Hellinger Distance Decision Trees for PU Learning in Imbalanced Data Sets

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Abstract

Learning from positive and unlabeled data, or PU learning, is the setting in which a binary classifier can only train from positive and unlabeled instances, the latter containing both positive as well as negative instances. Many PU applications, e.g., fraud detection, are also characterized by class imbalance, which creates a challenging setting. Not only are fewer minority class examples compared to the case where all labels are known, there is also only a small fraction of unlabeled observations that would actually be positive. Despite the relevance of the topic, only a few studies have considered a class imbalance setting in PU learning. In this paper, we propose a novel technique that can directly handle imbalanced PU data, named the PU Hellinger Decision Tree (PU-HDT). Our technique exploits the class prior to estimate the counts of positives and negatives in every node in the tree. Moreover, the Hellinger distance is used instead of more conventional splitting criteria because it has been shown to be class-imbalance insensitive. This simple yet effective adaptation allows PU-HDT to perform well in highly imbalanced PU data sets. We also introduce PU Stratified Hellinger Random Forest (PU-SHRF), which uses PU-HDT as its base learner and integrates a stratified bootstrap sampling. Our empirical analysis shows that PU-SHRF substantially outperforms state-of-the-art PU learning methods for imbalanced data sets in most experimental settings.

Keywords: PU Learning, Weakly Supervised Learning, Imbalanced Classification, Ensemble Learning

1 Introduction

Despite the ubiquity of supervised learning in practice, many real-world applications, including fraud detection (Li, Chen, Liu, Wei, & Shao, 2014; Stripling, Baesens, Chizi, & vanden Broucke, 2018), text classification (Liu, Lee, Yu, & Li, 2002; Yarowsky, 1995), and medical diagnosis (Chen et al., 2020; Claesen, De Smet, Suykens, & De Moor, 2015), suffer from inaccurate or incomplete label information. Moreover, these applications are often also characterized by high class imbalance. For example, in credit card fraud detection, fraudulent transactions represent less than one percent of the total transactions (Van Belle, Van Damme, Tytgat, & De Weerdt, 2022). These applications relate to two areas of research: positive and unlabeled (PU) learning and imbalanced learning. PU learning assumes that labeled examples are positive, but the unlabeled examples can belong to either the positive or negative class. Imbalanced learning aims to propose methods that handle settings in which the class distribution is significantly unequal. Accordingly, in this paper, we focus on the problem of learning from imbalanced data sets in which the negative class and a proportion of positives remain unlabeled.

PU learning has increasingly gained popularity in recent years, as demonstrated by the uptake in method development (Bekker & Davis, 2020). One approach that was first used in text classification identifies reliable negatives and learns from positives and the resulting reliable negatives (Liu et al., 2002; Yarowsky, 1995). Another approach assumes that all unlabeled examples are negative and applies standard classifiers (Lee & Liu, 2003; Mordelet & Vert, 2014). A last approach, with more recent developments, utilizes the class prior (i.e., positive class ratio) in existing algorithms to enable PU learning (Denis, Gilleron, & Letouzey, 2005; Du Plessis, Niu, & Sugiyama, 2015; Elkan & Noto, 2008; Kiryo, Niu, Plessis, & Sugiyama, 2017; Li et al., 2014). Other works have explored non-standard settings in PU learning motivated by domain applications. For example, a common assumption in PU learning is that the labeled examples are a random subset of the positive examples; however, this assumption is often violated in practice (Bekker, Robberechts, & Davis, 2019; He, Liu, Webb, & Tao, 2018).

Although most modern PU methods perform successfully in several benchmark data sets (Chen et al., 2020; Du Plessis et al., 2015; Kiryo et al., 2017), it remains unclear how well they perform in highly imbalanced data sets. Imbalanced PU classification poses new challenges that have not been sufficiently addressed. In this specific setting, the fact that only a few positive instances are known to the learner creates more severe class imbalance. A suitable PU method for an imbalanced setting should be able to exploit the small number of labeled positives and still learn from unlabeled instances. Only a few works have focused on imbalanced PU classification. Two works have proposed PU learning via optimizing an adaptation of the area under the receiver operating characteristic curve (AUC-ROC) for the semisupervised setting (Sakai, Niu, & Sugiyama, 2018; Xie & Li, 2018). However, optimizing the AUC-ROC does not guarantee optimization of more relevant metrics for imbalanced classification, such as the area under the precision-recall curve (Davis & Goadrich, 2006). A second approach, Cost-Sensitive Positive and Unlabeled learning (CSPU) (Chen, Gong, & Yang, 2021), introduces the use of misclassification costs to address class imbalance. While being conceptually appealing, CSPU's requirement to have misclassification costs available is not easily met given that in several domains these costs are difficult to determine. Lastly, the imbalanced nonnegative PU learning method relies on oversampling to balance the PU data (Su, Chen, & Xu, 2021). Nonetheless, oversampling might cause unnecessary overfitting, and the oversampling rate might need to be tuned as an extra hyper-parameter. Accordingly, we observe a gap in the literature for a technique that can perform well in highly imbalanced PU data without requiring resampling or misclassification costs.

Therefore, in this work, we introduce a novel tree-based technique that is designed to learn from imbalanced PU data, denoted as the PU Hellinger Decision Tree (PU-HDT). PU-HDT does not need to modify the imbalanced data distribution. Similar to other class-prior-based methods (Du Plessis et al., 2015; Kiryo et al., 2017; Su et al., 2021), PU-HDT exploits the class prior (i.e., the proportion of positive examples) to enable PU learning. At each node, the true positives are estimated from unlabeled instances rather than assuming that all unlabeled instances are negatives. Instead of using a traditional splitting criterion exhibiting demonstrated inferiority towards imbalanced data sets (e.g., Gini and entropy), PU-HDT uses the Hellinger distance (Cieslak & Chawla, 2008). The Hellinger distance has shown robustness to extreme degrees of class imbalance in previous studies (Cieslak, Hoens, Chawla, & Kegelmeyer, 2012; Dal Pozzolo et al., 2014; Lyon, Brooke, Knowles, & Stappers, 2014). These two improvements enable PU-HDT to handle highly imbalanced data sets effectively. The performance of PU-HDT can be further improved using an ensemble. We show that a modified random forest with PU-HDT as its base learner outperforms state-of-the-art PU learning methods under different experimental settings with class imbalance.

The remainder of this paper is organized as follows: Sect. 2 discusses different methods found in the imbalanced learning and PU learning literature. Section 3 introduces the PU-HDT algorithm and explains its inner working. Additionally, an ensemble method that uses PU-HDT as the base learner is presented. Section 4 describes the experimental setup, and Sect. 5 discusses the results. Section 6 provides general conclusions and implications based on the empirical analysis. Finally, we outline some possibilities for further research.

2 Related Work

In this section, we provide an overview of related work in the imbalanced and PU learning domains.

2.1 Imbalanced Learning

In numerous domain applications of binary classification, including medical diagnosis, churn prediction and fraud detection, the class of interest (i.e., minority class) is particularly rare. This constitutes a challenge for standard classifiers as most conventional algorithms are biased towards the majority class. Specifically, minority class examples are misclassified more often when compared to those from the majority class. Thus, several techniques have been proposed to address class imbalance. These methods can be divided into four main categories (Fernández et al., 2018): data-level methods, algorithm-level methods, cost-sensitive learning, and ensemble-based approaches, with the latter two being more sophisticated.

Data-level methods balance the class distribution by relying on a resampling strategy. An advantage of resampling is that the end-user can choose a standard classifier of preference. However, data-level approaches are sensitive to the specific settings: in the presence of outliers, sampling methods excessively distort the data distribution, which results in worse performance (Baesens, Höppner, Ortner, & Verdonck, 2021). A popular data-level method is the Synthetic Minority Oversampling Technique (SMOTE) (Chawla, Bowyer, Hall, & Kegelmeyer, 2002). SMOTE creates new minority instances close to other minority examples via interpolation. However, SMOTE resamples the minority class without considering the density of the data, which can create further overlap between classes. Consequently, several works have proposed extensions of SMOTE that aim to overcome this problem: some well-known extensions include MWMOTE (Barua, Islam, Yao, & Murase, 2012), Borderline-SMOTE (Han, Wang, & Mao, 2005), and Adaptive Synthetic Sampling (ADASYN) (He, Bai, Garcia, & Li, 2008). ADASYN adaptively generates new minority instances according to the class distribution and creates more minority examples when few minority are present in the neighborhood. In this paper, we consider ADASYN as the default data-level solution for class imbalance.

