
Semi-Supervised Classification Based on Classification from Positive and Unlabeled Data

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Abstract

Most of the semi-supervised classification methods developed so far use unlabeled data for regularization purposes under particular distributional assumptions such as the cluster assumption. In contrast, recently developed methods of *classification from positive and unlabeled data* (PU classification) use unlabeled data for risk evaluation, i.e., label information is directly extracted from unlabeled data. In this paper, we extend PU classification to also incorporate negative data and propose a novel semi-supervised classification approach. We establish a generalization error bound for our novel method and show that the bound decreases with respect to the number of unlabeled data *without* the distributional assumptions that are required in existing semi-supervised classification methods. Through experiments, we demonstrate the usefulness of the proposed methods.

1. Introduction

Collecting a large amount of labeled data is a critical bottleneck in real-world machine learning applications due to the laborious manual annotation. In contrast, unlabeled data can often be collected automatically and abundantly, e.g., by a web crawler. This has led to the development of various semi-supervised classification algorithms over the past decades.

To leverage unlabeled data in training, most of the existing semi-supervised classification methods rely on particular assumptions on the data distribution (Chapelle et al., 2006). For example, the *manifold assumption* supposes that samples are distributed on a low-dimensional manifold in the data space (Belkin et al., 2006). In the existing framework, such a distributional assumption is encoded as a reg-

ularizer for training a classifier and *biases* the classifier toward a better one under the assumption. However, if such a distributional assumption contradicts the data distribution, the bias behaves adversely, and the performance of the obtained classifier becomes worse than the one obtained with supervised classification (Cozman et al., 2003; Sokolovska et al., 2008; Li & Zhou, 2015; Krijthe & Loog, 2017).

Recently, *classification from positive and unlabeled data* (PU classification) has been gathering growing attention (Elkan & Noto, 2008; du Plessis et al., 2014; 2015; Jain et al., 2016), which trains a classifier only from positive and unlabeled data without negative data. In PU classification, the *unbiased* risk estimators proposed in du Plessis et al. (2014; 2015) utilize unlabeled data for *risk evaluation*, implying that label information is directly extracted from unlabeled data without restrictive distributional assumptions, unlike existing semi-supervised classification methods that utilize unlabeled data for *regularization*. Furthermore, theoretical analysis (Niu et al., 2016) showed that PU classification (or its counterpart, *NU classification*, classification from negative and unlabeled data) is likely to outperform classification from positive and negative data (*PN classification*, i.e., ordinary supervised classification) depending on the number of positive, negative, and unlabeled samples. It is thus naturally expected that combining PN, PU, and NU classification can be a promising approach to semi-supervised classification without restrictive distributional assumptions.

In this paper, we propose a novel semi-supervised classification approach by considering convex combinations of the risk functions of PN, PU, and NU classification. Without any distributional assumption, we theoretically show that the confidence term of the generalization error bounds decreases at the optimal parametric rate with respect to the number of positive, negative, and unlabeled samples, and the variance of the proposed risk estimator is almost always smaller than the plain PN risk function given an infinite number of unlabeled samples. Through experiments, we analyze the behavior of the proposed approach and demonstrate the usefulness of the proposed semi-supervised classification methods.

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2. Background

In this section, we first introduce the notation commonly used in this paper and review the formulations of PN, PU, and NU classification.

2.1. Notation

Let random variables $\mathbf{x} \in \mathbb{R}^d$ and $y \in \{+1, -1\}$ be equipped with probability density $p(\mathbf{x}, y)$, where d is a positive integer. Let us consider a binary classification problem from \mathbf{x} to y , given three sets of samples called the *positive* (P), *negative* (N), and *unlabeled* (U) data:

$$\begin{aligned}\mathcal{X}_P &:= \{\mathbf{x}_i^P\}_{i=1}^{n_P} \stackrel{\text{i.i.d.}}{\sim} p_P(\mathbf{x}) := p(\mathbf{x} \mid y = +1), \\ \mathcal{X}_N &:= \{\mathbf{x}_i^N\}_{i=1}^{n_N} \stackrel{\text{i.i.d.}}{\sim} p_N(\mathbf{x}) := p(\mathbf{x} \mid y = -1), \\ \mathcal{X}_U &:= \{\mathbf{x}_i^U\}_{i=1}^{n_U} \stackrel{\text{i.i.d.}}{\sim} p(\mathbf{x}) := \theta_P p_P(\mathbf{x}) + \theta_N p_N(\mathbf{x}),\end{aligned}$$

where

$$\theta_P := p(y = +1), \quad \theta_N := p(y = -1)$$

are the class-prior probabilities for the positive and negative classes such that $\theta_P + \theta_N = 1$.

Let $g: \mathbb{R}^d \rightarrow \mathbb{R}$ be an arbitrary real-valued decision function for binary classification, and classification is performed based on its sign. Let $\ell: \mathbb{R} \rightarrow \mathbb{R}$ be a loss function such that $\ell(m)$ generally takes a small value for large margin $m = yg(\mathbf{x})$. Let $R_P(g)$, $R_N(g)$, $R_{U,P}(g)$, and $R_{U,N}(g)$ be the risks of classifier g under loss ℓ :

$$\begin{aligned}R_P(g) &:= \mathbb{E}_P[\ell(g(\mathbf{x}))], & R_N(g) &:= \mathbb{E}_N[\ell(-g(\mathbf{x}))], \\ R_{U,P}(g) &:= \mathbb{E}_U[\ell(g(\mathbf{x}))], & R_{U,N}(g) &:= \mathbb{E}_U[\ell(-g(\mathbf{x}))],\end{aligned}$$

where \mathbb{E}_P , \mathbb{E}_N , and \mathbb{E}_U denote the expectations over $p_P(\mathbf{x})$, $p_N(\mathbf{x})$, and $p(\mathbf{x})$, respectively. Since we do not have any samples from $p(\mathbf{x}, y)$, the true risk $R(g) = \mathbb{E}_{p(\mathbf{x}, y)}[\ell(yg(\mathbf{x}))]$, which we want to minimize, should be recovered without using $p(\mathbf{x}, y)$ as shown below.

2.2. PN Classification

In standard supervised classification (PN classification), we have both positive and negative data, i.e., fully labeled data. The goal of PN classification is to train a classifier using labeled data.

The risk in PN classification (the PN risk) is defined as

$$\begin{aligned}R_{PN}(g) &:= \theta_P \mathbb{E}_P[\ell(g(\mathbf{x}))] + \theta_N \mathbb{E}_N[\ell(-g(\mathbf{x}))] \\ &= \theta_P R_P(g) + \theta_N R_N(g),\end{aligned}\tag{1}$$

which is equal to $R(g)$, but $p(\mathbf{x}, y)$ is not included. If we use the hinge loss function $\ell_H(m) := \max(0, 1 - m)$, the PN risk coincides with the risk of the support vector machine (Vapnik, 1995).

2.3. PU Classification

In PU classification, we do not have labeled data for the negative class, but we can use unlabeled data drawn from marginal density $p(\mathbf{x})$. The goal of PU classification is to train a classifier using only positive and unlabeled data. The basic approach to PU classification is to discriminate P and U data (Elkan & Noto, 2008). However, naively classifying P and U data causes a bias.

To address this problem, du Plessis et al. (2014; 2015) proposed a risk equivalent to the PN risk but where $p_N(\mathbf{x})$ is not included. The key idea is to utilize unlabeled data to evaluate the risk for negative samples in the PN risk. Replacing the second term in Eq. (1) with¹

$$\theta_N \mathbb{E}_N[\ell(-g(\mathbf{x}))] = \mathbb{E}_U[\ell(-g(\mathbf{x}))] - \theta_P \mathbb{E}_P[\ell(-g(\mathbf{x}))],$$

we obtain the risk in PU classification (the PU risk) as

$$\begin{aligned}R_{PU}(g) &:= \theta_P \mathbb{E}_P[\tilde{\ell}(g(\mathbf{x}))] + \mathbb{E}_U[\ell(-g(\mathbf{x}))] \\ &= \theta_P R_P^C(g) + R_{U,N}(g),\end{aligned}\tag{2}$$

where $R_P^C(g) := \mathbb{E}_P[\tilde{\ell}(g(\mathbf{x}))]$ and $\tilde{\ell}(m) = \ell(m) - \ell(-m)$ is a composite loss function.

Non-Convex Approach: If the loss function satisfies

$$\ell(m) + \ell(-m) = 1,\tag{3}$$

the composite loss function becomes $\tilde{\ell}(m) = 2\ell(m) - 1$. We thus obtain the *non-convex* PU risk as

$$R_{N-PU}(g) := 2\theta_P R_P(g) + R_{U,N}(g) - \theta_P.\tag{4}$$

This formulation can be seen as cost-sensitive classification of P and U data with weight $2\theta_P$ (du Plessis et al., 2014).

The ramp loss used in the robust support vector machine (Collobert et al., 2006),

$$\ell_R(m) := \frac{1}{2} \max(0, \min(2, 1 - m)),\tag{5}$$

satisfies the condition (3). However, the use of the ramp loss (and any other losses that satisfy the condition (3)) yields a non-convex optimization problem, which may be solved locally by the *concave-convex procedure* (CCCP) (Yuille & Rangarajan, 2002; Collobert et al., 2006; du Plessis et al., 2014).

Convex Approach: If a convex surrogate loss function satisfies

$$\ell(m) - \ell(-m) = -m,\tag{6}$$

¹The equation comes from the definition of the marginal density $p(\mathbf{x}) = \theta_P p_P(\mathbf{x}) + \theta_N p_N(\mathbf{x})$.

the composite loss function becomes a linear function $\tilde{\ell}(m) = -m$ (see Table 1 in du Plessis et al., 2015). We thus obtain the *convex* PU risk as

$$R_{C\text{-}PU}(g) := \theta_P R_P^L(g) + R_{U,N}(g),$$

where $R_P^L(g) := \mathbb{E}_P[-g(\mathbf{x})]$ is the risk with the linear loss $\ell_{\text{Lin}}(m) := -m$. This formulation yields the convex optimization problem that can be solved efficiently.

2.4. NU Classification

As a mirror of PU classification, we can consider NU classification. The risk in NU classification (the NU risk) is given by

$$\begin{aligned} R_{\text{NU}}(g) &:= \theta_N \mathbb{E}_N[\tilde{\ell}(-g(\mathbf{x}))] + \mathbb{E}_U[\ell(g(\mathbf{x}))] \\ &= \theta_N R_N^C(g) + R_{U,P}(g), \end{aligned}$$

where $R_N^C(g) := \mathbb{E}_N[\tilde{\ell}(-g(\mathbf{x}))]$ is the risk function with the composite loss. Similarly to PU classification, the non-convex and convex NU risks are expressed as

$$R_{N\text{-}NU}(g) := 2\theta_N R_N(g) + R_{U,P}(g) - \theta_N, \quad (7)$$

$$R_{C\text{-}NU}(g) := \theta_N R_N^L(g) + R_{U,P}(g), \quad (8)$$

where $R_N^L(g) := \mathbb{E}_N[g(\mathbf{x})]$ is the risk with the linear loss.

3. Semi-Supervised Classification Based on PN, PU, and NU Classification

In this section, we propose semi-supervised classification methods based on PN, PU, and NU classification.

3.1. PUNU Classification

A naive idea to build a semi-supervised classifier is to combine the PU and NU risks. For $\gamma \in [0, 1]$, let us consider a linear combination of the PU and NU risks:

$$R_{\text{PUNU}}^\gamma(g) := (1 - \gamma)R_{\text{PU}}(g) + \gamma R_{\text{NU}}(g).$$

We refer to this combined method as *PUNU classification*.

