Reproducible Bootstrap Aggregating

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Abstract

Heterogeneity between training and testing data degrades reproducibility of a well-trained predictive algorithm. In modern applications, how to deploy a trained algorithm in a different domain is becoming an urgent question raised by many domain scientists. In this paper, we propose a reproducible bootstrap aggregating (Rbagging) method coupled with a new algorithm, the iterative nearest neighbor sampler (INNs), effectively drawing bootstrap samples from training data to mimic the distribution of the test data. Rbagging is a general ensemble framework that can be applied to most classifiers. We further propose Rbagging+ to effectively detect anomalous samples in the testing data. Our theoretical results show that the resamples based on Rbagging have the same distribution as the testing data. Moreover, under suitable assumptions, we further provide a general bound to control the test excess risk of the ensemble classifiers. The proposed method is compared with several other popular domain adaptation methods via extensive simulation studies and real applications including medical diagnosis and imaging classifications.

Keywords: Bagging; Classification; Domain adaptation; Ensemble learning; Generalizability; Reproducibility.

1 Introduction

When the data distribution in the test domain differs from the training domain, there can be a dramatic increase in test misclassification error, particularly for highly flexible classifiers. This issue has led to a reproducibility crisis in many fields. For example, in automatic medical diagnosis, a predictive algorithm may initially be trained using data from a particular medical center or collected across a range of dates. Physicians would like to be able to apply this same predictive algorithm broadly for future patients including at different centers. However, these new patients may differ in

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subtle ways from the training patients. Highly flexible classifiers, such as deep neural networks, can be very sensitive to such differences, leading to a lack of reproducibility and generalizability.

This problem has been studied in the literature under different names, including class imbalance [Japkowicz and Stephen, 2002], label shift [Shimodaira, 2000], sample selection bias [Heckman, 1979, Huang et al., 2007], and domain adaptation [Daume III and Marcu, 2006, Blitzer et al., 2006]. There are also some closely-related statistical and machine learning problems including conformal prediction [Vovk et al., 2009, Lei et al., 2013], transfer learning [Torrey and Shavlik, 2010], and multi-task learning [Caruana, 1997]. In this work, we consider the reproducibility problem in the multi-class classification setting in which the training data and the testing data may be mismatched. Our goal is to adjust for a distribution shift correctly so that our classifier is designed to perform well on the testing data.

Let $X \in \mathbb{R}^p$ denote a continuous vector of covariates and $Y \in \{1, \ldots, L\}$ be a label. As a simplifying assumption, to allow a distributional shift, we suppose the training and testing data follow different mixture distributions as

$$f_{\text{tr}}(x) = \sum_{\ell=1}^{L} p_\ell f_\ell(x), \quad f_{\text{te}}(x) = \sum_{\ell=1}^{L} q_\ell f_\ell(x),$$

(1.1)

where $f_\ell$, $\ell = 1, \ldots, L$, are shared densities of $x$ from class $\ell$ for both the training and test covariates, $0 < p_\ell \leq 1$ is the label proportion for training data satisfying $\sum_{\ell=1}^{L} p_\ell = 1$, and $0 \leq q_\ell \leq 1$ is the label proportion for test data with $\sum_{\ell=1}^{L} q_\ell = 1$. In the literature, (1.1) is referred to as prior/label shifting, in the sense that the prior probabilities of the classes are different, but the conditional feature distributions are shared as $f(X_{\text{te}} = x|Y_{\text{te}} = y)$.

Under (1.1), Storkey [2009] proposed to use a (meta-)prior and infer the posterior distribution from unlabeled test data. Chan and Ng [2005] developed an EM algorithm to estimate $q_\ell$. These two approaches require explicit estimation of $f_\ell$, which may be infeasible in high-dimensional cases. Zhang et al. [2013] extended the kernel mean matching (KMM) approach to the label shift problem based on the minimum mean discrepancy introduced by Gretton et al. [2012]. This kernel based method suffers from high computational complexity, and is not scalable to massive datasets. Lipton et al. [2018] introduced black box shift estimation (BBSE) to estimate the label shifts based on a data-splitting strategy. However, the performance of BBSE varies with different black box predictors. Also, it is unstable when the sample size is small due to its splitting strategy. A practical question then arises: how can we leverage on the testing data to improve generalizability of predictive algorithms applied to the training data in a computationally efficient and stable way with statistical guarantees?

With this goal in mind, we develop a novel method “Reproducible Bootstrap Aggregating” (Rbagging) which draws bootstrap samples from the training data to effectively mimic the distribution
of the testing data. Classical Bagging [Breiman, 1996] (short for Bootstrap AGGregatING) is an ensemble learning method that is used primarily to reduce prediction variance. Bagging is particularly motivated as a fix-up to unstable predictive algorithms. Instead of making predictions from a single model fit on the observed data, multiple bootstrap samples are taken, the model is fit to each sample, and the predictions are averaged over all of the fitted models to get the bagged prediction. However, when the covariate distribution shifts between the training and testing set, training accuracy may decline dramatically on the testing set. Although Bagging is efficient at reducing the prediction variance in homogeneous data, it does not take into account the bias introduced by a distribution shift. In Rbagging, we propose an iterative nearest neighbor sampling (INNs) procedure to draw bootstrap samples from the training data with the guidance of the testing data, instead of uniformly sampling from the training data in classic bagging. Rbagging is a general ensemble framework that can be naturally equipped with any base classifiers, ranging from random forests [Breiman, 2001] to $k$-nearest neighbors [Hall et al., 2008]. Rbagging is computationally efficient and robust.

