 0 \) rules out classifiers with a negative estimate for the expected error on the negative examples. Note that \( Z_t \) may be less than or equal to 0. We stop adding weak classifiers whenever this happens.

We note that in PU learning, we often have a lot of unlabeled examples, and thus a large part of the weighted error \( e_t(h) \) is contributed by the unlabeled examples. The error \( e_t(h) \) can be relatively small when most of the unlabeled examples are classified as negative, but a small fraction of the positive examples are classified as positive. However, since the positive examples are indeed positive, while the unlabeled examples may be either positive or negative, it is more important to correctly classify the positive examples as positive. We thus introduce an error measure \( e_t(h) \) that better balance the influence of the positive examples and the unlabeled examples, as compared to \( e_t(h) \). Specifically, for any subset \( S \) of \( D \), let \( w^{(t)}(S) = \sum_{(x,y) \in S} w^{(t)}(x,y) \), and \( \epsilon_t(h; S) = \frac{1}{w^{(t)}(S)} \sum_{(x,y) \in S} w^{(t)}(x,y) \Pi(h(x) \neq y) \). We define \( \epsilon_t(h) \) by

\[
\epsilon_t(h) = \pi \epsilon_t(h; P^+) + \epsilon_t(h; U^-) - \pi \epsilon_t(h; P^-).
\]

The form is inspired by the uPU estimator for expected zero-one loss, which is

\[
L_{01}(h) = \pi \sum_{x \in P} \frac{\Pi(h(x) \neq +1)}{n_p} + \sum_{x \in U} \frac{\Pi(h(x) \neq -1)}{n_u} - \pi \sum_{x \in P} \frac{\Pi(h(x) \neq -1)}{n_p}
\]

Finally, we choose the weak classifier \( h_t \) and its weight \( \alpha_t \) by

\[
h_t = \arg\min_{h_{x,t}(h) \in [0,0.5], \epsilon_t^{nn}(h) \geq 0} E_t(h), \tag{16}
\]

\[
\alpha_t = \frac{1}{2} \ln \frac{1 - \epsilon_t(h_t)}{\epsilon_t(h_t)}.
\tag{17}
\]

where \( \epsilon_t^{nn} = \epsilon_t(h; U^-) - \pi \epsilon_t(h; P^-) \) is the counterpart of \( \epsilon_t^{nn} \).

We also implement an additional regularization mechanism by adding \( \beta \alpha_t h_t \) to \( H_{t-1} \) for some \( \beta \in [0,1] \), instead of adding \( \alpha_t h_t \) to \( H_{t-1} \). This is motivated by the regularization mechanism in [23], which is implemented in scikit-learn.

We provide a comparison between the updates in Eqs. (14) and (15) (which are said to use over-all normalization) and the updates in Eqs. (16) and (17) (which are said to use per-group normalization), in Section 4.4. Both variants have similar performance with a large number of weak classifiers, but per-group normalization seems to learn faster at the beginning. This suggests that balancing the contribution of the errors from \( P^+, P^- \) and \( U^- \) is helpful.

**An instantiation of the greedy minimization algorithm** We show how the greedy minimization approach discussed above can be instantiated when the weak classifiers are decision stumps. Decision stumps allow an efficient algorithm for the optimization problem in Eq. (16), yet shows strong empirical performance in our experiments. Our algorithm is shown in Algorithm 2. For computational efficiency, we do not consider all possible thresholds for all the features for the decision stumps considered. Instead, for each feature, we consider \( K \) random thresholds sampled in an interval that is slightly larger than the feature’s value range — note that a larger range is chosen to allow decision stumps that classify all examples as positive/negative. We then find \( h_t \) by considering only these candidate decision stumps. If
Algorithm 2 AdaPU StumpGenerator

\textbf{Input} $\pi; \ w^{(t)}; \mathcal{P}; \mathcal{U}; K$
\textbf{Output} $h_t, \alpha_t$

1: \textbf{procedure} StumpGenerator
2: \hskip 1em $E_{\text{min}} \leftarrow \infty; \ \epsilon_{\text{min}} \leftarrow 1/2; \ h_t \leftarrow 0$
3: \textbf{for} each feature $f$ \textbf{do}
4: \hskip 1em $n_f \leftarrow$ the number of $f$'s unique values.
5: \hskip 1em $v_r \leftarrow v_{\text{max}} - v_{\text{min}}, \text{where } [v_{\text{min}}, v_{\text{max}}] \text{ is } f$'s range.
6: \textbf{for} $k = 1, \ldots, K$ \textbf{do}
7: \hskip 1em $v \leftarrow$ a random value in $[v_{\text{min}} - \frac{v_r}{(n_f-1)}, v_{\text{min}} + \frac{v_r}{n_f-1}]$.
8: \hskip 1em $h_L, h_R \leftarrow$ the two decision stumps splitting $f$ with threshold $v$.
9: \textbf{for} $h$ in $[h_L, h_R]$ \textbf{do}
10: \hskip 1em if $\epsilon_t(h) \in [0, 0.5)$ and $\epsilon_t^{mn}(h) \geq 0$ and $E_t(h) < E_{\text{min}}$ then
11: \hskip 2em $E_{\text{min}} \leftarrow E_t; \ h_t \leftarrow h; \ \epsilon_{\text{min}} \leftarrow \epsilon_t$
12: \hskip 1em end if
13: \textbf{end for}
14: \textbf{end for}
15: \textbf{end for}
16: \alpha_t = 1/2 \ln[(1 - \epsilon_{\text{min}})/\epsilon_{\text{min}}]
17: \textbf{end procedure}