If we use a loss function satisfying the condition (3), the non-convex PUNU risk $R_{\text{N-PUNU}}^\gamma(g)$ can be expressed as

$$\begin{aligned} R_{\text{N-PUNU}}^\gamma(g) &= 2(1 - \gamma)\theta_P R_P(g) + 2\gamma\theta_N R_N(g) \\ &\quad + \mathbb{E}_U[(1 - \gamma)\ell(-g(\mathbf{x})) + \gamma\ell(g(\mathbf{x}))] \\ &\quad - (1 - \gamma)\theta_P - \gamma\theta_N. \end{aligned}$$

Here, $R_{\text{N-PUNU}}^{1/2}(g)$ agrees with $R_{\text{PN}}(g)$ due to the condition (3). Thus, when $\gamma = 1/2$, PUNU classification is reduced to ordinary PN classification.

On the other hand, $\gamma = 1/2$ is still effective when the condition (6) is satisfied. Its risk $R_{\text{C-PUNU}}^\gamma(g)$ can be expressed as

$$\begin{aligned} R_{\text{C-PUNU}}^\gamma(g) &= (1 - \gamma)\theta_P R_P^L(g) + \gamma\theta_N R_N^L(g) \\ &\quad + \mathbb{E}_U[(1 - \gamma)\ell(g(\mathbf{x})) + \gamma\ell(-g(\mathbf{x}))]. \end{aligned}$$

Here, $(1 - \gamma)\ell(g(\mathbf{x})) + \gamma\ell(-g(\mathbf{x}))$ can be regarded as a loss function for unlabeled samples with weight γ .

When $\gamma = 1/2$, unlabeled samples incur the same loss for the positive and negative classes. On the other hand, when $0 < \gamma < 1/2$, a smaller loss is incurred for the negative class than the positive class. Thus, unlabeled samples tend to be classified into the negative class. The opposite is true when $1/2 < \gamma < 1$.

3.2. PNU Classification

Another possibility of using PU and NU classification in semi-supervised classification is to combine the PN and PU/NU risks. For $\gamma \in [0, 1]$, let us consider linear combinations of the PN and PU/NU risks:

$$R_{\text{PNPU}}^\gamma(g) := (1 - \gamma)R_{\text{PN}}(g) + \gamma R_{\text{PU}}(g),$$

$$R_{\text{PNNU}}^\gamma(g) := (1 - \gamma)R_{\text{PN}}(g) + \gamma R_{\text{NU}}(g).$$

In practice, we combine PNPU and PNNU classification and adaptively choose one of them with a new trade-off parameter $\eta \in [-1, 1]$ as

$$R_{\text{PNU}}^\eta(g) := \begin{cases} R_{\text{PNPU}}^\eta(g) & (\eta \geq 0), \\ R_{\text{PNNU}}^{-\eta}(g) & (\eta < 0). \end{cases}$$

We refer to the combined method as *PNU classification*. Clearly, PNU classification with $\eta = -1, 0, +1$ corresponds to NU, PN, and PU classification. As η gets large/small, the effect of the positive/negative classes is more emphasized.

In the theoretical analyses in Section 4, we denote the combinations of the PN risk with the non-convex PU/NU risks by $R_{\text{N-PNPU}}^\gamma$ and $R_{\text{N-PNNU}}^\gamma$, and that with the convex PU/NU risks by $R_{\text{C-PNPU}}^\gamma$ and $R_{\text{C-PNNU}}^\gamma$.

3.3. Practical Implementation

We have so far only considered the true risks R (with respect to the expectations over true data distributions). When a classifier is trained from samples in practice, we use the empirical risks \widehat{R} where the expectations are replaced with corresponding sample averages.

More specifically, in the theoretical analysis in Section 4 and experiments in Section 5, we use a linear-in-parameter model given by $g(\mathbf{x}) = \sum_{j=1}^b w_j \phi_j(\mathbf{x}) = \mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x})$, where $^\top$ denotes the transpose, b is the number of basis

functions, $\mathbf{w} = (w_1, \dots, w_b)^\top$ is a parameter vector, and $\phi(\mathbf{x}) = (\phi_1(\mathbf{x}), \dots, \phi_b(\mathbf{x}))^\top$ is a basis function vector. The parameter vector \mathbf{w} is learned in order to minimize the ℓ_2 -regularized empirical risk:

$$\min_{\mathbf{w}} \widehat{R}(g) + \lambda \mathbf{w}^\top \mathbf{w},$$

where $\lambda \geq 0$ is the regularization parameter.

4. Theoretical Analyses

In this section, we theoretically analyze the behavior of the empirical versions of the proposed semi-supervised classification methods. We first derive generalization error bounds and then discuss variance reduction. Finally, we discuss whether PUNU or PNU classification is more promising. All proofs can be found in Appendix A.

4.1. Generalization Error Bounds

Let \mathcal{G} be a function class of bounded hyperplanes:

$$\mathcal{G} = \{g(\mathbf{x}) = \langle \mathbf{w}, \phi(\mathbf{x}) \rangle \mid \|\mathbf{w}\| \leq C_w, \|\phi(\mathbf{x})\| \leq C_\phi\},$$

where C_w and C_ϕ are certain positive constants. Since ℓ_2 -regularization is always included, we can naturally assume that the empirical risk minimizer g belongs to a certain \mathcal{G} . Denote by $\ell_{0-1}(m) = (1 - \text{sign}(m))/2$ the *zero-one loss* and $I(g) = \mathbb{E}_{p(\mathbf{x}, y)}[\ell_{0-1}(yg(\mathbf{x}))]$ the risk of g for binary classification, i.e., the generalization error of g . In the following, we study upper bounds of $I(g)$ holding uniformly for all $g \in \mathcal{G}$. We respectively focus on the *scaled ramp and squared losses* for the non-convex and convex methods due to limited space. Similar results can be obtained with a little more effort if other eligible losses are used. For convenience, we define a function as

$$\chi(c_P, c_N, c_U) = c_P \theta_P / \sqrt{n_P} + c_N \theta_N / \sqrt{n_N} + c_U / \sqrt{n_U}.$$

Non-Convex Methods: A key observation is that $\ell_{0-1}(m) \leq 2\ell_R(m)$, and consequently $I(g) \leq 2R(g)$. Note that by definition we have

$$R_{N-PUNU}^\gamma(g) = R_{N-PNPU}^\gamma(g) = R_{N-PNNU}^\gamma(g) = R(g).$$

The theorem below can be proven using the Rademacher analysis (see, for example, Mohri et al., 2012; Ledoux & Talagrand, 1991).

Theorem 1 *Let $\ell_R(m)$ be the loss for defining the empirical risks. For any $\delta > 0$, the following inequalities hold separately with probability at least $1 - \delta$ for all $g \in \mathcal{G}$:*

$$I(g) \leq 2\widehat{R}_{N-PUNU}^\gamma(g) + C_{w,\phi,\delta} \cdot \chi(2 - 2\gamma, 2\gamma, |2\gamma - 1|),$$

$$I(g) \leq 2\widehat{R}_{N-PNPU}^\gamma(g) + C_{w,\phi,\delta} \cdot \chi(1 + \gamma, 1 - \gamma, \gamma),$$

$$I(g) \leq 2\widehat{R}_{N-PNNU}^\gamma(g) + C_{w,\phi,\delta} \cdot \chi(1 - \gamma, 1 + \gamma, \gamma),$$

where $C_{w,\phi,\delta} = 2C_w C_\phi + \sqrt{2 \ln(3/\delta)}$.

Theorem 1 guarantees that when $\ell_R(m)$ is used, $I(g)$ can be bounded from above by two times the empirical risks, i.e., $2\widehat{R}_{N-PUNU}^\gamma(g)$, $2\widehat{R}_{N-PNPU}^\gamma(g)$, and $2\widehat{R}_{N-PNNU}^\gamma(g)$, plus the corresponding confidence terms of order

$$\mathcal{O}_p(1/\sqrt{n_P} + 1/\sqrt{n_N} + 1/\sqrt{n_U}).$$

Since n_P , n_N , and n_U can increase independently, this is already the optimal convergence rate without any additional assumption (Vapnik, 1998; Mendelson, 2008).

Convex Methods: Analogously, we have $\ell_{0-1}(m) \leq 4\ell_S(m)$ for the squared loss. However, it is too loose when $|m| \gg 0$. Fortunately, we do not have to use $\ell_S(m)$ if we work on the generalization error rather than the estimation error. To this end, we define the *truncated (scaled) squared loss* $\ell_{TS}(m)$ as

$$\ell_{TS}(m) = \begin{cases} \ell_S(m) & 0 < m \leq 1, \\ \ell_{0-1}(m)/4 & \text{otherwise,} \end{cases}$$

so that $\ell_{0-1}(m) \leq 4\ell_{TS}(m)$ is much tighter. For $\ell_{TS}(m)$, $R_{C-PU}(g)$ and $R_{C-NU}(g)$ need to be redefined as follows (see du Plessis et al., 2015):

$$R_{C-PU}(g) := \theta_P R'_P(g) + R_{U,N}(g),$$

$$R_{C-NU}(g) := \theta_N R'_N(g) + R_{U,P}(g),$$

where $R'_P(g)$ and $R'_N(g)$ are simply $R_P(g)$ and $R_N(g)$ w.r.t. the composite loss $\tilde{\ell}_{TS}(m) = \ell_{TS}(m) - \ell_{TS}(-m)$. The condition $\tilde{\ell}_{TS}(m) \neq -m$ means the loss of convexity, but the equivalence is not lost; indeed, we still have

$$R_{C-PUNU}^\gamma(g) = R_{C-PNPU}^\gamma(g) = R_{C-PNNU}^\gamma(g) = R(g).$$

Theorem 2 *Let $\ell_{TS}(m)$ be the loss for defining the empirical risks (where $R_{C-PU}(g)$ and $R_{C-NU}(g)$ are redefined). For any $\delta > 0$, the following inequalities hold separately with probability at least $1 - \delta$ for all $g \in \mathcal{G}$:*

$$I(g) \leq 4\widehat{R}_{C-PUNU}^\gamma(g) + C'_{w,\phi,\delta} \cdot \chi(1 - \gamma, \gamma, 1),$$

$$I(g) \leq 4\widehat{R}_{C-PNPU}^\gamma(g) + C'_{w,\phi,\delta} \cdot \chi(1, 1 - \gamma, \gamma),$$

$$I(g) \leq 4\widehat{R}_{C-PNNU}^\gamma(g) + C'_{w,\phi,\delta} \cdot \chi(1 - \gamma, 1, \gamma),$$

where $C'_{w,\phi,\delta} = 4C_w C_\phi + \sqrt{2 \ln(4/\delta)}$.

Theorem 2 ensures that when $\ell_{TS}(m)$ is used (for evaluating the empirical risks rather than learning the empirical risk minimizers), $I(g)$ can be bounded from above by four times the empirical risks plus confidence terms in the optimal parametric rate. As $\ell_{TS}(m) \leq \ell_S(m)$, Theorem 2 is valid (but weaker) if all empirical risks are w.r.t. $\ell_S(m)$.