We establish theoretical guarantees for Rbagging. We prove that the bootstrapped samples using INNs converge to the same distribution as $f_{te}(x)$ asymptotically as the iterations proceed. We control the difference between the expected test error of the ensemble classifier based on Rbagging and the Bayesian risk. This is accomplished by bounding the test error between the corresponding classifier and the Bayesian risk under the oracle distribution of $f_{te}$. Our general bounds can be applied to different base classifiers, including $k$-NN. Rbagging is essentially a weighted randomized ensemble method. We further quantify the convergence in terms of the algorithmic variance leveraging on recent results in Cannings and Samworth [2017] and Lopes [2020], showing that the algorithmic variance decreases as the number of bootstrap samples increases.

We additionally consider the case when the testing data include unobserved classes or outliers; that is, suppose the training and testing data follow distributions:

$$f_{tr}(x) = \sum_{\ell=1}^{L} p_{\ell} f_{\ell}(x), \quad f_{te}(x) = \sum_{\ell=1}^{L} q_{\ell} f_{\ell}(x) + \epsilon f_{out}(x),$$

which is related to the classic Huber-contamination model [Huber, 1992]. Expression (1.2) implies there exists a subset of test samples that do not share any information with the training set, and hence their labels cannot be reliably predicted. We propose a method Rbagging+, which first detects anomalies in the test data before conducting the Rbagging procedure. If the sample is labeled as an anomaly, we predict its label as $\{\emptyset\}$. Intuitively, if a sample from the testing dataset is an “inlier”, then its distance to its $k$-nearest neighbors in the training data will be small, otherwise this distance is large. Therefore, we propose a test statistic based on the distance of $X \sim f_{te}$ to its $k$-NN in the training data. Type I error for wrongly detecting anomalous samples is controlled at
the α-significance level, while proving the power is high.

Anomaly detection arises in many applications such as fraud detection in finance, automated medication systems, and failure detection for autonomous driving. Some well known methods, such as kNNG [Hero, 2007] and bi-KNNG [Sricharan and Hero, 2011], detect data using geometric entropy minimization (GEM) principles, assuming \( q = p_x \). Gu et al. [2019] introduced nearest neighbor methods for anomaly detection in unsupervised learning, i.e., only given the unlabeled datasets. Recently, Guan and Tibshirani [2019] proposed the BCOPS method, which generalizes BBSE methods [Lipton et al., 2018] to account for label shifting in the testing data with anomalies. However, inherited from the data-splitting strategy in BBSE, BCOPS also suffers from accuracy loss when the sample size is small. Moreover, BCOPS needs to estimate the ratio between \( f(Y|X) \) and \( f(Y|X) \), which depends on the performance of the classifiers, and hence may be unstable for unstable classifiers. In addition, BCOPS estimates \( q \) by taking the inverse of the estimated confusion matrix, which may suffer from large error in cases with some small \( q > 0 \) or collinearity.

The remainder of the paper is organized as follows. The Rbagging method and general theory are developed in Sections 2.2 and 3. Rbagging+ methods with anomaly detection are introduced in Section 4. In Section 5 we present results from an extensive empirical analysis on simulated data with several popular techniques. In Section 6, we demonstrate the performance of Rbagging and Rbagging+ in real data examples. In Section 7, we conclude with a discussion of various extensions and open problems.

2 Reproducible Bagging (Rbagging)

2.1 Notation and Preliminaries

Consider the multi-class classification problem where the training and testing data may be mismatched. Suppose we have \( n \) observed training data \( D_{tr} = \{(X_{tr}^{1}, Y_{tr}^{1}), \ldots, (X_{tr}^{n}, Y_{tr}^{n})\} \). Let \((X, Y)\), \((X_{tr}^{1}, Y_{tr}^{1})\), \((X_{tr}^{2}, Y_{tr}^{2})\), \ldots, \((X_{tr}^{n}, Y_{tr}^{n})\) be independent and identically distributed pairs taking values in \( \mathbb{R}^p \times \{1, \ldots, L\} \). We suppose that the label proportion \( P(Y = \ell) = p_{\ell} \) for some \( p_{\ell} \in (0, 1) \) satisfying \( \sum_{\ell=1}^{L} p_{\ell} = 1 \), and the conditional probability density function of \( X | Y = \ell \) is \( f_{\ell}(x) \). Then, the marginal distribution of \( X \) follows \( f_{tr}(x) = \sum_{\ell=1}^{L} p_{\ell} f_{\ell}(x) \); see (1.1). Denote i.i.d. observations of \( X_{te} \) as \( D_{te} = (X_{te}^{1}, \ldots, X_{te}^{m}) \), each \( X_{te}^{i} \) has a corresponding \( Y_{te}^{i} \) unobserved. Suppose \( X_{te} \) follows the marginal density \( f_{te}(x) = \sum_{\ell=1}^{L} q_{\ell} f_{\ell}(x) \). \( f_{te} \) is a mixture of \( f_{\ell}(x) \) shared with the training data, but with different mixture proportions \( q_{\ell} \) characterizing the distributional shift.

A classifier on \( \mathbb{R}^p \) is a Borel measurable function \( C : \mathbb{R}^p \to \{1, \ldots, L\} \) meaning that we assign a point \( X \in \mathbb{R}^p \) to class \( C(X) \). Given the training and testing datasets \( D_{tr} \) and \( D_{te} \), we aim to
predict $C(X)$ for $X \sim f_{te}$. The risk of $C$ is defined as

$$R(C) = \mathbb{E}[\mathbb{I}[C(X) \neq Y]] = \mathbb{P}(C(X) \neq Y),$$

where $\mathbb{E}$ and $\mathbb{P}$ take account of the randomness of both $X$ and $Y$.