all the candidate decision stumps do not satisfy the conditions $\epsilon_t(h) \in [0, 0.5)$ and $\epsilon_t^{mn}(h) \geq 0$, then $h_t = 0$ with $\alpha_t = 0$, thus $H_t$ is the same as $H_{t-1}$. Interestingly, this did not happen in our experiments.

4 Experiments

We perform experiments to compare AdaPU with (i) NN-based PU methods, and (ii) fully supervised boosting models. We also perform experiments to study how the performance of AdaPU is affected by the value of the regularization constant $\beta$, different feature threshold sampling methods and different normalization methods.

4.1 Datasets

We used PU datasets and PN datasets derived from the following four datasets.

- Epsilon\footnote{https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/binary.html}: a binary classification text dataset with 400,000 training and 100,000 test examples, each with 2,000 features. We use $n = 40,000$ training examples from the original dataset. $\pi_p = 0.5$.

- Breast Cancer\footnote{https://goo.gl/U2Uwz2}: a binary classification dataset with $n = 455$ training and 114 test examples. Each example has 30 features. $\pi_p = 0.59$.
• UNSW-NB15\textsuperscript{4}: a binary classification dataset with \( n = 175,340 \) training and 82,331 test examples. Each example has 39 features. \( \pi_p = 0.68 \).

• CIFAR-10\textsuperscript{5}: a multi-class dataset with \( n = 50,000 \) training and 10,000 test images. The input for NN-based methods (i.e., uPU and nnPU methods) are the images, and the input for non NN-based methods (i.e., AdaPU and PN boosting methods) are the 3,072 features provided by a pretrained all convolutional net [27]. To make it binary, we follow [18] treating classes ‘airplane’, ‘automobile’, ‘ship’ and ‘truck’ as the positive class. \( \pi_p = 0.4 \).

We follow [18] to generate the PU and PN data for our experiments below. To generate the PU data, we randomly sample \( n_p = 1000 \) positive examples, and use all training examples as unlabeled examples (i.e., we have \( n_u = n \) unlabeled examples). To generate the PN data, we randomly sample \( n_p = 1000 \) positive examples and \( n_n = (\pi_n/2\pi_p)^2n_p \) negative examples. A strong PU learning algorithm trained on the PU data with a large \( n_n \) is expected to perform competitively with a PN algorithm trained on such PN data [26]. The \( n_n \) values are 256, 55, and 562 respectively for Epsilon, UNSW-NB15 and CIFAR-10; we used \( n_p = 10 \) and \( n_n = 1 \) for the BreastCancer dataset as it only has 455 training examples.

4.2 Experimental settings

We run each algorithm five times with different random seeds, and report the means and standard deviations (std) of the performance metrics used.

AdaPU We sampled \( K = 10 \) candidate feature thresholds for each feature. The regularization constant \( \beta \) is an important parameter that needs to be tuned, as demonstrated in Section 4.4. We used 5-fold cross-validation to choose the best \( \beta \) value from The selected \( \beta \) values are as follows: \( \beta = 0.2 \) for Epsilon, \( \beta = 0.1 \) for UNSW-NB15, \( \beta = 0.001 \) for BreastCancer, and \( \beta = 0.2 \) for CIFAR-10.

PU methods We compared AdaPU with neural network based methods uPU [8] and nnPU [18]. For Epsilon, BreastCancer and UNSW-NB15, we follow [18] to use multilayer perceptron (MLP), where Epsilon uses Softsign [13] activations and the other two datasets use ReLU [25] activations. For CIFAR-10, we used Residual Network (ResNet) [15] and all convolutional net [27] (CNN) with ReLU [25] activations. All neural networks are trained using Adam [17] for 100 epochs to ensure convergence.