4.2. Variance Reduction

Our empirical risk estimators proposed in Section 3 are all unbiased. The next question is whether their variance can be smaller than that of $\widehat{R}_{\text{PN}}(g)$, i.e., whether \mathcal{X}_{U} can help reduce the variance in estimating $R(g)$. To answer this question, pick any g of interest. For simplicity, we assume that $n_{\text{U}} \rightarrow \infty$, to illustrate the maximum variance reduction that could be achieved. Due to limited space, we only focus on the non-convex methods.

Similarly to $R_{\text{P}}(g)$ and $R_{\text{N}}(g)$, let $\sigma_{\text{P}}^2(g)$ and $\sigma_{\text{N}}^2(g)$ be the corresponding variance:

$$\sigma_{\text{P}}^2(g) := \text{Var}_{\text{P}}[\ell(g(\mathbf{x}))], \quad \sigma_{\text{N}}^2(g) := \text{Var}_{\text{N}}[\ell(-g(\mathbf{x}))],$$

where Var_{P} and Var_{N} denote the variance over $p_{\text{P}}(\mathbf{x})$ and $p_{\text{N}}(\mathbf{x})$. Moreover, denote by $\psi_{\text{P}} = \theta_{\text{P}}^2 \sigma_{\text{P}}^2(g)/n_{\text{P}}$ and $\psi_{\text{N}} = \theta_{\text{N}}^2 \sigma_{\text{N}}^2(g)/n_{\text{N}}$ for short, and let Var be the variance over $p_{\text{P}}(\mathbf{x}_1^{\text{P}}) \cdots p_{\text{P}}(\mathbf{x}_{n_{\text{P}}}^{\text{P}}) \cdot p_{\text{N}}(\mathbf{x}_1^{\text{N}}) \cdots p_{\text{N}}(\mathbf{x}_{n_{\text{N}}}^{\text{N}}) \cdot p(\mathbf{x}_1^{\text{U}}) \cdots p(\mathbf{x}_{n_{\text{U}}}^{\text{U}})$.

Theorem 3 Assume $n_{\text{U}} \rightarrow \infty$. For any fixed g , let

$$\gamma_{\text{N-PUNU}} = \underset{\gamma}{\text{argmin}} \text{Var}[\widehat{R}_{\text{N-PUNU}}^{\gamma}(g)] = \frac{\psi_{\text{P}}}{\psi_{\text{P}} + \psi_{\text{N}}}. \quad (9)$$

Then, we have $\gamma_{\text{N-PUNU}} \in [0, 1]$. Further, $\text{Var}[\widehat{R}_{\text{N-PUNU}}^{\gamma}(g)] < \text{Var}[\widehat{R}_{\text{PN}}(g)]$ for all $\gamma \in (2\gamma_{\text{N-PUNU}} - 1/2, 1/2)$ if $\psi_{\text{P}} < \psi_{\text{N}}$, or for all $\gamma \in (1/2, 2\gamma_{\text{N-PUNU}} - 1/2)$ if $\psi_{\text{P}} > \psi_{\text{N}}$.²

Theorem 3 guarantees that the variance is always reduced by $\widehat{R}_{\text{N-PUNU}}^{\gamma}(g)$ if γ is close to $\gamma_{\text{N-PUNU}}$, which is optimal for variance reduction. The interval of such good γ values has the length $\min\{|\psi_{\text{P}} - \psi_{\text{N}}|/(\psi_{\text{P}} + \psi_{\text{N}}), 1/2\}$. In particular, if $3\psi_{\text{P}} \leq \psi_{\text{N}}$ or $\psi_{\text{P}} \geq 3\psi_{\text{N}}$, the length is $1/2$.

Theorem 4 Assume $n_{\text{U}} \rightarrow \infty$. For any fixed g , let

$$\gamma_{\text{N-PNPU}} = \underset{\gamma}{\text{argmin}} \text{Var}[\widehat{R}_{\text{N-PNPU}}^{\gamma}(g)] = \frac{\psi_{\text{N}} - \psi_{\text{P}}}{\psi_{\text{P}} + \psi_{\text{N}}}, \quad (10)$$

$$\gamma_{\text{N-PNNU}} = \underset{\gamma}{\text{argmin}} \text{Var}[\widehat{R}_{\text{N-PNNU}}^{\gamma}(g)] = \frac{\psi_{\text{P}} - \psi_{\text{N}}}{\psi_{\text{P}} + \psi_{\text{N}}}. \quad (11)$$

Then, we have $\gamma_{\text{N-PNPU}} \in [0, 1]$ if $\psi_{\text{P}} \leq \psi_{\text{N}}$ or $\gamma_{\text{N-PNNU}} \in [0, 1]$ if $\psi_{\text{P}} \geq \psi_{\text{N}}$. Additionally, $\text{Var}[\widehat{R}_{\text{N-PNPU}}^{\gamma}(g)] < \text{Var}[\widehat{R}_{\text{PN}}(g)]$ for all $\gamma \in (0, 2\gamma_{\text{N-PNPU}})$ if $\psi_{\text{P}} < \psi_{\text{N}}$, or $\text{Var}[\widehat{R}_{\text{N-PNNU}}^{\gamma}(g)] < \text{Var}[\widehat{R}_{\text{PN}}(g)]$ for all $\gamma \in (0, 2\gamma_{\text{N-PNNU}})$ if $\psi_{\text{P}} > \psi_{\text{N}}$.

Theorem 4 implies that the variance of $\widehat{R}_{\text{PN}}(g)$ is reduced by either $\widehat{R}_{\text{N-PNPU}}^{\gamma}(g)$ if $\psi_{\text{P}} \leq \psi_{\text{N}}$ or $\widehat{R}_{\text{N-PNNU}}^{\gamma}(g)$

²Being fixed means g is determined before seeing the data for evaluating the empirical risk. For example, if g is trained by some learning method, and the empirical risk is subsequently evaluated on the validation/test data, g is regarded as fixed in the evaluation.

if $\psi_{\text{P}} \geq \psi_{\text{N}}$, where γ should be close to $\gamma_{\text{N-PNPU}}$ or $\gamma_{\text{N-PNNU}}$. The range of such good γ values is of length $\min\{2|\psi_{\text{P}} - \psi_{\text{N}}|/(\psi_{\text{P}} + \psi_{\text{N}}), 1\}$. In particular, if $3\psi_{\text{P}} \leq \psi_{\text{N}}$, $\widehat{R}_{\text{N-PNPU}}^{\gamma}(g)$ given any $\gamma \in (0, 1)$ can reduce the variance, and if $\psi_{\text{P}} \geq 3\psi_{\text{N}}$, $\widehat{R}_{\text{N-PNNU}}^{\gamma}(g)$ given any $\gamma \in (0, 1)$ can reduce the variance.

As a corollary of Theorems 3 and 4, the minimum variance achievable by $\widehat{R}_{\text{N-PUNU}}^{\gamma}(g)$, $\widehat{R}_{\text{N-PNPU}}^{\gamma}(g)$, and $\widehat{R}_{\text{N-PNNU}}^{\gamma}(g)$ at their optimal $\gamma_{\text{N-PUNU}}$, $\gamma_{\text{N-PNPU}}$, and $\gamma_{\text{N-PNNU}}$ is exactly the same, namely, $4\psi_{\text{P}}\psi_{\text{N}}/(\psi_{\text{P}} + \psi_{\text{N}})$. Nevertheless, $\widehat{R}_{\text{N-PNPU}}^{\gamma}(g)$ and $\widehat{R}_{\text{N-PNNU}}^{\gamma}(g)$ have a much wider range of nice γ values than $\widehat{R}_{\text{N-PUNU}}^{\gamma}(g)$.

If we further assume that $\sigma_{\text{P}}(g) = \sigma_{\text{N}}(g)$, the condition in Theorems 3 and 4 as to whether $\psi_{\text{P}} \leq \psi_{\text{N}}$ or $\psi_{\text{P}} \geq \psi_{\text{N}}$ will be independent of g . Also, it will coincide with the condition in Theorem 7 in Niu et al. (2016) where the minimizers of $\widehat{R}_{\text{PN}}(g)$, $\widehat{R}_{\text{PU}}(g)$ and $\widehat{R}_{\text{NU}}(g)$ are compared.

A final remark is that learning is uninvolved in Theorems 3 and 4, such that $\ell(m)$ can be any loss that satisfies $\ell(m) + \ell(-m) = 1$, and g can be any fixed decision function. For instance, we may adopt $\ell_{0-1}(m)$ and pick some g resulted from some other learning methods. As a consequence, the variance of $\widehat{I}_{\text{PN}}(g)$ over the validation data can be reduced, and then the cross-validation should be more stable, given that n_{U} is sufficiently large. Therefore, even without being minimized, our proposed risk estimators are themselves of practical importance.

4.3. PUNU vs. PNU Classification

We discuss here which approach, PUNU or PNU classification, is more promising according to state-of-the-art theoretical comparisons (Niu et al., 2016), which are based on estimation error bounds.

Let \widehat{g}_{PN} , \widehat{g}_{PU} , and \widehat{g}_{NU} be the minimizers of $\widehat{R}_{\text{PN}}(g)$, $\widehat{R}_{\text{PU}}(g)$, and $\widehat{R}_{\text{NU}}(g)$, respectively. Let $\alpha_{\text{PU,PN}} := (\theta_{\text{P}}/\sqrt{n_{\text{P}}} + 1/\sqrt{n_{\text{U}}})/(\theta_{\text{N}}/\sqrt{n_{\text{N}}})$ and $\alpha_{\text{NU,PN}} := (\theta_{\text{N}}/\sqrt{n_{\text{N}}} + 1/\sqrt{n_{\text{U}}})/(\theta_{\text{P}}/\sqrt{n_{\text{P}}})$. The finite-sample comparisons state that if $\alpha_{\text{PU,PN}} > 1$ ($\alpha_{\text{NU,PN}} > 1$), PN classification is more promising than PU (NU) classification, i.e., $R(\widehat{g}_{\text{PN}}) < R(\widehat{g}_{\text{PU}})$ ($R(\widehat{g}_{\text{PN}}) < R(\widehat{g}_{\text{NU}})$); otherwise PU (NU) classification is more promising than PN classification (cf. Section 3.2 in Niu et al., 2016).

Suppose that n_{U} is not sufficiently large against n_{P} and n_{N} . According to the finite-sample comparisons, PN classification is most promising, and either PU or NU classification is the second best, i.e., $R(\widehat{g}_{\text{PN}}) < R(\widehat{g}_{\text{PU}}) < R(\widehat{g}_{\text{NU}})$ or $R(\widehat{g}_{\text{PN}}) < R(\widehat{g}_{\text{NU}}) < R(\widehat{g}_{\text{PU}})$. On the other hand, if n_{U} is sufficiently large ($n_{\text{U}} \rightarrow \infty$, which is faster than $n_{\text{P}}, n_{\text{N}} \rightarrow \infty$), we have the asymptotic comparisons: $\alpha_{\text{PU,PN}}^* = \lim_{n_{\text{P}}, n_{\text{N}}, n_{\text{U}} \rightarrow \infty} \alpha_{\text{PU,PN}}$, $\alpha_{\text{NU,PN}}^* =$

$\lim_{n_P, n_N, n_U \rightarrow \infty} \alpha_{\text{NU,PN}}$, and $\alpha_{\text{PU,PN}}^* \cdot \alpha_{\text{NU,PN}}^* = 1$. From the last equation, if $\alpha_{\text{PU,PN}}^* < 1$, then $\alpha_{\text{NU,PN}}^* > 1$, implying that PU (PN) classification is more promising than PN (NU) classification, i.e., $R(\hat{g}_{\text{PU}}) < R(\hat{g}_{\text{PN}}) < R(\hat{g}_{\text{NU}})$. Similarly, when $\alpha_{\text{PU,PN}}^* > 1$ and $\alpha_{\text{NU,PN}}^* < 1$, $R(\hat{g}_{\text{NU}}) < R(\hat{g}_{\text{PN}}) < R(\hat{g}_{\text{PU}})$ (cf. Section 3.3 in Niu et al., 2016).