Algorithm-level methods modify existing classifiers to improve the predictive performance on the minority class. Several algorithm-level methods have been proposed based on popular classifiers, including support vector machines (SVM) (Gonzalez-Abril, Nunez, Angulo, & Velasco, 2014), nearest-neighbor methods (Cano, Zafra, & Ventura, 2013; Liu & Chawla, 2011), and decision trees (Cieslak & Chawla, 2008; Liu, Chawla, Cieslak, & Chawla, 2010; Sardari, Eftekhari, & Afsari, 2017). In this work, we extend algorithmic methods based on decision trees. In particular, we focus on the splitting criterion, which is the main element that can be improved for the imbalanced setting. Decision trees such as C4.5 (Quinlan, 1993) and CART (Breiman, Friedman, Stone, & Olshen,

1984) utilize splitting functions that are sensitive to highly skewed distributions as both Information Gain and Gini Index are biased towards the majority class. Hellinger Decision Tree (HDT) (Cieslak & Chawla, 2008) and Class Confidence Proportion Decision Tree (Liu et al., 2010) rely on skew-insensitive splitting functions. For instance, HDT has been shown experimentally to outperform other decision trees such as C4.5 (Quinlan, 1993) and CART (Breiman et al., 1984). Other works have used cost-sensitive learning to adapt the splitting criterion (Bahnsen, Aouada, & Ottersten, 2015; Vadera, 2010). Moreover, decision tree methods have been used in an ensemble setup (Chen, Liaw, Breiman, et al., 2004; Cieslak et al., 2012; O'Brien & Ishwaran, 2019; Zelenkov, 2019).

Among the algorithm-level methods previously presented, HDT is one of the most popular in the literature. Motivated by HDT, several extensions have been proposed to handle different tasks under class imbalance: data streams (Grzyb, Klikowski, & Woźniak, 2021; Lyon et al., 2014), multilabel classification (Daniels & Metaxas, 2017), and multiclass classification (Hoens, Qian, Chawla, & Zhou, 2012). Other works have used the Hellinger distance to propose their own methods that aim to outperform the HDT (Akash, Kadir, Ali, & Shoyaib, 2019; Su & Cao, 2019). Despite the popularity of HDT in other domains, it is not yet explored in weakly supervised learning. In this paper, we focus on a special case of weakly supervised learning: PU learning. Our technique represents an extension of HDT that can effectively handle PU data in the imbalanced setting.

2.2 PU Learning

PU learning is a setting related to weakly supervised learning (Zhou, 2018), in which only positive and unlabeled examples exist. Different assumptions can be made regarding the observation of labeled positive examples or the underlying labeling mechanism. Most PU learning methods are built on the selected completely at random (SCAR) assumption. The SCAR assumption states that the positively labeled examples are a randomly selected subset of the set of positives. SCAR implies that supervised techniques can be used for PU learning because the ranking order of predictions is preserved as if the true label was known (Elkan & Noto, 2008). Selected at random (SAR) (Bekker et al., 2019) is a more realistic assumption regarding the labeling mechanism. For SAR, the probability of a positive observation being labeled depends on its features or attributes. The latter assumption is much more sensible for common PU learning applications, including recommendation systems, medical diagnosis, and fraud detection. One specific type of SAR is the probabilistic gap (PG), which assumes that the positive examples that more closely resemble negatives are less likely to be labeled (He et al., 2018). For instance, a fraudster is more likely to go unnoticed if their behavior mimics a normal profile.

PU learning methods can be divided into three categories: two-step techniques, biased learning, and class-prior-based methods (Bekker & Davis, 2020). Two-step techniques first identify the instances that are most likely to be negatives among the unlabeled; then, a model learns from the newly labeled negative and positive examples. A semisupervised technique can also be used to exploit the remaining unlabeled data (Liu, Dai, Li, Lee, & Yu, 2003). Early two-step techniques come from the text classification literature (Li & Liu, 2003; Liu et al., 2002; Yu & Li, 2007), in which models such as Naïve Bayes (NB) and SVM are often used. For instance, S-EM (Liu et al., 2002) first introduces labeled instances as "spies" to identify unreliable negatives and then applies semi-supervised NB to predict the labels of the unreliable negatives. A two-step approach works well as long as separability exists between the negative and positive classes (Bekker & Davis, 2020). Biased learning techniques consider unlabeled instances as negatives with label noise (Claesen et al., 2015; Lee & Liu, 2003; Mordelet & Vert, 2014). Most biased learning techniques place a high misclassification cost on false positives by either introducing asymmetric penalization (Liu et al., 2003) or by using bagging (Claesen et al., 2015; Mordelet & Vert, 2014). For instance, PU Bagging selects all labeled examples and takes bootstrap samples of the unlabeled examples. One advantage of PU Bagging is that it enables the user to choose any base learner: SVM is used in (Mordelet & Vert, 2014) but other models such as a decision tree can be selected as well. The class-prior-based methods utilize the class prior information to either preprocess the data or modify the algorithm (Bekker et al., 2019; Du Plessis et al., 2015; Elkan & Noto, 2008; Plessis, Niu, & Sugiyama, 2017). Among them, some techniques are based on the empirical minimization framework, which modifies the loss function to incorporate the class prior. Accordingly, well-known algorithms have been adapted for PU learning, e.g., logistic regression (Bekker et al., 2019; Du Plessis et al., 2015) and neural networks (Kiryo et al., 2017), which can be considered the state-of-the-art in the field.

Although the PU learning literature has developed a plethora of methods, most of the works have focused on a balanced setting. Likewise, no study has focused on the evaluation of well-known PU learning methods in highly imbalanced settings. Compared to imbalanced classification with complete label information, PU classification under class imbalance suffers from severe underrepresentation of the positive class. In such a scenario, the bias towards the majority class worsens for most of PU methods. A few studies have proposed methods to handle class imbalance. These PU methods for imbalanced setting have used cost-sensitive learning (Chen et al., 2021), algorithm-level approaches (Sakai et al., 2018; Xie & Li, 2018), and data-level approaches (Su et al., 2021). Motivated by previous work on the adaption to PU learning of the risk minimization framework (Du Plessis et al., 2015; Kiryo et al., 2017), CSPU introduces class-dependent costs to improve the performance of PU classification under class imbalance. However, this particular setting requires complete information of the misclassification costs, which might not be available; in some applications, such as credit scoring or fraud detection, the misclassification costs are better represented at the instance level (Bahnsen et al., 2015; Zelenkov, 2019). Based on the semisupervised learning literature, the risk minimization framework can be adapted to optimize a semisupervised variant of the AUC-ROC (Sakai et al., 2018; Xie & Li, 2018). Nevertheless, optimizing the AUC-ROC does not automatically lead to an optimization of relevant metrics for the imbalanced setting, such as the F-score (Chen et al., 2021) and the area under the precision-recall curve (Davis & Goadrich, 2006). Unlike the CSPU, imbalanced nonnegative PU learning (imbalanced nnPU) (Su et al., 2021) does not require misclassification information as it relies on oversampling to balance the class distribution. Oversampling, however, might create harmful overfitting because it creates exact copies of the positive labeled instances (Fernández et al., 2018): in order to avoid overfitting, the oversampling rate can be tuned as an additional hyperparameter. Our work contributes to the literature by introducing a Decision Tree technique that can natively handle imbalanced data without requiring complete information of misclassification costs or a resampling method. To the best of our knowledge, this is the first work that integrates the effectiveness of Hellinger Decision Trees for imbalanced classification into PU learning.