### 2.2 Methodology

We develop an iterative nearest neighbor sampling (INNs) procedure to draw bootstrap samples from the training data $D_{tr}$ with the guidance of the testing data $D_{te}$. For $X^{te} \sim f_{te}(x)$, we reorder the samples in $D_{tr}$ as $(X_1^{te}, Y_1^{te}), \ldots, (X_n^{te}, Y_n^{te})$, such that

$$\|X^{te} - X_1^{te}\| \leq \cdots \leq \|X^{te} - X_n^{te}\|,$$

and define its $k$-nearest neighbors in $D_{tr}$ as $N^k_{X^{te}_j} = (X_1^{te}, \ldots, X_k^{te})$.

For each $X_j^{te}$, we search its $k$-nearest neighbors in the training data denoted as $N^k_{X_j^{te}}$, and sample $\lceil n/m \rceil$ data points denoted as $D_{tr}^{(1)}$ with replacement from the $L$ classes with probability $\pi_j = \{\pi_{j,1}, \ldots, \pi_{j,L}\}$ where

$$\pi_{j,\ell} = \frac{1}{k} \# \{Y_i^{tr} = \ell \mid X_i^{tr} \in N^k_{X_j^{te}}\} \text{ for } \ell = 1, \ldots, L. \quad (2.1)$$

That is, in our sampling schedule, each $X_j^{te}$ contributes $\lceil n/m \rceil$ samples from the $L$ classes in $D_{tr}$, with the weight for class $\ell$ determined via the proportion of the labels $\ell$ in its $k$-nearest neighborhood $N^k_{X_j^{te}}$. Repeating for $j = 1, \ldots, m$, we have the sampled data $D_{tr}^{(1)} = (D_{tr,1}^{(1)}, \ldots, D_{tr,m}^{(1)})$. We view $D_{tr}^{(1)}$ as the “new” training data, and search the $k$-NN of $D_{te}$ in $D_{tr}^{(1)}$ iteratively. Repeating the procedure $T$ times for the purpose of refining, we obtain a final training dataset $D_{tr}^{(T)}$. In practice, we choose $T$ as the number of iterations when the changes of proportions of classes from $D_{tr}^{(T-1)}$ to $D_{tr}^{(T)}$ is controlled by a pre-specified threshold $\varepsilon_T$. Figure 1 (a) provides an illustrative example showing how the reproducible sampling works.

Let $\xi$ be a “randomizing parameter” controlling the mapping from the initial $D_{tr}$ to the sampled $D_{tr}^{(T)}$ under the above procedure; that is, $\xi : D_{tr} \rightarrow D_{tr}^{\xi} := D_{tr}^{(T)}$; see Figure 1 (b) for illustration. Implementing the procedure $B$ times, we obtain randomizations $\xi_1, \ldots, \xi_B$ and corresponding datasets $D_{tr}^{\xi_1}, \ldots, D_{tr}^{\xi_B}$. Parameters $\xi_1, \ldots, \xi_B$ are conditionally i.i.d. given $D_{tr}$ and $D_{te}$.

Based on each $D_{tr}^{\xi_b}$, we construct a base classifier $C^\xi_{n_b}(\cdot)$, and the prediction for any $X \sim f_{te}$ as

$$C^\xi_{n_b}(X) = C_{n,D_{tr}^{\xi_b}}(X) = C_n(X; D_{tr}, D_{te}, \xi_b).$$

The ensemble classifier $C^RB_n$ (RB is short for Rbagging) for any $X \sim f_{te}$ is then defined as

$$C^RB_n(X) = \arg\max_\ell \# \{b \in \{1, \ldots, B\} : C_{n}^{\xi_b}(X) = \ell\}. \quad (2.2)$$
Figure 1: (a) Flowchart of the nearest neighbor sampler. Blue and green dots represent data points in class \{1\} and class \{2\}. For each point in the test data, (shown as black circles in the training data), we seek its nearest neighbor in the training data and draw \(\lceil n/m \rceil\) samples from class \{\ell\}, where \(\ell\) is the label of its nearest neighbor. In the sampled data plot, we show the drawn sample where larger circles correspond to repeated data points. (b) Illustrative figure of the histogram of the training data, test data, and the first to fifth drawn samples by INNs.

Figure 2: Flowchart for Rbagging. First, draw \(T\) labeled training data by INNs. Second, train a classifier for each drawn sample. Third, ensemble all classifiers and make prediction for testing data.

Figure 2 shows the flowchart of the reproducible sampling schedule of Rbagging. The detailed algorithm is summarized in Algorithm 1.
Algorithm 1 Reproducible bagging

1. for Parallel $b = 1, \ldots, B$ do
   
   for Parallel $t = 1, \ldots, T - 1$ do
       for Parallel $j = 1, \ldots, m$ do
           (a) For $X_{te}^j$, find its $k$-nearest neighbor in $D_{tr}^{bs,(t)}$, denoted as $\{N_{X_{te}^j}^k\}$.
           (b) Define $\pi_j = (\pi_{j,1}, \ldots, \pi_{j,L})$ with $\pi_{j,\ell}$ defined as
               $\pi_{j,\ell} = \frac{1}{k} \# \{Y_{tr}^i = \ell \mid X_{tr}^i \in N_{X_{te}^j}^k\}$ for $\ell = 1, \ldots, L$.
           (c) Sample $(n_{j,1}, \ldots, n_{j,L})$ from Multinomial($\lceil n/m \rceil, \pi_j$).
           (d) For $\ell = 1, \cdots, L$, draw $n_{j,\ell}$ bootstrap samples with replacement from the $\ell$-th class in $D_{tr}^{bs,(t)}$.
       end
       