In real-world applications, since we do not know whether the number of unlabeled samples is sufficiently large or not, a practical approach is to combine the best methods in both the finite-sample and asymptotic comparisons cases. PNU classification is the combination of the best methods in both cases, but PUNU classification is not. In addition, PUNU classification includes the worst one in its combination in both cases. From this viewpoint, PNU classification would be more promising than PUNU classification, as demonstrated in the experiments shown in the next section.

5. Experiments

In this section, we first numerically analyze the proposed approach and then compare the proposed semi-supervised classification methods against existing methods. All experiments were carried out using a PC equipped with two 2.60GHz Intel® Xeon® E5-2640 v3 CPUs.

5.1. Experimental Analyses

Here, we numerically analyze the behavior of our proposed approach. Due to limited space, we show results on two out of six data sets and move the rest to Appendix C.

Common Setup: As a classifier, we use the Gaussian kernel model: $g(\mathbf{x}) = \sum_{i=1}^n w_i \exp(-\|\mathbf{x} - \mathbf{x}_i\|^2 / (2\sigma^2))$, where $n = n_P + n_N$, $\{w_i\}_{i=1}^n$ are the parameters, $\{\mathbf{x}_i\}_{i=1}^n = \mathcal{X}_P \cup \mathcal{X}_N$, and $\sigma > 0$ is the Gaussian bandwidth. The bandwidth candidates are $\{1/8, 1/4, 1/2, 1, 3/2, 2\} \times \text{median}(\|\mathbf{x}_i - \mathbf{x}_j\|_{i,j=1}^n)$. The classifier trained by minimizing the empirical PN risk is denoted by \hat{g}_{PN} . The number of labeled samples for training is 20, where the class-prior was 0.5. In all experiments, we used the squared loss for training. We note that the class-prior of test data was the same as that of unlabeled data.

Variance Reduction in Practice: Here, we numerically investigate how many unlabeled samples are sufficient in practice such that the variance of the empirical PNU risk is smaller than that of the PN risk: $\text{Var}[\hat{R}_{\text{PNU}}^\eta(g)] < \text{Var}[\hat{R}_{\text{PN}}(g)]$ given a fixed classifier g .

As the fixed classifier, we used the classifier \hat{g}_{PN} , where the hyperparameters were determined by five-fold cross-validation. To compute the variance of the empirical PN and PNU risks, $\text{Var}[\hat{R}_{\text{PN}}(\hat{g}_{\text{PN}})]$ and $\text{Var}[\hat{R}_{\text{PNU}}^\eta(\hat{g}_{\text{PN}})]$, we repeatedly drew additional $n_U^V = 10$ positive, $n_N^V = 10$

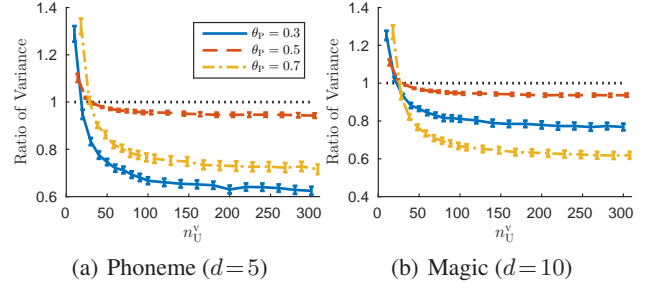


Figure 1. Average and standard error of the ratio between the variance of empirical PNU risk and that of PN risk, $\text{Var}[\hat{R}_{\text{PNU}}^\eta(\hat{g}_{\text{PN}})] / \text{Var}[\hat{R}_{\text{PN}}(\hat{g}_{\text{PN}})]$, as a function of the number of unlabeled samples over 100 trials. Although the variance reduction is proved for an infinite number of samples, it can be observed with a finite number of samples.

negative, and n_U^V unlabeled samples from the rest of the data set. The additional samples were also used for approximating $\hat{\sigma}_P(\hat{g}_{\text{PN}})$ and $\hat{\sigma}_N(\hat{g}_{\text{PN}})$ to compute η , i.e., γ in Eqs.(10) and (11).

Figure 1 shows the ratio between the variance of the empirical PNU risk and that of the PN risk, $\text{Var}[\hat{R}_{\text{PNU}}^\eta(\hat{g}_{\text{PN}})] / \text{Var}[\hat{R}_{\text{PN}}(\hat{g}_{\text{PN}})]$. The number of unlabeled samples for validation n_U^V increases from 10 to 300. We see that with a rather small number of unlabeled samples, the ratio becomes less than 1. That is, the variance of the empirical PNU risk becomes smaller than that of the PN risk. This implies that although the variance reduction is proved for an infinite number of unlabeled samples, it can be observed under a finite number of samples in practice.

Compared to when $\theta_P = 0.3$ and 0.7 , the effect of variance reduction is small when $\theta_P = 0.5$. This is because if we assume $\sigma_P(g) \approx \sigma_N(g)$, when $n_P \approx n_N$ and $\theta_P = 0.5$, we have $\gamma_{\text{N-PNPU}} \approx \gamma_{\text{N-PNNU}} \approx 0$ (because $\psi_P \approx \psi_N$. See Theorem 4). That is, the PNU risk is dominated by the PN risk, implying that $\text{Var}[\hat{R}_{\text{PNU}}^\eta(g)] \approx \text{Var}[\hat{R}_{\text{PN}}(g)]$. Note that the class-prior is not the only factor for variance reduction; for example, if $\theta_P = 0.5$, $n_P \gg n_N$, and $\sigma_P(g) \approx \sigma_N(g)$, then $\gamma_{\text{N-PNPU}} \not\approx 0$ (because $\psi_P \ll \psi_N$) and the variance reduction will be large.

PNU Risk in Validation: As discussed in Section 4, the empirical PNU risk will be a reliable validation score due to its having smaller variance than the empirical PN risk. We show here that the empirical PNU risk is a promising alternative to a validation score.

To focus on the effect of validation scores only, we trained two classifiers by using the same risk, e.g, the empirical PN risk. We then tune the classifiers with the empirical PN and PNU risks denoted by $\hat{g}_{\text{PN}}^{\text{PN}}$ and $\hat{g}_{\text{PN}}^{\text{PNU}}$, respectively. The number of validation samples was the same as in the previous experiment.

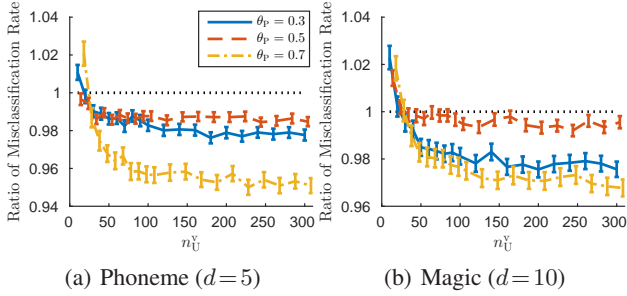


Figure 2. Average and standard error of the ratio between the misclassification rates of \hat{g}_{PN}^{PNU} and \hat{g}_{PN}^{PN} as a function of unlabeled samples over 1000 trials. In many cases, the ratio becomes less than 1, implying that the PNU risk is a promising alternative to the standard PN risk in validation if unlabeled data are available.

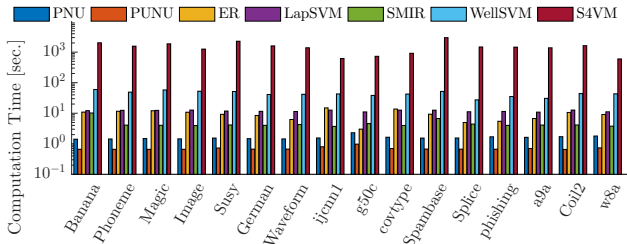


Figure 3. Average computation time over 50 trials for benchmark data sets when $n_L = 50$.

Figure 2 shows the ratio between the misclassification rate of \hat{g}_{PN}^{PNU} and that of \hat{g}_{PN}^{PN} . The number of unlabeled samples for validation increases from 10 to 300. With a rather small number of unlabeled samples, the ratio becomes less than 1, i.e., \hat{g}_{PN}^{PNU} achieves better performance than \hat{g}_{PN}^{PN} . In particular, when $\theta_P = 0.3$ and 0.7 , \hat{g}_{PN}^{PNU} improved substantially; the large improvement tends to give the large variance reduction (cf. Figure 1). This result shows that the use of the empirical PNU risk for validation improved the classification performance given a relatively large size of unlabeled data.

5.2. Comparison with Existing Methods

Next, we numerically compare the proposed methods against existing semi-supervised classification methods.

Common Setup: We compare our methods against five conventional semi-supervised classification methods: *entropy regularization* (ER) (Grandvalet & Bengio, 2004), the *Laplacian support vector machine* (LapSVM) (Belkin et al., 2006; Melacci & Belkin, 2011), *squared-loss mutual information regularization* (SMIR) (Niu et al., 2013), the *weakly labeled support vector machine* (WellSVM) (Li et al., 2013), and the *safe semi-supervised support vector machine* (S4VM) (Li & Zhou, 2015).

Among the proposed methods, PNU classification and

Table 1. Average and standard error of the misclassification rates of each method over 50 trials for benchmark data sets. Boldface numbers denote the best and comparable methods in terms of average misclassifications rate according to a t-test at a significance level of 5%. The bottom row gives the number of best/comparable cases of each method.