3 PU Hellinger Decision Tree (PU-HDT)

In this section, we introduce PU-HDT. Moreover, we illustrate its workings on a half-moons data set and expand the technique towards a PU Stratified Hellinger Random Forest.

3.1 The PU-HDT Algorithm

The Hellinger Decision Tree (HDT) exploits the Hellinger distance to improve the splitting mechanism in imbalanced settings. The goal of the Hellinger distance is to capture the divergence between the positive and negative class distribution without being dominated by the class imbalance. Equation (1) further illustrates the robustness to class imbalance. The Hellinger distance can be calculated in a parent node i as follows:

$$HD_i = \sqrt{\left(\sqrt{\frac{N_{left_i}}{N_i}} - \sqrt{\frac{P_{left_i}}{P_i}}\right)^2 + \left(\sqrt{\frac{N_{right_i}}{N_i}} - \sqrt{\frac{P_{right_i}}{P_i}}\right)^2}, \qquad (1)$$

where N_i and P_i are the counts of negatives and positives in the parent node i, N_{left_i} and P_{left_i} are the counts of the examples that fall into the left child node, and N_{right_i} and P_{right_i} the ones that fall into the right child node. Thus, there is no influence of the proportion of the majority class. In comparison, the Gini Index, as used in, e.g., CART, depends on p_j, the proportion of class j: $I_G = 1 - \sum_{j=1}^{2} p_j^2$. With the Hellinger distance, the HDT can create better splits during tree construction in imbalanced data sets; however, HDT is not directly applicable to PU data sets.

Therefore, we adapt the HDT (Cieslak & Chawla, 2008) to PU learning by exploiting the class prior, represented as α. Under the SCAR assumption, the class prior enables estimation of the label frequency c, the proportion of positive examples that are labeled in the data. Equation (2) illustrates the previous statement:

$$\begin{aligned} Pr(l=1) &= Pr(l=1 \mid y=1)Pr(y=1) + Pr(l=1 \mid y=0)Pr(y=0) \\ &= Pr(l=1 \mid y=1)Pr(y=1) \\ &= c\,\alpha, \end{aligned} \tag{2}$$

where l is the observed labeled and y is the true label. The proportion of labeled positives $Pr(l=1)$ can easily be estimated from the training data. In the PU setting, only the labeled instances can belong to the positive class, which implies that the conditional probability $Pr(l=1 \mid y=0)=0$. The label frequency c enables estimation of the counts of positives and negatives from PU data. In a given node i, the estimated count of positives $\hat{P}_i$ can be calculated as follows:

$$\begin{aligned} \hat{P}_i &= \min\left\{\frac{L_i}{c}, T_i\right\} \\ \hat{P}_i &= \min\left\{L_i \frac{\alpha}{Pr(l=1)}, T_i\right\}, \end{aligned} \tag{3}$$

where L_i is the count of labeled positives and T_i is the count of total instances in node i. Equation (3) indicates that, in a given node, the number of positives cannot exceed the total number of examples. The estimated count of negatives $\hat{N}_i$ can be computed from the difference between the total count of instances and the number of positives: $\hat{N}_i = T_i - \hat{P}_i$. This estimation is similar to the one found in POSC4.5 (Denis et al., 2005), but it is used to modify entropy as the splitting criterion. Moreover, Eq. (3) emphasizes the importance of the class prior for adapting the HDT to PU learning: this means that PU-HDT falls into the category of class-prior-based methods. Despite the relevance of the class prior in PU-HDT, it is often unavailable in PU learning, so we require domain knowledge or methods for class prior estimation (Bekker & Davis, 2018; Du Plessis & Sugiyama, 2014; Elkan & Noto, 2008; Plessis et al., 2017; Ramaswamy, Scott, & Tewari, 2016). Figure 1 illustrates the difference between Gini Index and Hellinger Distance in node splitting. The left tree is split according to the Gini Index whereas the right tree follows the Hellinger distance with the PU adaptation.

Algorithm 1 outlines how a PU-HDT is built based on the Hellinger Distance with the estimated counts of positive and negative instances. PU-HDT follows the same binary tree construction as other decision trees, such as CART (Breiman et al., 1984), C4.5 (Quinlan, 1993), and of course, HDT (Cieslak & Chawla, 2008). Algorithm 1 can limit the size of the tree to avoid overfitting if it is used as a stand-alone classifier. In the case of using PU-HDT in a bagging ensemble or Random Forest, the tree can fully grow, as overfitting is not longer an issue (Breiman, 2001). Figure 1 visualizes a scenario showing the advantage of the (PU-)Hellinger distance over the Gini Index. On the one hand, the Gini Index prefers a node split (left tree) that concentrates most of the positive and negative class in one single child node. On the another hand, the (PU-)Hellinger distance indicates a preference for a node split (right tree) that concentrates all the positives in one child node.

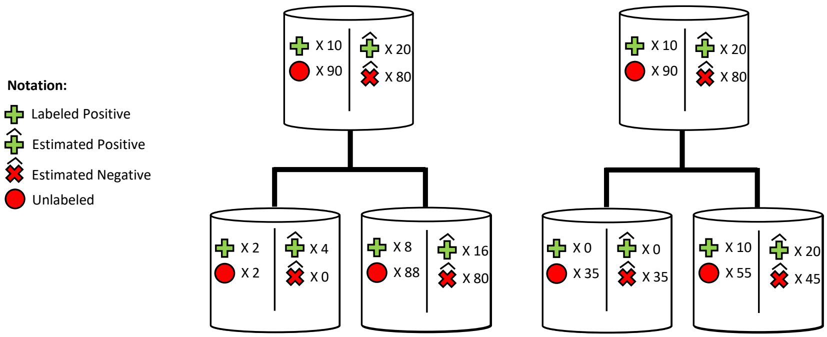


Fig. 1 Difference between Gini Index and Hellinger distance in node splitting. Gini Index is better in the left tree (0.166) compared to the right tree (0.169); PU Hellinger distance is better in the right tree (0.707) than in the left tree (0.459).

3.2 Half-Moons Data Set

As an illustrative example, we consider the popular "half-moons" data set that consists of two-dimensional points generated from two interleaved half circles. Figure 2 shows a class-imbalanced variant of the data set in which the class prior $\alpha = 5\%$: the upper half-moon corresponds to the negative class, whereas the lower half-moon corresponds to the positive class. Moreover, half of the positives are mislabeled (i.e., unlabeled in the PU setting). The only information on the positive class is the labeled positives (blue dots), while the rest remains unlabeled (orange and red dots). Three techniques are compared: PU-HDT, HDT, and CART. The CART decision tree cannot learn from PU data, so only a few unlabeled positives fall into the blue regions: the positive distribution is not well represented by the decision boundary of the CART decision tree. The HDT performs better because of the built-in insensitivity to the imbalanced setting; however, the algorithm cannot learn from positive and unlabeled data. In the region where unlabeled positives dominate (lower left), the HDT provides predictions with high uncertainty. Lastly, the PU-HDT can learn from PU data and is suitable for the imbalanced setting. Most of the unlabeled positives fall into the blue regions as the technique considers that some positives are unlabeled. We see a clearer representation of the positive distribution that follows a half-moon shape.