       Denote the $\{n_{j,\ell}\}$ samples together as $D_{tr}^{bs,(t+1)}$.
   end
   
   Define $D_{tr}^{bs,(T)}$ as $D_{tr}^{bs}$, and construct the classifier $C_n^{bs}(\cdot) = C_{n,D_{tr}^{bs}}(\cdot)$.
end

2. Build the ensemble classifier as the majority voting

$$C_n^{RB}(X) = \arg\max_\ell \# \{b \in \{1, \cdots, B\} : C_n^{bs}(X) = \ell\}.$$ 

3 Theoretical Results

In this section, we study the theoretical properties of Rbagging based on using $k = 1$ in $k$-NN in Algorithm 1. To simplify the presentation, we consider binary classification with the labels equal to 1 or 2. Then model (1.1) can be written as

$$f_{tr}(x) = p_1 f_1(x) + p_2 f_2(x) \quad \text{and} \quad f_{te}(x) = q_1 f_1(x) + q_2 f_2(x), \quad (3.1)$$

where $p_1 = \mathbb{P}(Y_{tr}^r = 1)$, $p_2 = 1 - p_1 = \mathbb{P}(Y_{tr}^r = 2)$, $q_1 = \mathbb{P}(Y_{te}^r = 1)$ and $q_2 = 1 - q_1 = \mathbb{P}(Y_{te}^r = 2)$.

We aim to show that the bootstrapped data $D_{tr}^{bs,1}, \ldots, D_{tr}^{bs,B}$ can represent the testing data with probability 1. Further, we establish the generalization error of general classifiers based on Rbagging, and characterize the algorithmic convergence.
3.1 Consistency of the representation of testing data

Letting \( k = 1 \) in Algorithm 1 and \( L = 2 \), the Rbagging algorithm based on 1-NN can be simplified as the following Algorithm 2. For each \( X^{te}_j \in D_{te} \), we find its 1-NN in \( D_{tr} \). If its nearest neighbor is from class \( \ell \in \{1, 2\} \), we randomly sample \( \lceil n/m \rceil \) data from class \( \ell \) with replacement. Repeat this procedure for all of the \( m \) testing samples, and collect the samples as \( D_{tr}^{1*,(1)} \), where 1* represents the 1st Bootstrap copy, and (1) means the first iteration in that bootstrap copy. Viewing \( D_{tr}^{1*,(1)} \) as the “new” training data, we search 1-NN of \( D_{te} \) in \( D_{tr}^{1*,(1)} \), and denote the re-sampled data as \( D_{tr}^{1*,(2)} \). Denote \( D_{tr}^{1*,(t)} \) as the sample from the \( t \)-th iteration \( D_{tr}^{1*,(t)} \). In Theorem 3.2, we show that for \( X \in D_{tr}^{1*,(t)} \), the corresponding density \( f_{(t)}(x) \) approaches to \( f_{te}(x) \) as \( t \) increases.

**Algorithm 2** R-bagging based on 1-NN with \( L = 2 

1. for Parallel \( b = 1, \ldots, B \) do
   for Parallel \( t = 1, \ldots, T - 1 \) do
      for Parallel \( j = 1, \ldots, m \) do
         (a) For \( X^{te}_j \in D_{te} \), find its nearest neighbor in \( D_{tr}^{bs,(t)} \), denoted as \( X^{(1)}(X^{te}_j) \), and the corresponding label as \( Y_{(1)} \).
         (b) Bootstrap \( n_j = \lceil n/m \rceil \) samples with replacement from the \( \ell \)-th class in \( D_{tr}^{bs,(t)} \), where \( \ell = Y_{(1)} \).
      end
      Collect the \( n_1, \ldots, n_m \) samples together as \( D_{tr}^{bs,(t+1)} \).
   end
   Denote \( D_{tr}^{bs,(T)} \) as \( D_{tr}^{\xi_b} \). Construct the classifier \( C_{n,D_{tr}^{\xi_b}}(\cdot) = C_{n,D_{tr}^{\xi_b}}(\cdot) \).
   end
2. Ensemble the classifiers based on \( D_{tr}^{\xi_1}, \ldots, D_{tr}^{\xi_B} \) as the majority voting

\[
C^{RB}_n(X) = \operatorname{argmax}_\ell \# \{ b \in \{1, \cdots, B\} : C^{\xi_b}_n(X) = \ell \}.
\]

We introduce some notation. Let \( X^{te} \) be the random variable with density \( f_{te}(x) \), and \( X_1, \cdots, X_n \in \mathbb{R}^p \) be i.i.d. random variables with density \( f_{tr}(x) \). Denote the nearest neighbor of \( X^{te} \) from the set \( \{X_1, \cdots, X_n\} \) as \( X_{(1)}(X^{te}) \); that is

\[
\min_{i \in \{1, \cdots, n\}} \|X_i - X^{te}\| = \|X_{(1)}(X^{te}) - X^{te}\|,
\]

where \( \| \cdot \| \) is a metric defined on \( \mathbb{R}^p \). We denote the corresponding label of \( X_{(1)}(X^{te}) \) as \( Y_{(1)}(X^{te}) \).

We first show that, under the distributional shifting from \( f_{tr} \) to \( f_{te} \) defined in (3.1), for any \( X \in D_{te} \), its nearest neighbor \( X_{(1)}(X^{te}) \) in \( D_{tr} \) converges to \( X^{te} \) with probability one.
Lemma 3.1. Assume $f_{tr}(x)$ and $f_{te}(x)$ follow (1.1). Let $X^{te} \sim f_{te}(x)$, and $X_1, \cdots, X_n \in \mathbb{R}^p$ be i.i.d. random variables with density $f_{tr}(x)$. Then $X(1)(X^{te}) \to X^{te}$ with probability 1.