Data set	n_L	PNU	PUNU	ER	LapSVM	SMIR	WellSVM	S4VM
Banana	10	30.1 (1.0)	32.1 (1.1)	35.8 (1.0)	36.9 (1.0)	37.7 (1.1)	41.8 (0.6)	45.3 (1.0)
	$d = 2$	50 19.0 (0.6)	26.4 (1.2)	20.6 (0.7)	21.3 (0.7)	21.1 (1.0)	42.6 (0.5)	38.7 (0.9)
Phoneme	10	32.5 (0.8)	33.5 (1.0)	33.4 (1.2)	36.5 (1.5)	36.4 (1.2)	28.4 (0.6)	33.7 (1.4)
	$d = 5$	50 28.1 (0.5)	32.8 (0.9)	27.8 (0.6)	27.0 (0.8)	28.6 (1.0)	26.8 (0.4)	25.1 (0.2)
Magic	10	31.7 (0.8)	34.1 (0.9)	34.2 (1.1)	37.9 (1.3)	36.0 (1.2)	30.1 (0.8)	33.3 (0.9)
	$d = 10$	50 29.9 (0.8)	33.4 (0.9)	30.9 (0.5)	31.0 (0.9)	30.8 (0.9)	28.8 (0.8)	29.2 (0.4)
Image	10	29.8 (0.9)	31.7 (0.8)	33.7 (1.1)	36.6 (1.2)	36.7 (1.2)	34.7 (1.1)	35.9 (1.0)
	$d = 18$	50 20.7 (0.8)	26.6 (1.1)	20.8 (0.8)	20.3 (1.0)	20.9 (0.9)	27.2 (1.0)	23.2 (0.7)
Susy	10	44.6 (0.6)	45.0 (0.6)	47.7 (0.4)	48.2 (0.4)	45.1 (0.7)	48.0 (0.3)	46.8 (0.3)
	$d = 18$	50 38.9 (0.6)	41.5 (0.6)	37.9 (0.7)	43.1 (0.6)	43.9 (0.8)	43.8 (0.7)	42.1 (0.4)
German	10	40.8 (0.9)	42.4 (0.7)	43.6 (0.9)	45.9 (0.7)	46.2 (0.8)	42.4 (0.8)	42.0 (0.7)
	$d = 20$	50 36.2 (0.8)	39.0 (0.8)	38.9 (0.6)	40.6 (0.6)	38.4 (1.1)	38.5 (1.0)	34.9 (0.5)
Waveform	10	17.4 (0.6)	18.0 (0.9)	18.5 (0.6)	24.9 (1.4)	18.0 (1.0)	16.7 (0.6)	20.8 (0.8)
	$d = 21$	50 16.3 (0.6)	23.7 (1.2)	14.2 (0.4)	18.1 (0.8)	15.4 (0.6)	15.5 (0.5)	15.3 (0.3)
ijcnn1	10	43.6 (0.6)	40.3 (1.0)	49.7 (0.1)	49.2 (0.3)	44.0 (1.0)	45.9 (0.7)	49.3 (0.8)
	$d = 22$	50 34.5 (0.8)	37.1 (0.9)	35.5 (0.8)	33.4 (1.1)	49.4 (0.3)	46.2 (0.8)	48.6 (0.4)
g50c	10	11.4 (0.6)	12.5 (0.6)	23.3 (2.3)	39.8 (1.6)	21.9 (1.3)	6.6 (0.4)	27.0 (1.4)
	$d = 50$	50 12.5 (1.1)	10.1 (0.6)	8.7 (0.4)	22.5 (1.5)	10.6 (0.6)	7.4 (0.4)	12.1 (0.5)
covtype	10	46.2 (0.4)	46.0 (0.4)	46.0 (0.5)	47.1 (0.5)	47.9 (0.5)	46.9 (0.6)	46.4 (0.4)
	$d = 54$	50 41.3 (0.5)	42.3 (0.5)	41.0 (0.4)	41.5 (0.5)	46.2 (0.8)	43.6 (0.6)	40.8 (0.4)
Spambase	10	27.2 (0.9)	28.1 (1.1)	31.8 (1.4)	39.7 (1.4)	30.9 (1.3)	23.8 (0.8)	36.1 (1.5)
	$d = 57$	50 23.4 (1.0)	26.6 (1.0)	22.1 (0.7)	28.5 (1.3)	20.9 (0.5)	19.1 (0.4)	24.5 (0.9)
Splice	10	38.3 (0.8)	39.3 (0.8)	43.9 (0.8)	47.9 (0.5)	41.6 (0.7)	42.0 (1.0)	42.4 (0.6)
	$d = 60$	50 30.6 (0.8)	34.7 (0.9)	30.9 (0.8)	38.8 (1.0)	30.6 (0.9)	40.9 (0.8)	35.9 (0.7)
phishing	10	24.2 (1.2)	25.8 (1.0)	27.3 (1.6)	37.2 (1.6)	27.6 (1.6)	27.5 (1.4)	31.7 (1.3)
	$d = 68$	50 15.8 (0.6)	18.3 (0.8)	15.4 (0.5)	21.1 (1.3)	14.7 (0.8)	17.2 (0.7)	16.7 (0.8)
a9a	10	31.4 (0.9)	31.3 (1.0)	34.3 (1.2)	41.0 (1.1)	37.3 (1.3)	33.1 (1.2)	34.3 (1.2)
	$d = 83$	50 27.9 (0.6)	29.9 (0.8)	28.6 (0.7)	33.3 (1.0)	26.9 (0.7)	28.9 (0.8)	26.2 (0.4)
Coil2	10	38.7 (0.8)	40.1 (0.8)	42.8 (0.7)	43.9 (0.8)	43.2 (0.8)	39.1 (0.9)	44.0 (0.8)
	$d = 241$	50 23.2 (0.6)	30.5 (0.9)	23.6 (0.9)	22.8 (0.9)	25.1 (0.9)	22.6 (0.8)	25.4 (0.8)
w8a	10	35.9 (0.9)	33.6 (1.0)	41.6 (1.0)	46.6 (0.8)	39.4 (0.9)	42.1 (0.8)	43.0 (0.8)
	$d = 300$	50 28.1 (0.7)	27.6 (0.6)	27.0 (0.9)	38.7 (0.8)	28.0 (0.9)	33.7 (0.8)	35.2 (1.0)
#Best/Comp.		23	13	11	4	9	13	7

PUNU classification with the squared loss were tested.³

Data Sets: We used sixteen benchmark data sets taken from the *UCI Machine Learning Repository* (Lichman, 2013), the *Semi-Supervised Learning book* (Chapelle et al., 2006), the *LIBSVM* (Chang & Lin, 2011), the *ELENA Project*,⁴ and a paper by Chapelle & Zien (2005).⁵ Each feature was scaled to $[0, 1]$. Similarly to the setting in Section 5.1, we used the Gaussian kernel model for all methods. The training data is $\{\mathbf{x}_i\}_{i=1}^n = \mathcal{X}_P \cup \mathcal{X}_N \cup \mathcal{X}_U$, where $n = n_P + n_N + n_U$. We selected all hyper-parameters with validation samples of size 20 ($n_P^V = n_N^V = 10$). For training, we drew n_L labeled and $n_U = 300$ unlabeled samples. The class-prior of labeled data was set at 0.7 and that of unlabeled samples was set at $\theta_P = 0.5$ that were assumed to be known. In practice, the class-prior, θ_P , can be estimated

³In preliminary experiments, we tested other loss functions such as the ramp and logistic losses and concluded that the difference in loss functions did not provide noticeable difference.

⁴<https://www.elen.ucl.ac.be/neural-nets/Research/Projects/ELENA/elena.htm>

⁵<http://olivier.chapelle.cc/lds/>

Table 2. Average and standard error of misclassification rates over 30 trials for the Places 205 data set. Boldface numbers denote the best and comparable methods in terms of the average misclassification rate according to a t-test at a significance level of 5%.

Data set	n_U	θ_P	$\hat{\theta}_P$	PNU	ER	LapSVM	SMIR	WellSVM
Arts	1000	0.50	0.49 (0.01)	27.4 (1.3)	26.6 (0.5)	26.1 (0.7)	40.1 (3.9)	27.5 (0.5)
	5000	0.50	0.50 (0.01)	24.8 (0.6)	26.1 (0.5)	26.1 (0.4)	30.1 (1.6)	N/A
	10000	0.50	0.52 (0.01)	25.6 (0.7)	25.4 (0.5)	25.5 (0.6)	N/A	N/A
Deserts	1000	0.73	0.67 (0.01)	13.0 (0.5)	15.3 (0.6)	16.7 (0.8)	17.2 (0.8)	18.2 (0.7)
	5000	0.73	0.67 (0.01)	13.4 (0.4)	13.3 (0.5)	16.6 (0.6)	24.4 (0.6)	N/A
	10000	0.73	0.68 (0.01)	13.3 (0.5)	13.7 (0.6)	16.8 (0.8)	N/A	N/A
Fields	1000	0.65	0.57 (0.01)	22.4 (1.0)	26.2 (1.0)	26.6 (1.3)	28.2 (1.1)	26.6 (0.8)
	5000	0.65	0.57 (0.01)	20.6 (0.5)	22.6 (0.6)	24.7 (0.8)	29.6 (1.2)	N/A
	10000	0.65	0.57 (0.01)	21.6 (0.6)	22.5 (0.6)	25.0 (0.9)	N/A	N/A
Stadiums	1000	0.50	0.50 (0.01)	11.4 (0.4)	11.5 (0.5)	12.5 (0.5)	17.4 (3.6)	11.7 (0.4)
	5000	0.50	0.50 (0.01)	11.0 (0.5)	10.9 (0.3)	11.1 (0.3)	13.4 (0.7)	N/A
	10000	0.50	0.51 (0.00)	10.7 (0.3)	10.9 (0.3)	11.2 (0.2)	N/A	N/A
Platforms	1000	0.27	0.33 (0.01)	21.8 (0.5)	23.9 (0.6)	24.1 (0.5)	30.1 (2.3)	26.2 (0.8)
	5000	0.27	0.34 (0.01)	23.3 (0.8)	24.4 (0.7)	24.9 (0.7)	26.6 (0.3)	N/A
	10000	0.27	0.34 (0.01)	21.4 (0.5)	24.3 (0.6)	24.8 (0.5)	N/A	N/A
Temples	1000	0.55	0.51 (0.01)	43.9 (0.7)	43.9 (0.6)	43.4 (0.6)	50.7 (1.6)	44.3 (0.5)
	5000	0.55	0.54 (0.01)	43.4 (0.9)	43.0 (0.6)	43.1 (1.0)	43.6 (0.7)	N/A
	10000	0.55	0.50 (0.01)	45.2 (0.8)	44.4 (0.8)	44.2 (0.7)	N/A	N/A

by methods proposed, e.g., by Blanchard et al. (2010), Ramaswamy et al. (2016), or Kawakubo et al. (2016).

Table 1 lists the average and standard error of the misclassification rates over 50 trials and the number of best/comparable performances of each method in the bottom row. The superior performance of PNU classification over PUNU classification agrees well with the discussion in Section 4.3. With the g50c data set, which well satisfies the low-density separation principle, the WellSVM achieved the best performance. However, in the Banana data set, where the two classes are highly overlapped, the performance of WellSVM was worse than the other methods. In contrast, PNU classification achieved consistently better/comparable performance and its performance did not degenerate considerably across data sets. These results show that the idea of using PU classification in semi-supervised classification is promising.

Figure 3 plots the computation time, which shows that the fastest computation was achieved using the proposed methods with the square loss.

Image Classification: Finally, we used the *Places 205 data set* (Zhou et al., 2014), which contains 2.5 million images in 205 scene classes. We used a 4096-dimensional feature vector extracted from each image by *AlexNet* under the framework of *Caffe*,⁶ which is available on the project website⁷. We chose two similar scenes to construct binary classification tasks (see the description of data sets in Appendix B.3). We drew 100 labeled and n_U unlabeled samples from each task; the class-prior of labeled and unlabeled data were respectively set at 0.5 and $\theta_P = m_P / (m_P + m_N)$, where m_P and m_N respectively denote the number of total samples in positive and negative scenes. We used a linear

⁶<http://caffe.berkeleyvision.org/>

⁷<http://places.csail.mit.edu/>

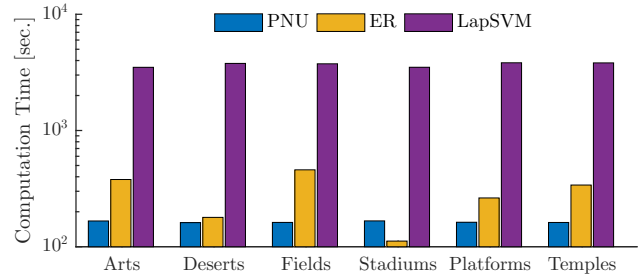


Figure 4. Average computation time over 30 trials for the Places 205 data set when $n_U = 10000$.

classifier $g(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + w_0$, where \mathbf{w} is the weight vector and w_0 is the offset (in the SMIR, the linear kernel model is used; see Niu et al. (2013) for details).