Algorithm 1: PU-HDT(X, L, α, h, ϕ)

Input: X - data, L - labels, α - class prior, h - depth, ϕ - number of considered features at each split

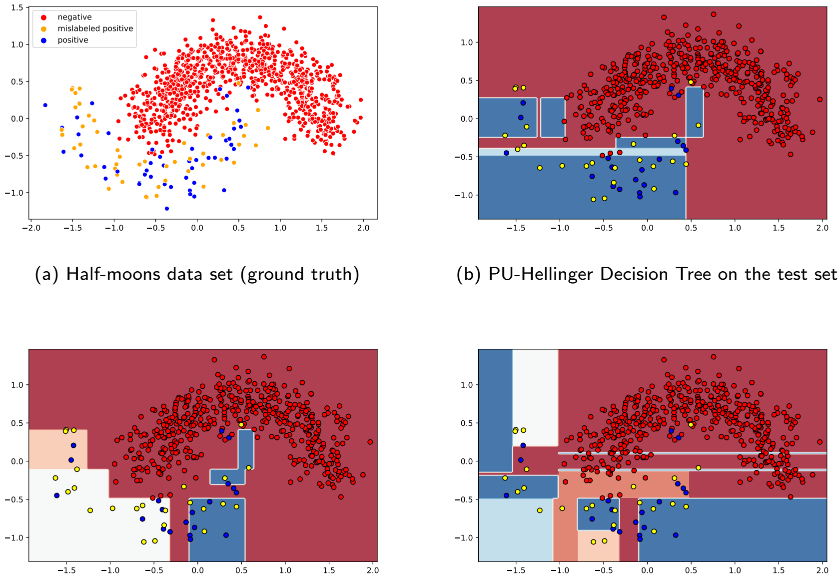
Output: PU-HDT - Hellinger Decision Tree for PU learning

create a tree node n
Initialize $e \leftarrow 0$
if $e > h$ **then**
  return
else
  $e \mathrel{+}= 1$
end
let F_X be the set of features from input X
$f_{sel} \leftarrow RandomSample(F_X, \phi)$
$f_{max} \leftarrow \text{argmax}_{f \in f_{sel}} PUHellingerDistance(X, f)$
let $x^*_{f_{max}}$ be the optimal split value in feature f_{max}
split X into $X_{left}(x_{f_{max}} < x^*_{f_{max}})$ and $X_{right}(x_{f_{max}} \geq x^*_{f_{max}})$
split L into $L_{left}(x_{f_{max}} < x^*_{f_{max}})$ and $L_{right}(x_{f_{max}} \geq x^*_{f_{max}})$
$n.left \leftarrow$ PU-HDT$(X_{left}, L_{left}, h, \phi)$
$n.right \leftarrow$ PU-HDT$(X_{right}, L_{right}, h, \phi)$

Function `PUHellingerDistance(`X, f`)`:
  Initialize $BestHellingerDistance \leftarrow -1$
  let V_f be the set of values of feature f
  for each value $v \in V_f$ **do**
    $w \leftarrow V_f \setminus v$
    estimate $\hat{P}_{f,v}$, $\hat{N}_{f,v}$, $\hat{P}_{f,w}$, and $\hat{N}_{f,w}$ according to Eq. (3)
    $\hat{P} \leftarrow \hat{P}_{f,v} + \hat{P}_{f,w}$
    $\hat{N} \leftarrow \hat{N}_{f,v} + \hat{N}_{f,w}$
    $HD \leftarrow \left(\sqrt{\hat{N}_{f,v}/\hat{N}} - \sqrt{\hat{P}_{f,v}/\hat{P}}\right)^2 + \left(\sqrt{\hat{N}_{f,w}/\hat{N}} - \sqrt{\hat{P}_{f,w}/\hat{P}}\right)^2$
    if $HD > BestHellingerDistance$ **then**
      $BestHellingerDistance \leftarrow HD$
    end
  end
return $\sqrt{BestHellingerDistance}$

3.3 PU Stratified Hellinger Random Forest

Ensemble learning generally improves the performance of a single learner by training several base learners and combining their output. A well-known ensemble method is Random Forest (Breiman, 2001), which extends bagging by incorporating randomized feature selection, with the base learner being a decision tree. Thus, we can use the PU-HDT as the base learner in a Random Forest. Moreover, we can further modify the ensemble algorithm based on



(a) Half-moons data set (ground truth)

(b) PU-Hellinger Decision Tree on the test set

(c) Hellinger Decision Tree on the test set

(d) CART on the test set

Fig. 2 Comparison of decision boundaries of decision trees, including PU-Hellinger decision tree, to illustrate the challenge of learning from positive and unlabeled data in an imbalanced setting. The red and orange dots represent the negative and hidden positives whereas the blue ones refer to the positive class. The areas with darker color (blue or red) points out more certainty regarding the classification into the positive (blue) or negative class (red). The lighter color, consequently, implies a higher uncertainty of the classifier.

the insights from PU Bagging (Mordelet & Vert, 2014): PU Bagging is naturally suitable for imbalanced learning because each bootstrap sample consists of all the available labeled positives and a subsample of the unlabeled data so that a balanced training set can be achieved. Although PU-HDT can handle imbalanced data, there is a practical reason to obtain bootstrap samples from the unlabeled data: the capability of PU-HDT to learn from PU data can be hindered by a bootstrap sample that contains a sparser representation of the positive distribution. For example, in Fig. 2b, the PU-HDT fails to learn the complete true positive distribution (ideally a blue half-moon shape) because there is a small region on the left that does not contain any labeled positives that can be exploited to estimate the true positives. Therefore, we propose the PU Stratified Hellinger Random Forest (PU-SHRF), ensuring that all labeled positives are represented in each bootstrap sample. Algorithm 2 outlines how PU-SHRF is designed based on PU-HDT and the stratified bootstrap sampling. Compared to standard Random Forest, PU-SHRF requires two extra hyperparameters: the size of stratified bootstrap sample K_U and the class prior α.

Algorithm 2: PU-SHRF(X, L, t, K_U, α)

Input: X - training data, L - labels, t - number of trees, K_U - size of bootstrap sample from unlabeled data, α - class prior

Output: Forest - set of t PU Hellinger trees

Initialize Forest
let $\mid F_X \mid$ be the number of features from input X
$\phi \leftarrow \sqrt{\mid F_X \mid}$
for $i \leftarrow 1$ **to** t **do**
    $X'_U,\ L'_U \leftarrow BootstrapSamp(X_{unl},\ L_{unl},\ K_U)$
    $X' \leftarrow X'_U \cup X_{lab}$
    $L' \leftarrow L'_U \cup L_{lab}$
    Forest $\leftarrow$ Forest $\cup$ PU-HDT(X', L', α, ϕ)
    randomly select a set of features x' at each node split
end

4 Experimental Setup

The main goal of the experimental evaluation is to demonstrate the classification performance benefit of PU-HDT when applied to imbalanced PU data, i.e., data sets in which only a small percentage of positive observations is present and only a small percentage of the unlabeled observations would actually be a positive observation if the label were known. Therefore, we compare PU-HDT, PU-HRF, and PU-SHRF with fifteen benchmark techniques detailed in Sect. 4.2. We use two evaluation metrics that are commonly used in imbalanced learning (Cieslak & Chawla, 2008; Davis & Goadrich, 2006; Fernández et al., 2018), namely, the area under the precision-recall curve (AUC-PR) and the F1-score, representing the harmonic mean between precision and recall. In contrast to AUC-PR, the F1-score depends on a threshold that might disadvantage techniques that do not provide calibrated scores, for instance, tree-based methods. Thus, the threshold is optimized according to a validation set to maximize the F1-score for all techniques for each experimental setting. Furthermore, hypothesis testing is applied to statistically validate the empirical results, following the recommendation of Demšar (2006). First, the Iman-Davenport test is applied to determine whether all methods perform the same, as expressed in the null hypothesis. Then, the Holm's post hoc test is used to compare the best performing model with the other techniques. The source code for our techniques and the experimental setup are publicly available on GitHub [1].