Theorem 3.2. Under Algorithm 2, denote $D_{tr}^{b} = \{(X_{1}^{\xi_b}, y_{1}^{\xi_b}), \ldots, (X_{n}^{\xi_b}, y_{n}^{\xi_b})\}$. Denote the conditional density of $X_{i}^{\xi_b}|Y_i^{\xi_b} = \ell$ as $f_{b}^{(T)}(x)$, and the marginal distribution of $X_{i}^{\xi_b}$ as $f^{(T)}$. Then we have $\{(X_{i}^{\xi_b}, Y_{i}^{\xi_b})\}$ are i.i.d, $P(Y_i^{\xi_b} = \ell) = q_{\ell}$, $f_{b}^{(T)}(x) = f_{\ell}(x)$, and hence,

$$f^{(T)}(x) = \lim_{t \to \infty} f^{(t)}(x) = \sum_{\ell=1}^{L} q_{\ell} f_{\ell}(x).$$

Theorem 3.2 shows that in the bootstrapped data $D_{tr}^{b}$ with sample size $n$ for $b = 1, \ldots, B$, each sample in $D_{tr}^{b}$ follows the same distribution as the testing data, that $P(Y^{te} = \ell) = q_{\ell}$, $X^{te}Y = \ell \sim f_{\ell}$ and the marginal density $f_{te}(x) = \sum_{\ell=1}^{L} q_{\ell} f_{\ell}(x)$.

### 3.2 Prediction error based on Rbagging

In this section, we analyze the testing error of basic classifiers based on Rbagging. To distinguish between different sources of randomness, we denote $P, E$ as the probability and expectation respectively, taken over the randomness from the random sampling parameters $\xi_1, \ldots, \xi_B$ conditional on the observed training and testing data $(D_{tr}, D_{te})$. We define $P, E$ as the probability and expectation respectively, taken over all random quantities.

Considering model (3.1), the test error of a classifier $C$ is defined as

$$R(C) := q_1 \int 1[C(x) = 2] f_1(x) dx + q_2 \int 1[C(x) = 1] f_2(x) dx. \quad (3.2)$$

$R(C)$ is minimized by the Bayes classifier defined as

$$C_{Bayes}^{Bayes}(x) := \begin{cases} 1 & \text{if } \eta(x) \geq 1/2 \\ 2 & \text{otherwise} \end{cases}$$

where $\eta(x) = P(Y^{te} = 1|X^{te} = x) = \frac{q_1 f_1(x)}{q_1 f_1(x) + q_2 f_2(x)}$. The corresponding Bayes risk for $C_{Bayes}^{Bayes}$ is

$$R(C_{Bayes}^{Bayes}) = E_{X \sim f_{te}} \left[ \min\{\eta(X), 1 - \eta(X)\} \right] = \int \min\{q_1 f_1(x), q_2 f_2(x)\} dx.$$

Given a base classifier $C$ and the new training samples $D_{tr}^{b}$ ($b = 1, \ldots, B$) obtained in Algorithm 2, we have a sequence of trained classifiers $C_{n}^{b_1}, \ldots, C_{n}^{b_B}$. We define $\Lambda_n(x) = \frac{1}{B} \sum_{b=1}^{B} 1\{C_{n}^{b}(x) = 1\}$, and the ensemble classifier $C_{n}^{RB}$ based on the reproducible bootstrapping as

$$C_{n}^{RB}(x) := \begin{cases} 1 & \text{if } \Lambda_n(x) \geq 1/2, \\ 2 & \text{otherwise}. \end{cases}$$
In Theorem 3.3, we show the test excess risk, i.e., the difference between the expected test error of \( C_{RB}^n \) and the Bayes risk, can be controlled in terms of the expected test excess risk of the classifier \( C_{\xi_b}^n \) based on a single randomized sampling \( \xi_b \).

**Theorem 3.3.** Assume model (3.1) holds. Based on Algorithm 2, for \( 1 \leq b \leq B \), we have

\[
E\{R(C_{RB}^n)\} - R(C_{Bayes}) \leq 2[E\{R(C_{\xi_b}^n)\} - R(C_{Bayes})].
\] (3.3)

Theorem 3.3 provides a general bound for different choices of base classifiers. Note that \( C_{\xi_b}^n \) is trained based on \( D_{\xi_b}^{tr} = ((X_{1}^{\xi_b}, Y_{1}^{\xi_b}), \ldots, (X_{n}^{\xi_b}, Y_{n}^{\xi_b})) \). By Theorem 3.2, the marginal distribution of \( X_{i}^{\xi_b} \) follows \( f_{te}(x) \) defined in (3.1). On the other hand, by definition (3.2), calculating \( R(C_{Bayes}) \) only involves the density function \( f_{te} \). Therefore, viewing \( D_{\xi_b}^{tr} \) as the training data, we remove the distributional shifting in the upper bound in (3.3) in Theorem 3.3. Once the training and test data have the same distribution, the existing literature on theoretical performance of previously proposed classifiers can be used to provide explicit bounds on the expectation of the test excess risk.