We selected hyper-parameters in PNU classification by applying five-fold cross-validation with respect to $R_{\text{PNU}}^{\bar{\eta}}(g)$ with the zero-one loss, where $\bar{\eta}$ was set at Eq.(10) or Eq.(11) with $\sigma_P(g) = \sigma_N(g)$. The class-prior $p(y = +1) = \theta_P$ was estimated using the method based on energy distance minimization (Kawakubo et al., 2016).

Table 2 lists the average and standard error of the misclassification rates over 30 trials, where methods taking more than 2 hours were omitted and indicated as *N/A*. The results show that PNU classification was most effective. The average computation times are shown in Figure 4, revealing again that PNU classification was the fastest method.

6. Conclusions

In this paper, we proposed a novel semi-supervised classification approach based on classification from positive and unlabeled data. Unlike most of the conventional methods, our approach does not require strong assumptions on the data distribution such as the cluster assumption. We theoretically analyzed the variance of risk estimators and showed that unlabeled data help reduce the variance without the conventional distributional assumptions. We also established generalization error bounds and showed that the confidence term decreases with respect to the number of positive, negative, and unlabeled samples without the conventional distributional assumptions in the optimal parametric order. We experimentally analyzed the behavior of the proposed methods and demonstrated that one of the proposed methods, termed PNU classification, was most effective in terms of both classification accuracy and computational efficiency. It was recently pointed out that PU classification can behave undesirably for very flexible models and a modified PU risk has been proposed (Kiryo et al., 2017). Our future work is to develop a semi-supervised classification method based on the modified PU classification.

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Supplementary Material for “Semi-Supervised Classification Based on Classification from Positive and Unlabeled Data”

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A. Proofs of Theorems

In this section, we give the proofs of Theorems in Section 4.

A.1. Proof of Theorem 1

Recall that

$$\begin{aligned}
 R_{\text{N-PUNU}}^\gamma(g) &= (1 - \gamma)R_{\text{N-PU}}(g) + \gamma R_{\text{N-NU}}(g) \\
 &= (2 - 2\gamma)\theta_{\text{P}}R_{\text{P}}(g) + 2\gamma\theta_{\text{N}}R_{\text{N}}(g) + (1 - \gamma)R_{\text{U,N}}(g) + \gamma R_{\text{U,P}}(g) + \text{Const}, \\
 R_{\text{N-PNPU}}^\gamma(g) &= (1 - \gamma)R_{\text{PN}}(g) + \gamma R_{\text{N-PU}}(g) \\
 &= (1 + \gamma)\theta_{\text{P}}R_{\text{P}}(g) + (1 - \gamma)\theta_{\text{N}}R_{\text{N}}(g) + \gamma R_{\text{U,N}}(g) + \text{Const}, \\
 R_{\text{N-PNNU}}^\gamma(g) &= (1 - \gamma)R_{\text{PN}}(g) + \gamma R_{\text{N-NU}}(g) \\
 &= (1 - \gamma)\theta_{\text{P}}R_{\text{P}}(g) + (1 + \gamma)\theta_{\text{N}}R_{\text{N}}(g) + \gamma R_{\text{U,P}}(g) + \text{Const}.
 \end{aligned}$$

Let $\widehat{R}_{\text{P}}(g)$, $\widehat{R}_{\text{N}}(g)$, $\widehat{R}_{\text{U,P}}(g)$ and $\widehat{R}_{\text{U,N}}(g)$ be the empirical risks. In order to prove Theorem 1, the following concentration lemma is needed:

Lemma 1 *For any $\delta > 0$, we have these uniform deviation bounds with probability at least $1 - \delta/3$:*

$$\begin{aligned}
 \sup_{g \in \mathcal{G}} (R_{\text{P}}(g) - \widehat{R}_{\text{P}}(g)) &\leq \frac{C_w C_\phi}{\sqrt{n_{\text{P}}}} + \sqrt{\frac{\ln(3/\delta)}{2n_{\text{P}}}}, \\
 \sup_{g \in \mathcal{G}} (R_{\text{N}}(g) - \widehat{R}_{\text{N}}(g)) &\leq \frac{C_w C_\phi}{\sqrt{n_{\text{N}}}} + \sqrt{\frac{\ln(3/\delta)}{2n_{\text{N}}}}, \\
 \sup_{g \in \mathcal{G}} (R_{\text{U,P}}(g) - \widehat{R}_{\text{U,P}}(g)) &\leq \frac{C_w C_\phi}{\sqrt{n_{\text{U}}}} + \sqrt{\frac{\ln(3/\delta)}{2n_{\text{U}}}}, \\
 \sup_{g \in \mathcal{G}} (R_{\text{U,N}}(g) - \widehat{R}_{\text{U,N}}(g)) &\leq \frac{C_w C_\phi}{\sqrt{n_{\text{U}}}} + \sqrt{\frac{\ln(3/\delta)}{2n_{\text{U}}}}.
 \end{aligned}$$

All inequalities in Lemma 1 are from the basic *uniform deviation bound* using the Rademacher complexity (Mohri et al., 2012), *Talagrand’s contraction lemma* (Ledoux & Talagrand, 1991), as well as the fact that the Lipschitz constant of ℓ_{R} is 1/2. For these reasons, the detailed proof of Lemma 1 is omitted.

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Consider $R_{N\text{-PNPU}}^\gamma(g)$. It is clear that

$$\begin{aligned} & \sup_{g \in \mathcal{G}} (R_{N\text{-PNPU}}^\gamma(g) - \widehat{R}_{N\text{-PNPU}}^\gamma(g)) \\ & \leq (1 + \gamma)\theta_P \sup_{g \in \mathcal{G}} (R_P(g) - \widehat{R}_P(g)) + (1 - \gamma)\theta_N \sup_{g \in \mathcal{G}} (R_N(g) - \widehat{R}_N(g)) + \gamma \sup_{g \in \mathcal{G}} (R_{U,N}(g) - \widehat{R}_{U,N}(g)). \end{aligned}$$

Therefore, by applying Lemma 1, for any $\delta > 0$, it holds with probability at least $1 - \delta$ that

$$\sup_{g \in \mathcal{G}} (R_{N\text{-PNPU}}^\gamma(g) - \widehat{R}_{N\text{-PNPU}}^\gamma(g)) \leq \frac{1}{2} C_{w,\phi,\delta} \cdot \chi(1 + \gamma, 1 - \gamma, \gamma).$$

Since $I(g) \leq 2R_{N\text{-PNPU}}^\gamma$, with the same probability,

$$\sup_{g \in \mathcal{G}} (I(g) - 2\widehat{R}_{N\text{-PNPU}}^\gamma(g)) \leq C_{w,\phi,\delta} \cdot \chi(1 + \gamma, 1 - \gamma, \gamma).$$

Similarly, $\sup_{g \in \mathcal{G}} (I(g) - 2\widehat{R}_{N\text{-PUNU}}^\gamma(g)) \leq C_{w,\phi,\delta} \cdot \chi(1 - \gamma, 1 + \gamma, \gamma)$ with probability at least $1 - \delta$.

Finally, $R_{N\text{-PUNU}}^\gamma(g)$ is slightly more involved, for that there are both $R_{U,P}(g)$ and $R_{U,N}(g)$. From $\ell_R(m) + \ell_R(-m) = 1$, we can know $R_{U,P}(g) + R_{U,N}(g) = 1$ and then

$$(1 - \gamma)R_{U,N}(g) + \gamma R_{U,P}(g) = \begin{cases} (2\gamma - 1)R_{U,P}(g) + \text{Const} & \gamma \geq 1/2, \\ (1 - 2\gamma)R_{U,N}(g) + \text{Const} & \gamma < 1/2. \end{cases}$$

As a result, $\sup_{g \in \mathcal{G}} (I(g) - 2\widehat{R}_{N\text{-PUNU}}^\gamma(g)) \leq C_{w,\phi,\delta} \cdot \chi(2 - 2\gamma, 2\gamma, |2\gamma - 1|)$ with probability at least $1 - \delta$.

A.2. Proof of Theorem 2

In fact,

$$\ell_{\text{TS}}(m) = \begin{cases} 1/4 & m \leq 0, \\ (m - 1)^2/4 & 0 < m \leq 1, \\ 0 & m > 1, \end{cases}$$

and after plugging this $\ell_{\text{TS}}(m)$ into $\widetilde{\ell}_{\text{TS}}(m)$,

$$\begin{aligned} \widetilde{\ell}_{\text{TS}}(m) &= \ell_{\text{TS}}(m) - \ell_{\text{TS}}(-m) \\ &= \begin{cases} 1/4 & m \leq -1, \\ 1/4 - (m + 1)^2/4 & -1 < m \leq 0, \\ (m - 1)^2/4 - 1/4 & 0 < m \leq 1, \\ -1/4 & m > 1. \end{cases} \end{aligned}$$

It is easy to see that $\ell_{\text{TS}}(m)$ and $\widetilde{\ell}_{\text{TS}}(m)$ are Lipschitz continuous with the same Lipschitz constant $1/2$.

Next, recall that

$$\begin{aligned} R_{C\text{-PUNU}}^\gamma(g) &= (1 - \gamma)R_{C\text{-PU}}(g) + \gamma R_{C\text{-NU}}(g) \\ &= (1 - \gamma)\theta_P R'_P(g) + \gamma\theta_N R'_N(g) + (1 - \gamma)R_{U,N}(g) + \gamma R_{U,P}(g), \\ R_{C\text{-PNPU}}^\gamma(g) &= (1 - \gamma)R_{PN}(g) + \gamma R_{C\text{-PU}}(g) \\ &= (1 - \gamma)\theta_P R_P(g) + (1 - \gamma)\theta_N R_N(g) + \gamma\theta_P R'_P(g) + \gamma R_{U,N}(g), \\ R_{C\text{-PUNU}}^\gamma(g) &= (1 - \gamma)R_{PN}(g) + \gamma R_{C\text{-NU}}(g) \\ &= (1 - \gamma)\theta_P R_P(g) + (1 - \gamma)\theta_N R_N(g) + \gamma\theta_N R'_N(g) + \gamma R_{U,P}(g). \end{aligned}$$

Let $\widehat{R}_P(g)$, $\widehat{R}_N(g)$, $\widehat{R}_{U,P}(g)$, $\widehat{R}_{U,N}(g)$, $\widehat{R}'_P(g)$ and $\widehat{R}'_N(g)$ be the empirical risks. Again, the following concentration lemma is needed:

Lemma 2 For any $\delta > 0$, we have these uniform deviation bounds with probability at least $1 - \delta/4$:

$$\begin{aligned} \sup_{g \in \mathcal{G}} (R_P(g) - \widehat{R}_P(g)) &\leq \frac{C_w C_\phi}{\sqrt{n_P}} + \sqrt{\frac{\ln(4/\delta)}{32n_P}}, \\ \sup_{g \in \mathcal{G}} (R_N(g) - \widehat{R}_N(g)) &\leq \frac{C_w C_\phi}{\sqrt{n_N}} + \sqrt{\frac{\ln(4/\delta)}{32n_N}}, \\ \sup_{g \in \mathcal{G}} (R_{U,P}(g) - \widehat{R}_{U,P}(g)) &\leq \frac{C_w C_\phi}{\sqrt{n_U}} + \sqrt{\frac{\ln(4/\delta)}{32n_U}}, \\ \sup_{g \in \mathcal{G}} (R_{U,N}(g) - \widehat{R}_{U,N}(g)) &\leq \frac{C_w C_\phi}{\sqrt{n_U}} + \sqrt{\frac{\ln(4/\delta)}{32n_U}}, \\ \sup_{g \in \mathcal{G}} (R'_P(g) - \widehat{R}'_P(g)) &\leq \frac{C_w C_\phi}{\sqrt{n_P}} + \sqrt{\frac{\ln(4/\delta)}{8n_P}}, \\ \sup_{g \in \mathcal{G}} (R'_N(g) - \widehat{R}'_N(g)) &\leq \frac{C_w C_\phi}{\sqrt{n_N}} + \sqrt{\frac{\ln(4/\delta)}{8n_N}}. \end{aligned}$$

The detailed proof of Lemma 2 is omitted for the same reason as Lemma 1. The difference is due to that $0 \leq \ell_{TS}(m) \leq 1/4$ and $-1/4 \leq \widetilde{\ell}_{TS}(m) \leq 1/4$ whereas $0 \leq \ell_R(m) \leq 1$ just like $0 \leq \ell_{0-1}(m) \leq 1$. For convenience, we will relax $1/32$ to $1/8$ in the square root for $R_P(g)$, $R_N(g)$, $R_{U,P}(g)$, $R_{U,N}(g)$.