4.1 Data

Fifteen data sets, summarized in Table 1, covering different applications such as churn prediction, fraud detection and image recognition, are considered. The churn data sets stem from the telecommunications industry, the credit card

[1] A software implementation of our two-step method is available at https://github.com/CarlosOrtegaV/PU_Hellinger_Trees

Table 1 Summary of data sets

Data set	Examples	Features	$P(y=1)$
Car Good (CGO)	1728	6	3.99%
Churn Chile (CCH)	5263	42	5.00%
Forest Cover (FCO)	286048	10	0.96%
Fraud Car Insurance (FCI)	15420	30	5.98%
Fraud Card Credit (FCC)	282982	8	0.16%
KDDCup land vs portsweep (KDD)	1061	41	1.97%
Churn Korean (CKO)	2221	8	5.00%
Mammography (MAM)	11183	6	2.32%
Pendigits (PEN)	6870	16	2.27%
Pizza Cutter 1 (PCU)	661	37	7.87%
Poker 8 vs 6 (POK)	1477	10	1.15%
Satellite (SAT)	5000	36	1.48%
Shuttle (SHU)	49097	9	7.15%
Thyroid (THY)	7200	21	7.41%
Yeast 6 (YEA)	1484	8	2.35%

fraud data set is provided by Wordline and ULB (MLG, 2018) on Kaggle, and the car insurance fraud data set is provided by Oracle (Oracle, 2015). Pizza Cutter 1, and Satellite are OpenML data sets (Vanschoren, van Rijn, Bischl, & Torgo, 2013). Forest Cover, Shuttle, Pendigits and Mammography are found in ODDS (Shebuti, 2016). Poker 8 vs 6, Car Good, KDD Cup land-vs-portsweep data sets are available on the KEEL repository (Alcalá-Fernandez et al., 2011). Finally, the Thyroid data set is found in UCI repository (Dua et al., 2019). The selection of the data sets is driven by our goal to compare techniques in a highly imbalanced setting. In previous works (Akash et al., 2019; Grzyb et al., 2021; Su et al., 2021), the class imbalance in benchmark data sets is not always extreme: several data sets show an imbalance ratio below 10. However, we are particularly interested in a more extreme setting. Thus, we select some of the most imbalanced data sets on the aforementioned public repositories.

To create the PU data, we flip completely at random (i.e., SCAR) some positives into unlabeled observations in each of the data sets. In the experiments, the number of labeled positives is determined by the flip ratio, which is the proportion of positives to be unlabeled. Three values of the flip ratio are considered: 25, 50, and 75%. For each data set, we perform 20 repetitions of a holdout validation that splits the data into a training set (70%) and test set (30%). The large number of repetitions is needed as training from imbalanced PU data might lead to unstable performance (Mordelet & Vert, 2014). For the data sets that contain more than 10,000 examples, we sample 10,000 observations without replacement to be used in each repetition to limit the computation time of the experiments. In total, there are 600 settings (10 datasets $\times$ 20 repetitions $\times$ 3 flip ratios).

4.2 Techniques

We compare our PU Hellinger-based techniques with eight well-known PU learning techniques: imbalanced nonnegative PU learning (imbalanced nnPU) (Su et al., 2021), nonnegative PU learning (nnPU) (Kiryo et al., 2017), unbiased PU learning (uPU) (Du Plessis et al., 2015), PU Bagging (Mordelet & Vert, 2014), Rank Pruning (Northcutt, Wu, & Chuang, 2017), PU Weighted Logistic Regression (Lee & Liu, 2003), Elkan-Noto's method, that is, the preprocessing method using label probabilities (Elkan & Noto, 2008), and Spy-EM (Liu et al., 2002). We also include two non-PU baselines: Random Forest (Breiman, 2001) combined with ADASYN (He et al., 2008) and a standard HDT (Cieslak & Chawla, 2008).

Table 2 summarizes the hyperparameter configuration of the methods in the experimental setup. PU learning methods in our experimental setup require hyperparameters that need to be specified by the end-user. However, the authors have suggested values for most of the hyper-parameters that have shown good results in previous experiments. For the PU Hellinger-based techniques and unbiased PU learning, along with its extensions, the class prior is an essential hyperparameter, as it enables the labeled positives to be weighted to enable PU learning. In this work, we assume that the class prior is known at training time. In practice, the class prior can be estimated using several methods from the literature (Bekker & Davis, 2018; Du Plessis & Sugiyama, 2014; Elkan & Noto, 2008; Plessis et al., 2017; Ramaswamy et al., 2016). Another important hyperparameter for PU-SHRF is K_U, which is the number of unlabeled examples in each bootstrap. PU Bagging also uses K_U; however, it subsamples the unlabeled examples to balance the training data and avoid sample contamination by hidden positives. PU-SHRF can increase the number of unlabeled examples in the bootstrap samples because it can naturally address class imbalance and PU data. Thus, we opt for $K_U = U_{training}$ as the default value, which leads to stratified bootstrap samples for each PU Hellinger tree in the ensemble. For the PU-HDT and HDT, the max depth of the tree is set to 5 to avoid overfitting. Rank pruning, PU-weighted logistic regression, Elkan-Noto's method and Spy-EM follow the hyperparameters recommended by the authors. The rest of the hyperparameters are set to the default values in `scikit-learn`.

Table 2 Experimental hyperparameters

Technique	Setting
PU-SHRF	$K_U = U_{training}$, trees = 100, $\alpha = \alpha_{groundtruth}$
PU-HRF	trees = 100, $\alpha = \alpha_{groundtruth}$
ADASYN + Random Forest	neighbors = 5, sampling strategy = balanced ratio, trees = 100
PU-HDT	max depth = 5, $\alpha = \alpha_{groundtruth}$
HDT	max depth = 5
uPU	base learner = XGBoost,
nnPU	base learner = XGBoost, $\alpha = \alpha_{groundtruth}$
imbalanced uPU	base learner = XGBoost, $\alpha = \alpha_{groundtruth}$
PU Bagging	hyperparameters recommended by authors
Rank Pruning	hyperparameters recommended by authors
PU Weighted Logistic Regression	hyperparameters recommended by authors
Elkan-Noto's Method	hyperparameters recommended by authors
Spy-EM	hyperparameters recommended by authors

5 Results & Discussion

The average and standard deviation of the F1-score and AUC-PR are shown in Tables 3 and 4. We also report on the average F1-score and AUC-PR per data set in the appendix. Additionally, results on the AUC-ROC are presented in Table A1. The bold and underlined value indicates the best performing model for a given flip ratio. Based on the average rank of each technique's metrics over all data sets, the Iman-Davenport test (Demšar, 2006) rejects the null hypothesis that all methods perform equally ($p < 0.01$). Furthermore, we apply Holm's post hoc test to identify the sources of the differences in performance. The best-performing model is used as the control classifier in the pairwise comparison with all other models.

PU-SHRF and PU-HRF outperform all other techniques in terms of the F1-score with the optimized threshold. Furthermore, at low and medium levels of the flip ratio (i.e., 25% and 50%), PU-SHRF and PU-HRF statistically outperform the rest of techniques at the 5% significance level according to Holm's post hoc test. PU Bagging is the only PU method that is not statistically outperformed at the highest flip ratio. The uPU, nnPU and imbalanced nnPU, considered to be state-of-the-art in the literature, generally perform better than earlier PU methods. Moreover, we observe the benefit of using imbalanced nnPU, designed for imbalanced data sets, over nnPU: imbalanced nnPU performs better than nnPU at every flip ratio. PU Bagging remains a competitive alternative at the highest flip ratio. A possible explanation is that PU Bagging naturally handles the class imbalance because each of the bootstrap samples consists of a balanced subset of the training data. The fact that ADASYN + Random Forest outperforms most of the PU methods emphasizes the weakness of conventional PU methods for imbalanced classification.

In terms of AUC-PR, PU-SHRF and PU-HRF stand out as the best technique at every flip ratio. The stratified bootstrap sampling in PU-SHRF appears to provide an additional performance enhancement. Similar to the F1-score performance at the low and medium flip ratios, all techniques are statistically outperformed at the 5% significance level by PU-SHRF. However, nnPU and imbalanced nnPU remain competitive at the highest flip ratio, as they are not statistically outperformed. Despite the good performance in terms of F1-score, PU Bagging performs poorly with respect to AUC-PR. This might suggest that the balanced bootstrap improves recall at the expense of precision. Furthermore, the use of a traditional data-level method for handling class imbalance together with a standard classifier, for instance ADASYN + Random Forest, is a good alternative that outperforms most older PU techniques. Based on the results in Table 4, we can observe that techniques that natively handle class imbalance perform especially well in terms of AUC-PR.