In the following Corollary 3.4, we bound the excess risk in (3.3) by considering a concrete example, that is, using \( k \)-nearest neighbors as the base classifier. Given \( X_{te} \in \mathbb{R}^p \) generated from the density \( f_{te}(x) \) in (3.1), we first order the data in \( D_{\xi_b}^{tr} \) as \( (X_{(1)}^{\xi_b}, Y_{(1)}^{\xi_b}), \ldots, (X_{(n)}^{\xi_b}, Y_{(n)}^{\xi_b}) \) such that \( \|X_{(1)}^{\xi_b} - X_{te}\| \leq \cdots \leq \|X_{(n)}^{\xi_b} - X_{te}\| \), with ties split at random. The \( k \)-nearest neighbor classifier is defined as

\[
C_{\xi_b}^n(X_{te}) = \begin{cases} 1 & \text{if } \frac{1}{k} \sum_{i=1}^{k} I[Y_{(i)}^{\xi_b}] \geq 1/2, \\ 2 & \text{otherwise.} \end{cases}
\]

Hall et al. [2008] established the rate of convergence of the excess risk with the optimal choice of \( k \). Combining with Theorem 3.3, we have the following Corollary.

**Corollary 3.4.** Suppose \( X \in \mathbb{R}^p \) with fixed \( p \) is a random variable with density \( f_{te}(x) \) in (3.1). Under regularity conditions, if \( k \) is chosen as \( O(n^{4/(p+4)}) \), then we have

\[
E\{R(C_{RB}^n)\} - R(C_{Bayes}) \leq 2[E\{R(C_{\xi_b}^n)\} - R(C_{Bayes})] = O(n^{-4/(p+4)}).
\]

Algorithmic convergence has been studied for randomized ensembles to analyze the effect of the ensemble size \( B \) on prediction error; see Cannings and Samworth [2017] and Lopes [2020]. Define \( \mu_n(X_{te}) := E\{\Lambda_n(X_{te})\} = P\{C_{\xi_b}^n(X_{te}) = 1\} \). Intuitively, \( \mu_n(X_{te}) \) represents infinite bootstrap samples with \( B \to \infty \). Define the classifier with infinite ensemble size as \( C_{RB^*}^n \), i.e.,

\[
C_{RB^*}^n(X_{te}) = \begin{cases} 1 & \text{if } \mu_n(X_{te}) \geq 1/2, \\ 2 & \text{otherwise.} \end{cases}
\]


In the following Theorem 3.5, we characterize how the test error of $C_n^{RB}$ based on an ensemble of size $B$ converges to the ideal level of an infinite ensemble of $C_n^{RB^*}$, in terms of the algorithmic randomness introduced by $\xi_0$, given the observations $(D_{tr}, D_{te})$.

We first introduce an assumption regarding the distribution of $\mu_n(X)$. Define the distribution functions of $\mu_n(X)$ conditional on $Y$ as $L_{\mu_n}(t | (D_{tr}, D_{te}), Y = \ell)$ for $\ell = 1, 2$. That is,

$$L_{\mu_n,1}(t | (D_{tr}, D_{te}), Y = 1) = \mathbb{P}\{X \in \mathbb{R}^p : \mu_n(X) \leq t\} | (D_{tr}, D_{te}), Y = 1;$$

$$L_{\mu_n,2}(t | (D_{tr}, D_{te}), Y = 2) = \mathbb{P}\{X \in \mathbb{R}^p : \mu_n(X) \leq t\} | (D_{tr}, D_{te}), Y = 2.$$

**Assumption A1.** For $\ell \in \{1, 2\}$, the distribution $L_{\mu_n,\ell}(t | (D_{tr}, D_{te}), Y = \ell)$ is twice differentiable at $t = 1/2$.

**Theorem 3.5.** Consider model (3.1), and under Algorithm 2, suppose Assumption A1 holds. Then, as $B \to \infty$,

$$E\{R(C_n^{RB})\} - R(C_n^{RB^*}) = \frac{\gamma_n}{B} + o(B)$$

$$\lim_{B \to \infty} B \text{Var}\{R(C_n^{RB})\} \leq 1/4\eta_n^2(1/2),$$

where $E(\cdot)$ and $\text{Var}(\cdot)$ are calculated conditional on $(D_{tr}, D_{te})$, $\gamma_n = (1/2 - (B/2 - [B/2]))\{q_1 g_{n,1}(1/2) - q_2 g_{n,2}(1/2)\} + \frac{1}{5}\{q_1 \dot{g}_{n,1}(1/2) - q_2 \dot{g}_{n,2}(1/2)\}$, and $\eta_n(1/2) = q_1 g_{n,1}(1/2) + q_2 g_{n,2}(1/2)$. Here $g_{n,\ell}$ and $\dot{g}_{n,\ell}$ are the first and second order derivative of $L_{\mu_n,\ell}(t | (D_{tr}, D_{te}), Y = \ell)$ for $\ell = 1, 2$.

Theorem 3.5 shows that the bias and the variance of the test error is of order $O(1/B)$. Note that $\xi_1, \ldots, \xi_B$ are independent conditional on $(D_{tr}, D_{te})$. The proof of Theorem 3.5 follows from Theorem 1 in Cannings and Samworth [2017].

### 4 Rbagging with Anomaly

In this section, we consider the situation in which anomalous samples are present in the testing data, with ‘anomalous’ meaning that these samples would be considered as outliers if they were observed in the training sample. In particular, we consider the model

$$f_{tr}(x) = \sum_{\ell=1}^{L} p_{\ell} f_{\ell}(x), \quad f_{te}(x) = \sum_{\ell=1}^{L} q_{\ell} f_{\ell}(x) + \epsilon f_{out}(x), \quad (4.1)$$

where $p_{\ell} > 0$ satisfying $\sum_{\ell=1}^{L} p_{\ell} = 1$ and $q_{\ell} \geq 0, \epsilon \geq 0$ satisfying $\sum_{\ell=1}^{L} q_{\ell} + \epsilon = 1$. Denote $\mathbb{P}_{\ell}$ as the probability measure of $X \sim f_{\ell}(x)$ for $\ell = 0, \ldots, L$, and $\mathbb{P}_0$ as the probability measure of $X \sim f_{out}(x)$. This model allows not only changes in the mixture proportions between training and test but also
an additional mixture component for the test data corresponding to anomalous observations that may be dissimilar to any of the training samples.