Consider $R_{C-PUNU}^\gamma(g)$. By applying Lemma 2, for any $\delta > 0$, it holds with probability at least $1 - \delta$ that

$$\sup_{g \in \mathcal{G}} (R_{C-PUNU}^\gamma(g) - \widehat{R}_{C-PUNU}^\gamma(g)) \leq \frac{1}{4} C'_{w,\phi,\delta} \cdot \chi(1 - \gamma, \gamma, 1).$$

Since $I(g) \leq 4R_{C-PUNU}^\gamma$, with the same probability,

$$\sup_{g \in \mathcal{G}} (I(g) - 4\widehat{R}_{C-PUNU}^\gamma(g)) \leq C'_{w,\phi,\delta} \cdot \chi(1 - \gamma, \gamma, 1).$$

The other two generalization error bounds can be proven similarly.

A.3. Proofs of Theorems 3 and 4

Note that g is independent of the data for evaluating $\widehat{R}_{N-PUNU}^\gamma(g)$, since it is fixed in the evaluation. Thus, $\text{Var}_P[\widehat{R}_P(g)] = \sigma_P^2(g)/n_P$ and $\text{Var}_N[\widehat{R}_N(g)] = \sigma_N^2(g)/n_N$. When $n_U \rightarrow \infty$,

$$\begin{aligned} \text{Var}[\widehat{R}_{N-PUNU}^\gamma(g)] &= 4(1 - \gamma)^2 \theta_P^2 \text{Var}_P[\widehat{R}_P(g)] + 4\gamma^2 \theta_N^2 \text{Var}_N[\widehat{R}_N(g)] \\ &= 4(1 - \gamma)^2 \psi_P + 4\gamma^2 \psi_N \\ &= 4(\psi_P + \psi_N)\gamma^2 - 8\psi_P\gamma + 4\psi_P, \end{aligned}$$

and it is obvious that $\gamma_{N-PUNU} \in [0, 1]$. All other claims in Theorem 3 follow from that $\text{Var}[\widehat{R}_{N-PUNU}^\gamma(g)]$ is quadratic in γ , that $\text{Var}[\widehat{R}_{N-PUNU}^\gamma(g)] = \text{Var}[\widehat{R}_{PN}(g)]$ at $\gamma = 1/2$, and that $\gamma_{N-PUNU} < 1/2$ if $\psi_P < \psi_N$ or $\gamma_{N-PUNU} > 1/2$ if $\psi_P > \psi_N$.

Likewise, when $n_U \rightarrow \infty$,

$$\begin{aligned} \text{Var}[\widehat{R}_{N-PNPU}^\gamma(g)] &= (1 + \gamma)^2 \psi_P + (1 - \gamma)^2 \psi_N, \\ \text{Var}[\widehat{R}_{N-PNNU}^\gamma(g)] &= (1 - \gamma)^2 \psi_P + (1 + \gamma)^2 \psi_N, \end{aligned}$$

and $\gamma_{N-PNPU} \geq 0$ if $\psi_P \leq \psi_N$ or $\gamma_{N-PNNU} \geq 0$ if $\psi_P \geq \psi_N$. The rest of proof of Theorem 4 is analogous to that of Theorem 3.

B. Experimental Setting

Here, we summarized the experimental settings.

B.1. Implementation in Our Experiments

We implemented the ER by ourselves, and for the other methods, we used the codes available at the authors’ websites:

- LapSVM: <http://www.dii.unisi.it/~melacchi/lapsvmp/>
- SMIR: <http://www.ms.k.u-tokyo.ac.jp/software/SMIR.zip>
- WellSVM: http://lamda.nju.edu.cn/code_WellSVM.ashx
- S4VM: <http://lamda.nju.edu.cn/files/s4vm.rar>.

Note that we modified the original code of the S4VM for transductive learning to inductive learning according to Li & Zhou (2015).

B.2. Parameter Candidates in Our Experiments

The regularization parameters for all the methods were chosen from $\{10^{-5}, 10^{-4}, \dots, 10^2\}$, except the regularization parameter of the SMIR for the squared loss mutual information (SMI) and that of the S4VM for labeled data. The number of nearest-neighbors to construct Laplacian matrix for the LapSVM was chosen from the candidates $\{5, 6, \dots, 10\}$. The combination parameter η of PNU classification was chosen from $\{-1, -0.9, \dots, 1\}$, and γ of PUNU classification was chosen from $\{0, 0.05, \dots, 1\}$. We chose these hyper-parameters by five-fold cross-validation. The parameter for the ℓ_2 -regularizer of the SMIR is set at $\gamma_S / (n \cdot \min_{k \in \{\pm 1\}} p(y = k)) + 0.001$, where γ_S is the regularization parameter for the SMI. The regularization parameter of the S4VM for the labeled data is set at 1. The other parameters were set at the default values.

B.3. Data Set Description of Image Classification Data Set

Table 1 is the description of the data sets used in the image classification experiment.

Table 1. The description of the data set used in the image classification experiment.

Data set	Data sources	#Samples
Arts	Art Gallery	$(m_P = 15000)$
	vs. Art Studio	$(m_N = 15000)$
Deserts	Desert Sand	$(m_P = 15000)$
	vs. Desert Vegetation	$(m_N = 5556)$
Fields	Field Wild	$(m_P = 15000)$
	vs. Field Cultivated	$(m_N = 8117)$
Stadiums	Stadium Baseball	$(m_P = 15000)$
	vs. Stadium Football	$(m_N = 15000)$
Platforms	Subway Station	$(m_P = 5597)$
	vs. Train Station	$(m_N = 15000)$
Temples	Temple East Asia	$(m_P = 8691)$
	vs. Temple South Asia	$(m_N = 7178)$

C. Supplementary Results for Experimental Analyses

Figure 1 and Figure 2 respectively show the results of variance reduction and comparison of validation scores. The details of experimental setting and the interpretation of results can be found in Section 5.1.

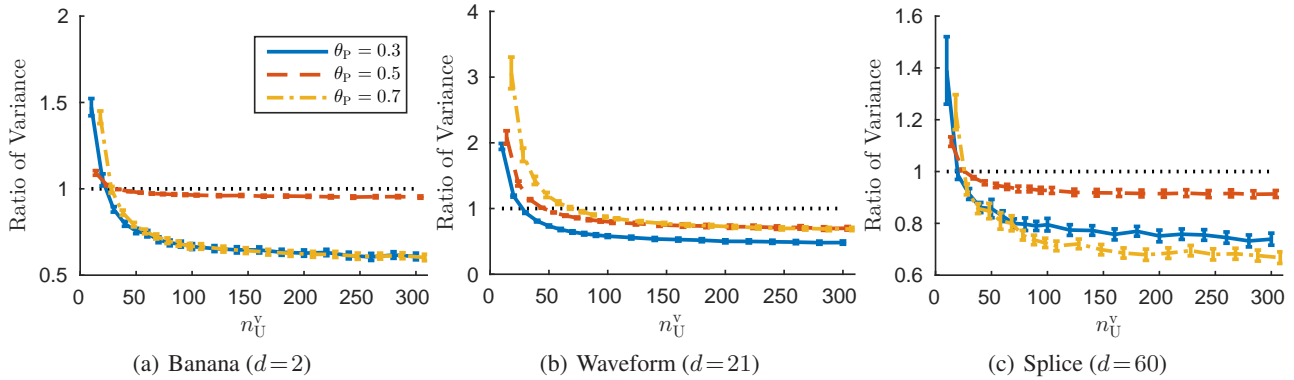


Figure 1. Average and standard error of the ratio between the variance of the empirical PNU risk and that of the PN risk, $\text{Var}[\widehat{R}_{\text{PNU}}^\eta(\widehat{g}_{\text{PN}})] / \text{Var}[\widehat{R}_{\text{PN}}(\widehat{g}_{\text{PN}})]$, as a function of the number of unlabeled samples over 100 trials. Although the variance reduction is proved for an infinite number of samples, it can be observed with a finite number of samples.

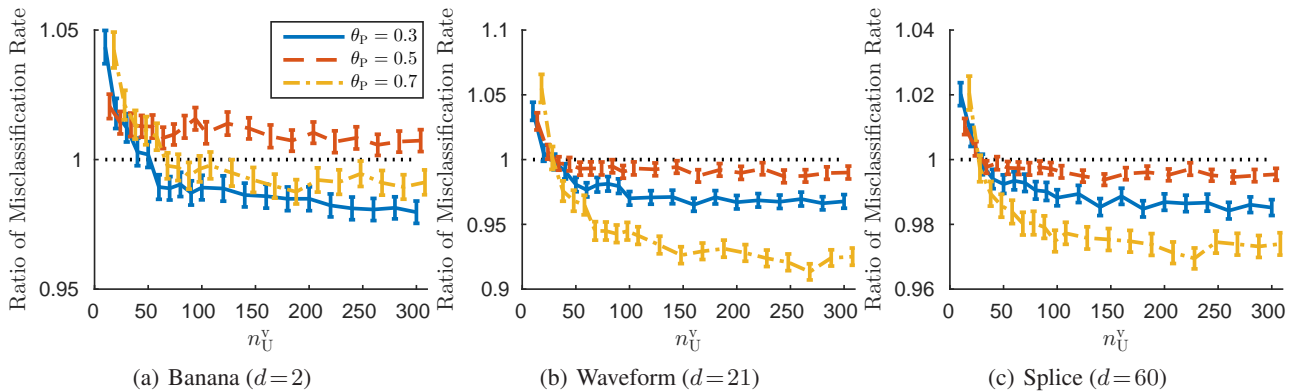


Figure 2. Average and standard error of the ratio between the misclassification rate of $\widehat{g}_{\text{PNU}}^{\text{PN}}$ and that of $\widehat{g}_{\text{PN}}^{\text{PN}}$ as a function of unlabeled samples over 1000 trials. In many cases, the ratio becomes less than 1 or at worst almost 1, implying that the PNU risk is a promising alternative to the standard PN risk in validation if unlabeled data is available.

D. Magnified Versions of Experimental Results

Here, we show magnified versions of the experimental results in Section 5.

Table 2. Magnified version of Table 1: Average and standard error of the misclassification rates of each method over 50 trials for benchmark data sets. Boldface numbers denote the best and comparable methods in terms of average misclassifications rate according to a t-test at a significance level of 5%. The bottom row gives the number of best/comparable cases of each method.