The results per data set also give more insights about the techniques' performance. The best performing technique remains consistent at low and medium flip ratios in most data sets: in the PEN data set, PU-SHRF outperforms all other techniques in F1-score, except for the setting with the high flip ratio where PU bagging dominates. This might explain that PU bagging becomes a competitive alternative to our methods in the aggregate results (Table 3) at the high flip ratio. Moreover, PU-HRF and PU-SHRF show strong performance in both F1-score and PR-AUC compared to other PU methods: in FCC, the most imbalanced data set, PU-HRF and PU-SHRF substantially outperform the benchmark techniques. Another observation comes from the churn data sets in which our methods are preferred in the CCH data set whereas imbalanced nnPU is the best classifier in CKO, in terms of PR-AUC. Both data sets share the same level of class imbalance and domain application but differ in terms of the number of features and examples.

From the empirical analysis, we can derive some general insights that highlight the advantages of PU-SHRF and PU-HRF. PU classification under high class imbalance poses a challenge to most PU methods. Despite not being able to learn from PU data, a resampling strategy might be sufficient to outperform most PU methods. The PU methods that perform well in imbalanced data sets are those that have integrated a specialized mechanism that diminishes the bias towards the majority class: imbalanced nnPU incorporates oversampling in the risk minimization, whereas PU Bagging exploits balanced bootstrap sampling. However, each of these strategies achieves either better recall (i.e., F1-score) or better precision (i.e., AUC-PR). PU-SHRF achieves state-of-the-art performance because it combines the strategies by incorporating PU-HDT, which is a strong base learner for imbalanced PU data, and by relying on a tailored bootstrap sampling.

Table 3 Average F1-score (%) with optimal threshold and standard deviation at different flip ratios

		F1-score (SD)		
Model	Flip Ratio:	25%	50%	75%
PU-HDT		62.2 ± 7.0	59.1 ± 8.3	55.4 ± 10.6
PU-HRF		$\underline{\mathbf{75.0 \pm 5.7}}$	$\underline{\mathbf{71.9 \pm 6.2}}$	$\mathbf{64.1 \pm 7.6}$
PU-SHRF		$\mathbf{74.7 \pm 5.7}$	$\mathbf{71.3 \pm 6.0}$	$\underline{\mathbf{64.5 \pm 7.4}}$
imbalanced nnPU		71.4 ± 5.3	67.6 ± 7.8	60.5 ± 8.5
nnPU		70.8 ± 5.7	67.3 ± 7.7	58.0 ± 9.0
uPU		69.9 ± 5.7	65.9 ± 7.3	58.1 ± 7.8
Ranking Pruning		61.6 ± 7.3	58.0 ± 8.5	53.6 ± 9.5
PU Bagging		63.4 ± 6.3	63.7 ± 6.1	$\mathbf{63.9 \pm 6.7}$
Elkan-Noto's Method		41.6 ± 12.0	33.7 ± 18.3	11.1 ± 12.7
PU Weighted Logistic Regression		59.1 ± 6.0	55.6 ± 8.3	50.5 ± 8.9
Spy-EM		32.6 ± 4.9	32.6 ± 6.1	34.4 ± 9.1
ADASYN+RF		73.3 ± 6.3	69.5 ± 6.8	62.2 ± 7.8
HDT		62.0 ± 7.5	58.6 ± 8.0	51.3 ± 11.3
Iman-Davenport test		$p < 0.01$	$p < 0.01$	$p < 0.01$

Best-performing model is indicated by **<u>bold and underlined</u>** in each column. Values in **bold** indicate that the best-performing model does not outperform the classifier in the model column at the 5% significance level

Table 4 Average AUC-PR (%) with standard deviation at different flip ratios

		AUC-PR (SD)		
Model	Flip Ratio:	25%	50%	75%
PU-HDT		53.3 ± 8.1	48.8 ± 8.9	43.9 ± 10.9
PU-HRF		$\underline{\mathbf{73.3 \pm 6.7}}$	$\underline{\mathbf{70.0 \pm 7.4}}$	$\mathbf{60.4 \pm 8.5}$
PU-SHRF		$\mathbf{72.6 \pm 6.5}$	$\mathbf{69.4 \pm 7.0}$	$\underline{\mathbf{61.1 \pm 8.4}}$
imbalanced nnPU		69.7 ± 6.2	66.4 ± 8.1	$\mathbf{60.4 \pm 9.0}$
nnPU		69.2 ± 6.6	66.3 ± 8.0	$\mathbf{59.1 \pm 8.8}$
uPU		67.0 ± 7.5	61.9 ± 9.1	51.9 ± 9.2
Ranking Pruning		57.6 ± 7.9	54.3 ± 8.2	49.5 ± 10.5
PU Bagging		54.4 ± 6.9	55.7 ± 7.2	56.3 ± 7.7
Elkan-Noto's Method		54.7 ± 9.0	44.1 ± 14.2	26.3 ± 16.3
PU Weighted Logistic Regression		55.4 ± 6.3	51.9 ± 8.6	46.5 ± 9.7
Spy-EM		35.5 ± 6.9	35.2 ± 9.1	36.5 ± 11.2
ADASYN+RF		71.5 ± 7.4	67.2 ± 8.0	58.8 ± 8.8
HDT		52.7 ± 8.8	47.9 ± 8.8	40.3 ± 10.4
Iman-Davenport test		$p < 0.01$	$p < 0.01$	$p < 0.01$

Best-performing model is indicated by **<u>bold and underlined</u>** in each column. Values in **bold** indicate that the best-performing model does not outperform the classifier in the model column at the 5% significance level

6 Conclusions

In this paper, we introduce a novel PU learning technique to handle highly imbalanced data sets: PU Hellinger Decision Tree (PU-HDT). PU-HDT utilizes the Hellinger distance as the splitting criterion, which shows robustness to extreme class imbalance. Furthermore, PU-HDT can learn from PU data by means of the estimation of positives from unlabeled instances at each node of the tree. Unlike other PU methods for imbalanced learning, the PU-HDT does not entail additional misclassification costs or require a resampling strategy. By using PU-HDT as the base learner, we propose the PU Hellinger Stratified Random Forest (PU-SHRF). The empirical analysis suggests that PU-SHRF generally outperforms all well-known PU methods under all experimental settings. Moreover, we emphasize the weakness of most PU methods to the imbalanced setting. Statistical hypothesis testing is applied to further validate the empirical findings.

There are several possible research directions for future work. In this work, we assume that labeled positives represent a random subset of the positive class: this scenario refers to the selected completely at random (SCAR) assumption. However, the SCAR assumption does not hold in most real-world applications. Thus, we could extend the current work to accommodate more realistic assumptions. Another interesting line of work relates to imbalanced data streams. Previous works have already exploited HDTs in imbalanced data streams. To the best of our knowledge, no work has yet explored PU learning in imbalanced data streams.

Appendix A

Table A1 Average AUC-ROC (%) with standard deviation at different flip ratios

		AUC-ROC (SD)		
Model	Flip Ratio:	25%	50%	75%
PU-HDT		85.3 ± 4.7	82.2 ± 5.1	78.5 ± 6.4
PU-HRF		<u>**93.5 ± 3.2**</u>	<u>**92.6 ± 3.5**</u>	88.3 ± 4.0
PU-SHRF		**93.2 ± 3.0**	**92.5 ± 3.0**	88.8 ± 4.0
imbalanced nnPU		91.9 ± 3.2	90.6 ± 3.9	88.4 ± 4.8
nnPU		92.0 ± 2.9	90.8 ± 3.8	87.3 ± 5.7
uPU		91.8 ± 3.5	89.7 ± 4.3	85.7 ± 5.7
Ranking Pruning		87.6 ± 3.9	86.9 ± 4.4	83.6 ± 5.8
PU Bagging		90.5 ± 3.7	90.9 ± 3.0	<u>**89.9 ± 3.8**</u>
Elkan-Noto's Method		83.5 ± 7.2	78.3 ± 12.3	67.1 ± 18.9
PU Weighted Logistic Regression		87.6 ± 3.9	85.9 ± 4.9	82.6 ± 6.0
Spy-EM		82.2 ± 5.3	82.4 ± 7.0	81.1 ± 8.3
ADASYN+RF		93.8 ± 2.9	93.0 ± 3.0	88.9 ± 4.1
HDT		85.2 ± 4.9	81.9 ± 5.1	76.1 ± 6.6
Iman-Davenport test		$p < 0.01$	$p < 0.01$	$p < 0.01$