We first detect the anomalies before conducting the reproducible sampling. Denote $\mathcal{D}_{tr} = (\mathcal{D}_{tr,1}, \ldots, \mathcal{D}_{tr,L})$, where $\mathcal{D}_{tr,\ell}$ only contain the training data with label $\{\ell\}$, having sample size $|\mathcal{D}_{tr,\ell}| = n_\ell$. For any $x$, define the squared distance between $x$ and its $k$-nearest neighbors in $\mathcal{D}_{tr,\ell}$ as

$$\hat{d}^2_\ell(x) = \frac{1}{k} \sum_{X_i \in \mathcal{N}_x^{k,\ell}} \|X_i - x\|^2,$$  \hspace{1cm} (4.2)

where $\mathcal{N}_x^{k,\ell}$ are the $k$-nearest neighbors of $x$ in $\mathcal{D}_{tr,\ell}$. Intuitively, if $x$ is an anomaly, then for any $\ell \in \{1, \ldots, L\}$, $\hat{d}^2_\ell(x)$ is large. A population version of $\hat{d}^2_\ell(x)$ is called the distance-to-measure (DTM) ([Chazal et al., 2011] [Chazal et al., 2017]) defined as

$$d^2_\ell(x) = \frac{1}{m_\ell} \int_0^{m_\ell} r_{\ell,t}(x) dt,$$  \hspace{1cm} (4.3)

where $m_\ell = \frac{k}{n_\ell}$ and $r_{\ell,t}(x) = \text{argmin}\{r : P_\ell(\|X - x\|^2 \leq r) > t\}$. By the definition of $d^2_\ell(x)$ in equation (4.3), a relatively large DTM happens in two situations: (1) $x$ is a tail sample from $f_\ell(x)$; (2) $x$ is an anomaly. Letting $P_{n_\ell}$ be the empirical probability measure that puts mass $1/n_\ell$ on each $X_i \in \mathcal{D}_{tr,\ell}$, the distance to the measure $P_{n_\ell}$ at resolution $m_\ell$ is exactly equation (4.2).

Observing this, for each $X_{te} \sim f_{te}(x)$, we construct a statistic for anomaly detection as

$$T(X_{te}) = \prod_{\ell=1}^L \mathbb{1}_{\{\hat{d}_\ell(X_{te}) > c_\ell\}},$$  \hspace{1cm} (4.4)

where $c_\ell$ is a constant threshold that will be specified later. In Lemma 1, we show that $\hat{d}_\ell(x)$ is a consistent estimator of $d_\ell(x)$. Then for any $X_{te} \in \mathcal{D}_{te}$, $T(X_{te}) = 1$ if and only if $d_\ell(X_{te}) > c_\ell$ ($\hat{d}_\ell(X_{te}) > c_\ell$) for all $\ell \in \{1, \ldots, L\}$.

Given $X_{te} \in \mathcal{D}_{te}$ with unobserved label $Y_{te}$, we propose a detection rule as $\Psi(X_{te}) = \mathbb{1}_{\{T(X_{te}) > c\}}$ for $0 < c < 1$. The type I error refers to the probability of wrongly detecting the anomaly, i.e., $P(T(X_{te}) > c | Y_{te} \in \{1, \ldots, L\})$. The power of $\Psi(X_{te})$ is expressed as $P(T(X_{te}) > c | Y_{te} \notin \{1, \ldots, L\})$. In Theorem 4.1, we show that the type I error can be controlled at a nominal level $\alpha$ by properly choosing the thresholds $c_\ell$s, while guaranteeing high power. Before the formal statement of Theorem 4.1, we first state some assumptions regarding the distribution of DTM and the separation between the normal and abnormal samples.

**Assumption A2.** (a) For each $\ell = 1, \ldots, L$, given a nominal level $\alpha$ where $0 < \alpha < 1$, there exists a positive finite constant $c_\ell$ satisfying $c_\ell = \text{argmin}\{c : P_\ell(X : d_\ell(X) \leq c) \geq 1 - \alpha\}$. 

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For any $\delta \in (0, 1)$, denote $\beta_n^\ell = \sqrt{(4/n^\ell)((p + 1)\log(2n^\ell) + \log(8/\delta))}$. There exists a constant $M$ satisfying $M \geq 2c^\ell + C\beta_n^\ell(\beta_n^\ell + \sqrt{m^\ell})$, such that given the anomaly $x_{out}$ sampled from $P_0$, $P_{\ell}(\|X - x_{out}\|^2 \leq M) \leq \epsilon$, where $C$ is a constant and $\epsilon < m^\ell/2$.

Assumption A2 (a) defines a safety zone for $X \sim P_\ell$, that is, $A_\ell^\ell = \{X : X \sim f_\ell(x), d_\ell(X) \leq c_\ell\}$. Based on $A_\ell^\ell$, Assumption A2 (a) separates $X \sim P_\ell$ into two parts: one with DTM smaller than $c_\ell$ and the other with DTM greater than $c_\ell$. Of course it is intrinsically hard or even impossible to distinguish between a sample from the tail of $f_\ell(x)$ and a true anomaly, as in both cases the DTMs are relatively large. Assumption A2 (b) requires that the distance between anomalies sampled from $f_{out}$ and samples from $f_\ell$ can be lower bounded with large probability.