Note that we tune the hyperparameters, including the number of layers for MLP and ResNet, based on the test performance of nnPU and uPU. Specifically, for MLP, the number of hidden layers is chosen from \{1, 3, 6, 7, 9\}. For ResNet, we consider variants with 18, 32, 56, and 110 layers. For CNN, we used the same architecture as in [18]. For each MLP and ResNet architecture, we tune the hyperparameters learning rate from \{10^{-2}, 10^{-3}, 10^{-4}\} and weight decay from \{5 \times 10^{-8}, 5 \times 10^{-9}\} and then select the best-performed hyperparameters under that architecture. The architectures of nnPU with the best test accuracies are selected: ResNet 18 for CIFAR-10, 3-hidden-layer MLP for both Epsilon and BreastCancer, and 9-hidden-layer MLP for UNSW-NB15. While the architectures of uPU with the best test accuracies are: ResNet 110 for CIFAR-10, 3-hidden-layer MLP for BreastCancer, and 9-hidden-layer MLP

\textsuperscript{4}https://research.unsw.edu.au/projects/unsw-nb15-dataset
\textsuperscript{5}https://www.cs.toronto.edu/~kriz/cifar.html
Table 1: The best model architectures, weight decay, and learning rates for each dataset after hyperparameter tuning and architecture selection for both nnPU and uPU.

| Dataset     | Model Architecture | Weight Decay | Learning Rate |
|-------------|--------------------|--------------|---------------|
| **nnPU**    |                    |              |               |
| CIFAR-10    | ResNet 18          | $5 \times 10^{-8}$ | $1 \times 10^{-4}$ |
| Epsilon     | 3-hidden-layer MLP  | $5 \times 10^{-8}$ | $1 \times 10^{-3}$ |
| UNSW-NB15   | 9-hidden-layer MLP  | $5 \times 10^{-8}$ | $1 \times 10^{-2}$ |
| BreastCancer| 3-hidden-layer MLP  | $5 \times 10^{-8}$ | $1 \times 10^{-3}$ |
| **uPU**     |                    |              |               |
| CIFAR-10    | ResNet 110         | $5 \times 10^{-8}$ | $1 \times 10^{-3}$ |
| Epsilon     | 9-hidden-layer MLP  | $5 \times 10^{-9}$ | $1 \times 10^{-2}$ |
| UNSW-NB15   | 9-hidden-layer MLP  | $5 \times 10^{-8}$ | $1 \times 10^{-2}$ |
| BreastCancer| 3-hidden-layer MLP  | $5 \times 10^{-8}$ | $1 \times 10^{-4}$ |

Table 2: Accuracy in the form of the mean (std) for all compared methods.

| Method | CIFAR-10 % | Epsilon % | UNSW-NB15 % | BreastCancer % |
|--------|------------|-----------|-------------|----------------|
| **PU** |            |           |             |                |
| nnPU   | **87.17 (1.14)** | 70.38 (1.92) | 74.61 (0.26) | 90.35 (8.48)   |
| uPU    | 82.97 (4.42) | 61.53 (2.20) | 74.54 (0.49) | 76.84 (10.22)  |
| **PN** |            |           |             |                |
| XGBoost| 85.29 (0.57) | 63.78 (0.58) | **77.46 (0.60)** | 77.19 (0.00)   |
| GBDT   | 86.46 (0.36) | 58.71 (1.58) | 76.59 (1.26) | 90.70 (2.82)   |
| AdaBoost| 86.10 (0.54) | 63.83 (1.13) | 77.13 (0.36) | 75.96 (10.32)  |
| **AdaPU** |            |           |             |                |
| Over-ALL| 84.83 (0.13) | 71.60 (1.08) | 76.60 (0.0)  | **93.86 (1.64)** |
| PER-GROUP| 85.77 (0.08) | **72.01 (0.91)** | 76.60 (0.0)  | 92.28 (2.09)   |

for both UNSW-NB15 and Epsilon. The selected model architectures and its corresponding hyperparameters are shown in Table 1. Note that the test accuracies of these architectures are the same or better than architectures chosen using any model selection method, thus the results reported below for nnPU and uPU are optimistic estimates on their generalization performances.

**PN methods** We compare our proposed AdaPU with XGBoost [1], AdaBoost [31] and GBDT [12] implemented in scikit-learn using default parameters. The number of iterations is set as 100, which is the same as the number of epochs in neural networks.

### 4.3 Results

**Comparison with NN-based PU methods** The results of AdaPU and NN-based PU learning methods are shown in Fig. 1 and Table 2. AdaPU outperforms nnPU, and uPU on Epsilon, UNSW-NB15, and BreastCancer. AdaPU performs similarly as nnPU on CIFAR-10. In particular, AdaPU clearly outperformed all NN-based PU learning methods on tabular data.