Best-performing model is indicated by <u>**bold and underlined**</u> in each column.
Values in **bold** indicate that the best-performing model does not outperform the classifier in the model column at the 5% significance level

Table A2 Average F1-score (%) with optimal threshold over holdout 20 repetitions at 25% flip ratio

Model	CGO	CCH	FCO	FCI	FCC	KDD	CKO	MAM	PEN	PCU	POK	SAT	SHU	THY	YEA
PU-HDT	56.1	46.4	88.9	25.6	57.3	87.8	**83.4**	55.3	91.1	26.9	6.1	61.8	98.8	95.7	51.6
PU-HRF	78.4	66.0	94.6	**26.8**	**85.0**	99.2	81.3	68.1	**98.4**	**44.7**	**50.1**	77.7	**99.5**	96.6	58.4
PU-SHRF	79.9	**67.0**	**94.8**	26.6	84.9	99.2	80.2	67.3	**98.4**	44.5	44.8	**78.3**	**99.5**	**96.8**	57.5
imbalanced nnPU	**81.7**	65.3	94.3	25.7	80.0	98.1	82.2	65.2	97.1	41.1	20.0	74.2	99.2	94.3	52.2
nnPU	79.7	65.7	93.9	25.7	80.1	97.7	81.5	65.7	96.9	42.6	14.8	74.9	99.1	94.9	49.3
uPU	79.0	61.0	91.7	26.6	78.0	96.8	82.3	**65.9**	90.9	37.6	28.1	70.2	98.0	91.5	50.6
Ranking Pruning	66.4	43.9	92.8	26.7	61.6	95.9	22.6	63.1	92.7	35.1	18.1	69.9	98.1	80.5	56.0
PU Bagging	59.4	46.3	90.8	22.5	64.1	**100.0**	29.9	44.3	93.9	41.4	36.2	75.6	97.9	88.5	**59.9**
Elkan-Noto's Method	29.9	26.1	92.6	14.1	24.9	97.7	10.2	12.8	93.8	28.0	0.0	67.4	80.9	15.3	30.8
PU Weighted LR	68.1	43.3	91.9	27.0	42.1	91.8	22.6	59.4	89.2	38.9	6.2	73.2	97.9	82.9	51.3
Spy-EM	54.2	13.0	48.5	14.3	4.8	90.7	14.9	27.2	65.1	26.2	5.2	6.3	93.9	16.3	8.1
ADASYN+RF	79.0	62.7	93.6	25.1	80.3	98.9	69.4	62.9	98.0	43.7	62.3	72.6	99.0	96.5	55.6
HDT	56.1	46.3	88.3	25.4	52.5	87.9	82.9	57.8	90.5	26.3	6.1	63.8	99.0	96.4	51.4

Best-performing model is indicated by **bold** in each column.

Table A3 Average AUC-PR (%) with optimal threshold over holdout 20 repetitions at 25% flip ratio

Model	CGO	CCH	FCO	FCI	FCC	KDD	CKO	MAM	PEN	PCU	POK	SAT	SHU	THY	YEA
PU-HDT	43.4	40.6	80.1	18.0	39.8	79.2	74.3	47.9	87.1	17.8	3.2	45.8	97.7	92.2	31.9
PU-HRF	78.6	69.6	**97.7**	20.8	**77.6**	99.7	**80.0**	**69.0**	99.4	38.0	39.7	80.2	**99.9**	**98.8**	**51.0**
PU-SHRF	77.8	**71.5**	97.9	**21.0**	77.1	99.8	78.2	68.1	99.5	38.4	31.2	**80.7**	**99.9**	**98.8**	49.1
imbalanced nnPU	**79.7**	70.2	96.6	19.0	74.8	98.3	**80.0**	64.2	98.6	36.1	12.4	76.6	**99.9**	97.0	41.7
nnPU	75.9	70.9	96.5	19.1	74.5	97.6	79.5	64.6	98.8	**36.9**	9.7	75.7	**99.9**	97.1	41.2
uPU	76.4	63.3	91.5	**21.0**	72.3	97.2	77.0	63.0	92.5	30.8	19.1	69.9	99.2	90.3	40.7
Ranking Pruning	52.2	39.2	96.0	17.7	52.3	98.9	15.4	60.2	96.0	28.4	11.8	68.3	97.1	84.2	47.0
PU Bagging	42.4	34.0	87.0	12.4	49.5	**100.0**	16.4	27.0	92.4	28.7	26.3	72.4	96.9	87.1	44.0
Elkan-Noto's Method	49.3	37.5	95.2	9.0	37.1	98.9	6.9	54.3	95.8	30.5	13.5	71.8	97.1	87.3	36.5
PU Weighted LR	54.1	37.2	96.1	17.5	34.5	95.4	15.6	53.5	92.5	33.1	1.9	75.5	97.0	85.7	40.5
Spy-EM	55.2	9.8	40.4	11.7	3.4	84.5	8.3	29.3	76.4	16.2	2.7	6.1	95.6	43.0	49.5
ADASYN+RF	79.9	64.2	97.3	17.6	72.0	99.5	67.2	60.9	**99.6**	36.4	**57.2**	75.4	99.9	98.6	47.3
HDT	43.4	38.4	80.4	17.7	37.1	79.5	73.6	48.6	83.0	17.8	3.2	46.7	97.9	93.4	30.4

Best-performing model is indicated by **bold** in each column.

Table A4 Average F1-score (%) with optimal threshold over holdout 20 repetitions at 50% flip ratio

Model	CGO	CCH	FCO	FCI	FCC	KDD	CKO	MAM	PEN	PCU	POK	SAT	SHU	THY	YEA
PU-HDT	56.0	47.3	85.5	24.3	44.0	69.3	79.0	55.8	88.9	26.8	6.6	62.4	98.1	94.8	47.3
PU-HRF	75.1	62.7	92.2	24.9	82.7	94.5	73.4	65.8	95.9	**41.4**	42.5	**76.8**	**99.1**	94.8	56.4
PU-SHRF	74.4	**63.0**	92.5	25.3	**85.1**	95.8	73.0	64.6	**96.5**	39.4	34.9	75.8	99.0	**95.4**	55.6
imbalanced nnPU	**77.5**	59.1	91.4	23.9	74.2	91.8	73.5	60.4	93.2	39.5	15.1	73.9	98.5	91.8	49.6
nnPU	75.0	59.4	91.4	23.4	74.0	91.8	71.7	60.7	93.1	39.4	15.0	74.8	98.1	92.1	49.1
uPU	72.1	52.2	87.2	23.9	71.3	93.6	75.5	**62.7**	84.6	35.7	35.3	64.3	96.5	87.4	45.7
Ranking Pruning	65.4	45.2	90.7	**25.5**	57.1	79.9	20.0	62.0	89.8	32.7	12.4	59.9	97.7	74.6	56.4
PU Bagging	55.7	46.3	91.2	22.6	68.9	**100.0**	34.4	46.6	92.7	40.2	38.7	75.0	97.6	86.7	**59.3**
Elkan-Noto's Method	23.2	20.3	69.2	12.9	23.5	79.1	9.4	15.5	69.7	23.7	2.9	60.9	56.4	24.2	15.0
PU Weighted LR	68.6	42.5	**92.6**	25.7	32.6	74.0	21.1	57.9	87.9	36.3	7.4	61.9	97.5	76.8	51.7
Spy-EM	54.5	12.2	48.9	18.8	5.2	82.3	14.5	29.3	66.1	24.1	6.4	7.8	94.0	15.7	8.6
ADASYN+RF	74.8	57.8	90.8	24.7	82.2	96.3	58.9	58.3	96.0	38.4	**46.8**	68.6	97.9	95.0	56.8
HDT	56.0	45.5	85.1	24.3	46.4	70.3	**80.2**	55.4	87.8	26.3	6.6	56.2	97.7	**95.4**	46.6

Best-performing model is indicated by **bold** in each column.