Data set	n_L	PNU	PUNU	ER	LapSVM	SMIR	WellSVM	S4VM
Banana	10	30.1 (1.0)	32.1 (1.1)	35.8 (1.0)	36.9 (1.0)	37.7 (1.1)	41.8 (0.6)	45.3 (1.0)
	$d = 2$	50	19.0 (0.6)	26.4 (1.2)	20.6 (0.7)	21.3 (0.7)	21.1 (1.0)	42.6 (0.5)
Phoneme	10	32.5 (0.8)	33.5 (1.0)	33.4 (1.2)	36.5 (1.5)	36.4 (1.2)	28.4 (0.6)	33.7 (1.4)
	$d = 5$	50	28.1 (0.5)	32.8 (0.9)	27.8 (0.6)	27.0 (0.8)	28.6 (1.0)	26.8 (0.4)
Magic	10	31.7 (0.8)	34.1 (0.9)	34.2 (1.1)	37.9 (1.3)	36.0 (1.2)	30.1 (0.8)	33.3 (0.9)
	$d = 10$	50	29.9 (0.8)	33.4 (0.9)	30.9 (0.5)	31.0 (0.9)	30.8 (0.9)	28.8 (0.8)
Image	10	29.8 (0.9)	31.7 (0.8)	33.7 (1.1)	36.6 (1.2)	36.7 (1.2)	34.7 (1.1)	35.9 (1.0)
	$d = 18$	50	20.7 (0.8)	26.6 (1.1)	20.8 (0.8)	20.3 (1.0)	20.9 (0.9)	27.2 (1.0)
Susy	10	44.6 (0.6)	45.0 (0.6)	47.7 (0.4)	48.2 (0.4)	45.1 (0.7)	48.0 (0.3)	46.8 (0.3)
	$d = 18$	50	38.9 (0.6)	41.5 (0.6)	37.9 (0.7)	43.1 (0.6)	43.9 (0.8)	43.8 (0.7)
German	10	40.8 (0.9)	42.4 (0.7)	43.6 (0.9)	45.9 (0.7)	46.2 (0.8)	42.4 (0.8)	42.0 (0.7)
	$d = 20$	50	36.2 (0.8)	39.0 (0.8)	38.9 (0.6)	40.6 (0.6)	38.4 (1.1)	38.5 (1.0)
Waveform	10	17.4 (0.6)	18.0 (0.9)	18.5 (0.6)	24.9 (1.4)	18.0 (1.0)	16.7 (0.6)	20.8 (0.8)
	$d = 21$	50	16.3 (0.6)	23.7 (1.2)	14.2 (0.4)	18.1 (0.8)	15.4 (0.6)	15.5 (0.5)
ijcnn1	10	43.6 (0.6)	40.3 (1.0)	49.7 (0.1)	49.2 (0.3)	44.0 (1.0)	45.9 (0.7)	49.3 (0.8)
	$d = 22$	50	34.5 (0.8)	37.1 (0.9)	35.5 (0.8)	33.4 (1.1)	49.4 (0.3)	46.2 (0.8)
g50c	10	11.4 (0.6)	12.5 (0.6)	23.3 (2.3)	39.8 (1.6)	21.9 (1.3)	6.6 (0.4)	27.0 (1.4)
	$d = 50$	50	12.5 (1.1)	10.1 (0.6)	8.7 (0.4)	22.5 (1.5)	10.6 (0.6)	7.4 (0.4)
covtype	10	46.2 (0.4)	46.0 (0.4)	46.0 (0.5)	47.1 (0.5)	47.9 (0.5)	46.9 (0.6)	46.4 (0.4)
	$d = 54$	50	41.3 (0.5)	42.3 (0.5)	41.0 (0.4)	41.5 (0.5)	46.2 (0.8)	43.6 (0.6)
Spambase	10	27.2 (0.9)	28.1 (1.1)	31.8 (1.4)	39.7 (1.4)	30.9 (1.3)	23.8 (0.8)	36.1 (1.5)
	$d = 57$	50	23.4 (1.0)	26.6 (1.0)	22.1 (0.7)	28.5 (1.3)	20.9 (0.5)	19.1 (0.4)
Splice	10	38.3 (0.8)	39.3 (0.8)	43.9 (0.8)	47.9 (0.5)	41.6 (0.7)	42.0 (1.0)	42.4 (0.6)
	$d = 60$	50	30.6 (0.8)	34.7 (0.9)	30.9 (0.8)	38.8 (1.0)	30.6 (0.9)	40.9 (0.8)
phishing	10	24.2 (1.2)	25.8 (1.0)	27.3 (1.6)	37.2 (1.6)	27.6 (1.6)	27.5 (1.4)	31.7 (1.3)
	$d = 68$	50	15.8 (0.6)	18.3 (0.8)	15.4 (0.5)	21.1 (1.3)	14.7 (0.8)	17.2 (0.7)
a9a	10	31.4 (0.9)	31.3 (1.0)	34.3 (1.2)	41.0 (1.1)	37.3 (1.3)	33.1 (1.2)	34.3 (1.2)
	$d = 83$	50	27.9 (0.6)	29.9 (0.8)	28.6 (0.7)	33.3 (1.0)	26.9 (0.7)	28.9 (0.8)
Coil2	10	38.7 (0.8)	40.1 (0.8)	42.8 (0.7)	43.9 (0.8)	43.2 (0.8)	39.1 (0.9)	44.0 (0.8)
	$d = 241$	50	23.2 (0.6)	30.5 (0.9)	23.6 (0.9)	22.8 (0.9)	25.1 (0.9)	22.6 (0.8)
w8a	10	35.9 (0.9)	33.6 (1.0)	41.6 (1.0)	46.6 (0.8)	39.4 (0.9)	42.1 (0.8)	43.0 (0.8)
	$d = 300$	50	28.1 (0.7)	27.6 (0.6)	27.0 (0.9)	38.7 (0.8)	28.0 (0.9)	33.7 (0.8)
#Best/Comp.		23	13	11	4	9	13	7

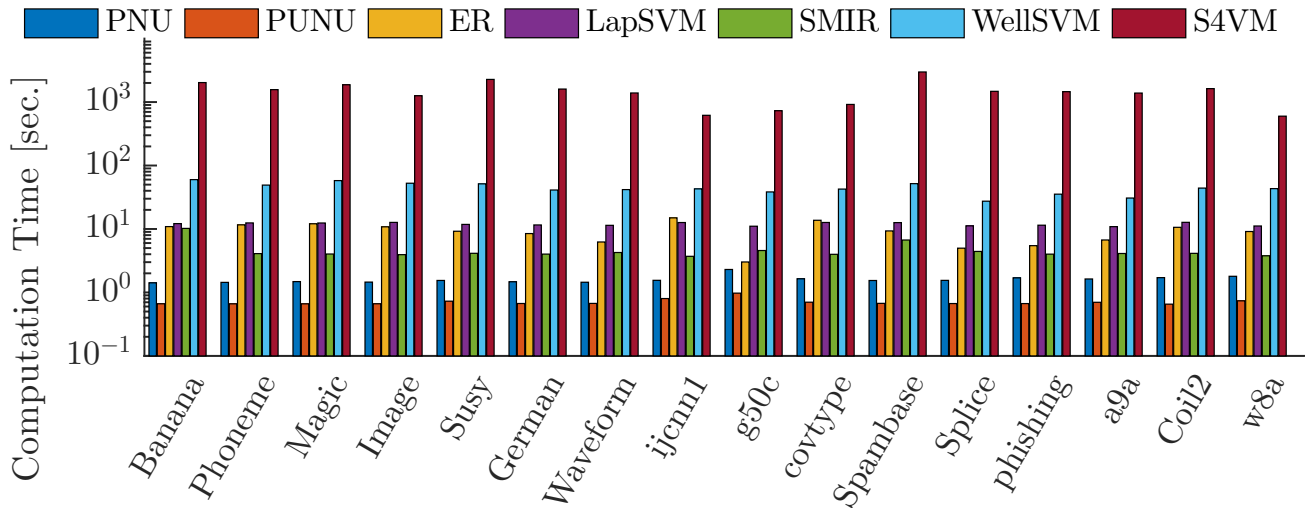

 Figure 3. Magnified version of Figure 3: Average computation time over 50 trials for benchmark data sets when $n_L = 50$.

Table 3. Magnified version of Table 2: Average and standard error of misclassification rates over 30 trials for the Places 205 data set. Boldface numbers denote the best and comparable methods in terms of the average misclassification rate according to a t-test at a significance level of 5%.

Data set	n_U	θ_P	$\hat{\theta}_P$	PNU	ER	LapSVM	SMIR	WellSVM
Arts	1000	0.50	0.49 (0.01)	27.4 (1.3)	26.6 (0.5)	26.1 (0.7)	40.1 (3.9)	27.5 (0.5)
	5000	0.50	0.50 (0.01)	24.8 (0.6)	26.1 (0.5)	26.1 (0.4)	30.1 (1.6)	N/A
	10000	0.50	0.52 (0.01)	25.6 (0.7)	25.4 (0.5)	25.5 (0.6)	N/A	N/A
Deserts	1000	0.73	0.67 (0.01)	13.0 (0.5)	15.3 (0.6)	16.7 (0.8)	17.2 (0.8)	18.2 (0.7)
	5000	0.73	0.67 (0.01)	13.4 (0.4)	13.3 (0.5)	16.6 (0.6)	24.4 (0.6)	N/A
	10000	0.73	0.68 (0.01)	13.3 (0.5)	13.7 (0.6)	16.8 (0.8)	N/A	N/A
Fields	1000	0.65	0.57 (0.01)	22.4 (1.0)	26.2 (1.0)	26.6 (1.3)	28.2 (1.1)	26.6 (0.8)
	5000	0.65	0.57 (0.01)	20.6 (0.5)	22.6 (0.6)	24.7 (0.8)	29.6 (1.2)	N/A
	10000	0.65	0.57 (0.01)	21.6 (0.6)	22.5 (0.6)	25.0 (0.9)	N/A	N/A
Stadiums	1000	0.50	0.50 (0.01)	11.4 (0.4)	11.5 (0.5)	12.5 (0.5)	17.4 (3.6)	11.7 (0.4)
	5000	0.50	0.50 (0.01)	11.0 (0.5)	10.9 (0.3)	11.1 (0.3)	13.4 (0.7)	N/A
	10000	0.50	0.51 (0.00)	10.7 (0.3)	10.9 (0.3)	11.2 (0.2)	N/A	N/A
Platforms	1000	0.27	0.33 (0.01)	21.8 (0.5)	23.9 (0.6)	24.1 (0.5)	30.1 (2.3)	26.2 (0.8)
	5000	0.27	0.34 (0.01)	23.3 (0.8)	24.4 (0.7)	24.9 (0.7)	26.6 (0.3)	N/A
	10000	0.27	0.34 (0.01)	21.4 (0.5)	24.3 (0.6)	24.8 (0.5)	N/A	N/A
Temples	1000	0.55	0.51 (0.01)	43.9 (0.7)	43.9 (0.6)	43.4 (0.6)	50.7 (1.6)	44.3 (0.5)
	5000	0.55	0.54 (0.01)	43.4 (0.9)	43.0 (0.6)	43.1 (1.0)	43.6 (0.7)	N/A
	10000	0.55	0.50 (0.01)	45.2 (0.8)	44.4 (0.8)	44.2 (0.7)	N/A	N/A

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