**Comparison with PN boosting methods** The results of AdaPU and PN boosting methods are shown in Fig. 2 and Table 2. AdaPU performs better on Epsilon and BreastCancer, and is comparable to PN boosting methods on CIFAR-10 and UNSW-NB15. This is consistent with the theoretical and experimental results in [26], which demonstrates that having a large amount of unlabeled data may be better than having a small amount of negative data.
Figure 1: Training zero-one loss and test zero-one loss of AdaPU and NN-based methods, on CIFAR-10, Epsilon, UNSW-NB15, and BreastCancer. The lines and shaded areas show the averages and standard deviations for 5 trials.

4.4 Additional experiments on AdaPU

**Effects of feature threshold selection strategy.** Algorithm 2 uses randomly sampled feature thresholds. A natural alternative is to sample evenly spaced threshold values. Fig. 3 compares these two different threshold selection strategies on CIFAR-10 and Epsilon. The random strategy leads to improved accuracies. To understand how the different threshold selection strategies affect the performance of AdaPU, we plotted the number of times that a feature is used as a splitting feature in the trees, for both datasets. We can see that with randomly sampled thresholds, the number of times that features are selected are more uniform, while with fixed thresholds, some features are selected much more frequently as compared to other features. This suggests that spikes in feature frequencies may be related to overfitting and poorer generalization.

**Effects of $\beta$.** We explore how the $\beta$ affects the performance of AdaPU. We evaluate the performance of AdaPU with $\beta \in \{0.0001, 0.001, 0.01, 0.1, 0.2, 0.5, 0.7, 0.9, 1.0\}$ in the experiment. Fig. 4 summarizes the comparison results of AdaPU with different $\beta$ on CIFAR-10, Epsilon, UNSW-NB15 and BreastCancer. The results show that AdaPU has a better performance with a suitable $\beta$.

**Effects of normalization method.** As mentioned in Section 3, we experimented with two different ways of estimating a weak classifier $h$’s performance: one with over-all normalization (i.e., using $e_t(h)$ to measure $h$’s classification error), the other with per-group normalization (i.e., using $\epsilon_t(h)$ to measure $h$’s classification error). We also used 5-fold cross-validation to select the $\beta$ values of AdaPU with over-all normalization. The selected $\beta$ values are as follows:
Figure 2: Test accuracy of AdaPU and PN boosting methods, on CIFAR-10, Epsilon, UNSW-NB15, and BreastCancer. The lines and shaded areas show the averages and standard deviations for 5 trials.

\( \beta = 0.1 \) for Epsilon, \( \beta = 0.01 \) for UNSW-NB15, \( \beta = 0.0001 \) for BreastCancer, and \( \beta = 0.01 \) for CIFAR-10. Fig. 5 shows that per-group normalization tends to have a faster convergence rate in general. However, the final performance of both methods after training 100 weak classifiers are comparable, as shown in Table 2. We further plotted the percentages of positives classified as positive and the percentages of unlabeled classified as negative, as we add more classifiers, in Fig. 6. We can see that with per-group normalization, AdaPU tends to be more accurate in classifying positive examples, particularly for CIFAR-10 and Epsilon. At the same time, per-group normalization seems to have a mixed effect on AdaPU’s tendency’s to classify unlabeled examples as negative. Overall, higher accuracy in classifying positive examples seem to be associated with faster learning, as seen on CIFAR-10 and Epsilon. Given the same accuracy on positive examples, a method which is less aggressive in trying to classify unlabeled examples seem to perform better, as seen on BreastCancer. This is likely a desirable behavior as discussed in Section 3, because unlabeled examples can be either positive or negative.

5 Conclusion

We proposed a novel boosting PU learning method AdaPU in this paper. AdaPU shares some similarities with AdaBoost at a high level but significantly differs from AdaBoost in how weak classifiers and their weights are learned. For computational efficiency, we focused on using decision stumps as the weak classifiers. The results show that AdaPU has strong performance on tabular data, even with very simple weak classifiers. It will be interesting to investigate the use of more complex weak classifiers in AdaPU.
Figure 3: The test accuracies of AdaPU under different feature value selection strategies. The lines and shaded areas show the averages and standard deviations for 5 trials. The bar charts show the number of times features are used as splitting features in the trees in one trial.

Figure 4: Test accuracies of AdaPU for $\beta \in \{0.0001, 0.001, 0.01, 0.1, 0.2, 0.5, 0.7, 0.9, 1.0\}$ on CIFAR-10, Epsilon, UNSW-NB15 and BreastCancer. The lines and shaded areas show the averages and standard deviations for 5 trials.
Figure 5: Comparison of the test accuracies for the per-group normalization variant and the over-all normalization variant of Algorithm 2. Per-group normalization is better than over-all normalization.

Figure 6: Comparison of training set predictions on the positive and unlabeled examples for the per-group normalization variant and the over-all normalization variant of Algorithm 2. The per-group normalization variant has a higher accuracy on positive examples in general.
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