Table A5 Average AUC-PR (%) with optimal threshold over holdout 20 repetitions at 50% flip ratio

Model	CGO	CCH	FCO	FCI	FCC	KDD	CKO	MAM	PEN	PCU	POK	SAT	SHU	THY	YEA
PU-HDT	43.7	37.7	74.1	16.6	28.8	57.1	66.3	45.8	81.4	18.0	3.6	45.8	96.3	90.8	26.6
PU-HRF	73.5	63.4	95.2	18.5	77.3	96.3	72.3	**65.1**	97.7	**34.7**	31.5	**76.8**	**99.8**	97.9	49.4
PU-SHRF	72.5	**65.2**	95.4	**18.9**	**79.0**	97.2	71.7	64.0	98.1	33.1	22.8	76.4	99.7	97.9	48.6
imbalanced nnPU	**76.6**	62.7	94.6	16.8	69.3	92.3	**74.6**	58.6	96.7	32.6	9.6	74.6	99.7	95.0	42.9
nnPU	73.4	63.6	94.5	16.9	71.2	91.2	72.3	58.9	96.8	33.5	9.0	74.7	99.7	95.7	42.7
uPU	70.4	49.7	85.4	17.9	64.8	93.8	73.0	57.0	85.6	25.5	24.4	63.4	98.1	85.0	34.7
Ranking Pruning	54.5	40.7	91.7	16.7	48.7	89.7	12.6	61.0	91.4	23.4	6.6	55.8	96.0	79.5	46.5
PU Bagging	38.7	37.4	88.9	12.5	56.6	**100.0**	19.8	29.5	93.1	29.2	27.9	73.6	96.5	88.4	44.0
Elkan-Noto's Method	36.6	23.6	89.6	8.1	30.8	85.5	6.5	24.4	84.7	25.7	9.6	60.1	92.0	61.3	23.3
PU Weighted LR	54.5	37.9	**95.6**	16.4	23.6	81.1	13.6	52.0	90.2	28.0	3.6	61.8	96.1	81.2	43.2
Spy-EM	55.8	10.5	41.9	13.5	3.8	73.0	8.7	31.0	69.4	17.2	4.2	11.7	95.3	39.2	**53.0**
ADASYN+RF	75.1	57.4	94.7	16.4	76.8	98.1	52.3	55.5	**98.6**	31.0	**35.8**	70.1	99.6	**98.1**	48.1
HDT	43.7	34.7	74.3	16.5	31.1	56.3	66.8	44.3	79.0	16.7	3.6	39.3	95.5	91.4	25.6

Best-performing model is indicated by **bold** in each column.

Table A6 Average F1-score (%) with optimal threshold over holdout 20 repetitions at 75% flip ratio

Model	CGO	CCH	FCO	FCI	FCC	KDD	CKO	MAM	PEN	PCU	POK	SAT	SHU	THY	YEA
PU-HDT	56.9	39.3	78.1	23.3	36.2	69.8	74.7	52.1	86.6	24.1	11.1	57.4	97.2	89.9	34.0
PU-HRF	60.0	49.1	84.8	22.4	81.5	93.8	56.0	**57.8**	90.4	32.0	32.1	**70.6**	95.3	89.0	46.8
PU-SHRF	61.4	**50.4**	84.7	23.3	**82.2**	95.0	58.6	56.6	90.9	34.6	26.9	67.3	95.9	90.2	50.1
imbalanced nnPU	61.3	46.8	82.5	19.1	69.8	91.7	62.3	51.7	84.4	33.9	14.2	67.2	94.4	82.8	45.7
nnPU	63.1	44.6	80.6	18.9	62.1	89.1	58.0	51.7	80.6	31.9	16.7	65.1	89.9	80.4	37.2
uPU	58.6	42.3	81.5	21.5	58.9	90.0	65.8	54.3	77.1	30.9	18.5	57.7	94.5	83.5	35.7
Ranking Pruning	63.0	39.0	84.5	24.7	51.5	75.2	17.8	**62.3**	85.0	26.0	17.7	45.0	97.3	65.1	49.3
PU Bagging	56.2	41.3	**88.9**	23.3	77.0	**100.0**	39.9	51.8	**92.6**	**36.4**	**42.7**	**70.6**	**97.4**	80.9	**58.9**
Elkan-Noto's Method	3.6	6.6	7.5	3.4	15.5	30.1	0.5	1.6	28.8	10.3	1.4	27.0	14.0	14.2	2.6
PU Weighted LR	**65.8**	37.8	86.5	**25.3**	25.5	63.2	20.5	57.0	85.7	24.8	14.1	43.0	97.2	63.5	48.1
Spy-EM	52.5	10.1	46.4	17.9	5.4	80.2	13.0	30.8	77.5	23.4	7.4	26.4	95.4	15.0	15.3
ADASYN+RF	59.1	48.2	85.0	23.3	77.4	93.7	47.7	50.4	91.7	33.8	28.9	58.1	95.9	90.9	49.1
HDT	56.6	37.0	71.2	23.1	24.8	53.4	**75.3**	51.0	82.5	19.6	10.3	44.4	94.7	**93.3**	32.1

Best-performing model is indicated by **bold** in each column.

Table A7 Average AUC-PR (%) with optimal threshold over holdout 20 repetitions at 75% flip ratio

Model	CGO	CCH	FCO	FCI	FCC	KDD	CKO	MAM	PEN	PCU	POK	SAT	SHU	THY	YEA
PU-HDT	42.3	26.0	62.6	14.4	23.8	58.3	60.5	38.8	76.5	15.0	7.5	38.2	94.5	82.0	17.7
PU-HRF	57.8	44.0	86.4	14.1	72.2	95.6	50.8	54.9	91.2	23.9	21.2	66.7	96.5	93.4	36.8
PU-SHRF	58.9	**46.9**	86.4	15.2	**74.8**	97.0	53.7	52.9	92.2	26.5	16.0	65.7	97.5	94.4	38.1
imbalanced nnPU	58.5	46.7	89.8	13.9	64.8	90.5	**63.1**	49.3	92.5	**29.5**	11.7	**67.1**	**99.1**	90.3	39.0
nnPU	**61.1**	47.3	**91.0**	14.5	59.6	88.2	56.6	46.4	93.4	28.8	11.8	64.7	98.7	90.3	34.0
uPU	50.3	32.4	77.8	14.3	57.1	89.0	59.9	41.8	74.8	19.0	12.9	48.8	95.9	79.3	25.5
Ranking Pruning	52.6	32.9	86.4	15.9	49.3	74.7	10.9	**60.2**	87.6	17.6	13.8	35.7	95.2	70.4	39.7
PU Bagging	39.2	35.2	88.7	13.2	65.1	**100.0**	25.8	34.4	94.5	24.9	**31.2**	64.8	96.7	85.0	45.2
Elkan-Noto's Method	31.1	11.3	28.7	8.8	29.0	74.6	5.5	11.0	52.9	13.9	13.8	33.7	55.2	8.3	17.0
PU Weighted LR	53.3	31.1	88.5	**16.1**	19.1	69.7	11.8	51.0	88.0	17.9	12.0	39.5	95.2	68.8	36.0
Spy-EM	53.8	9.9	37.6	12.3	4.0	70.6	10.7	33.1	82.4	17.0	4.7	48.2	95.8	21.2	**46.7**
ADASYN+RF	55.2	42.4	85.9	14.4	73.0	95.2	43.2	45.7	**95.3**	23.2	20.6	57.0	97.7	**95.1**	38.0
HDT	41.8	24.0	55.7	14.5	15.8	42.8	60.6	36.6	70.6	11.6	7.3	28.4	90.5	87.7	16.6

Best-performing model is indicated by **bold** in each column.

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Code Availability

Code used for this research is available at https://github.com/CarlosOrtegaV/PU_Hellinger_Trees.

Conflicts of Interest

The authors have no competing interests to declare that are relevant to the content of this article.

Ethics approval

Not applicable.

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