Assumption A3. (a) There exist positive constants $C = C(P_\ell)$ and $\epsilon_0 = \epsilon_0(P_\ell)$, such that for all $0 < \epsilon < \epsilon_0$ and $\eta \in \mathbb{R}$, for any $x$, and $0 < t < m$,

$$P_{\ell}(\|X - x\| \leq r_{\ell,t}(x) + \eta) - P_{\ell}(\|X - x\| \leq r_{\ell,t}(x)) \leq \epsilon,$$

then $|\eta| < C\epsilon$.

(b) For any $x$ sampled from $P_{\ell}$, if $\kappa < C\epsilon$, then

$$P_{\ell}(d_{\ell}(x) > c_\ell - \kappa) - P_{\ell}(d_{\ell}(x) > c_\ell) \leq \epsilon.$$

Assumption A3 implies that $P_\ell$ has non-zero probability around the boundary of the ball centered at $x$ with radius $r_{\ell,t}(x)$.

**Theorem 4.1.** Consider model (4.1). Suppose Assumptions A2 and A3 hold.

(a) As $n \to \infty$, for $X^{te} \in D_{te}$ with unobserved label $Y^{te} \in \{1, \ldots, L\}$, for $0 < c < 1$, $P(T(X^{te}) > c|Y^{te} \in \{1, \ldots, L\}) \leq \alpha$.

(b) For $X^{te} \in D_{te}$, $0 < c < 1$, we have $P(T(X^{te}) > c|Y^{te} \notin \{1, \ldots, L\}) \geq 1 - L\delta$, where $\delta$ is specified in Assumption A2 (b).

In practice, we cannot directly calculate $c_\ell$ since it depends on the unknown density $f_\ell$. Instead, we introduce a bootstrap method with data-splitting to approximate $c_\ell$ within each $D_{tr,\ell}$. Algorithm 3 summarizes the detailed procedure of approximating the cutoff $c_\ell$ and detecting anomalies. Denote the detected anomaly set as $D_0$. Then we conduct the Rbagging on the set $D_{te} \setminus D_0$. 

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**Algorithm 3** Anomaly Detection

| Input: labeled training data $D_{tr, \ell}$, testing data $D_{te}$, $k$, $\alpha$ |
| --- |
| **1.** for $\ell = 1, \ldots, L$ do |
| Split $D_{tr, \ell}$ as $D_{tr, \ell}^{(1)}$ and $D_{tr, \ell}^{(2)}$. |
| for $i = 1, \ldots, |D_{tr, \ell}^{(1)}|$ do |
| For each $z_i \in D_{tr, \ell}^{(1)}$, find its $k$-NN in $D_{tr, \ell}^{(2)}$ denoted as $\mathcal{N}_z^k$, and calculate |
| $\hat{d}_2^\ell(z_i) = \frac{1}{k} \sum_{X_j \in \mathcal{N}_z^k} \|X_j - z_i\|^2$. |
| end |
| Set $\hat{c}_\ell$ as the $(1 - \alpha)$-th quantile of $(\hat{d}_1(z_1), \ldots, \hat{d}_L(z_{|D_{tr, \ell}^{(1)}|}))$. |
| end |
| **2.** for $i = 1, \ldots, |D_{te}|$ do |
| Find the $k$-NN of $X_{te}^i \in D_{tr}$ denoted as $\mathcal{N}_X^k$, and calculate |
| $\hat{d}_2^\ell(X_{te}^i) = \frac{1}{k} \sum_{X_j \in \mathcal{N}_X^k} \|X_j - X_{te}^i\|^2$. |
| Calculate the test statistics $T(X_{te}^i) = \prod_{\ell=1}^L \mathbb{1}_{\{\hat{d}_\ell(X_{te}^i) > \hat{c}_\ell\}}$. |
| Set $X_{te}^i \in D_0$ if $T(X_{te}^i) = 1$. |
| end |

## 5 Simulation Study

### 5.1 An Illustrative Example

We first consider a toy example to compare the performance of Rbagging with the classical bagging classifier when a distribution shift exists. Classical bagging refers to uniformly sampling from the training data $B$ times, and averaging classifiers trained to each bootstrap replicate. We generate the training data with sample size $n = 300$ from the joint distribution $f_{tr}(x, y) = P_{tr}(Y = y)f(x|Y = y) = \frac{1}{3}f_y(x)$ for $y = 1, 2, 3$, with $f_1$ the density function of $N((1, 1)^T, \Sigma)$, $f_2$ the density of $N((1, 4)^T, \Sigma)$, and $f_3$ the density of $N((1, 7)^T, \Sigma)$. We set $\Sigma$ as a $2 \times 2$ matrix with diagonal entries as 1 and off-diagonal entries as 0.2. We further generate the testing data with sample size $m = 300$ from the joint distribution $f_{te}(x, y) = P_{te}(Y = y)f(x|Y = y) = P_{te}(Y = y)f_y(x)$ with $P_{te}(Y = 1) = P_{te}(Y = 2) = \frac{10}{21}$ and $P_{te}(Y = 3) = \frac{1}{21}$. That is, the testing data set also contains the classes $\{1, 2, 3\}$ but with proportions varying. We use multinomial regression as the base classifier.
We implement Rbagging based on Algorithm 1 with $k = 5$. Repeat $B = 10$ times. Figure 3 (a) and (b) show the generated training and testing data. Figure 3 (c) shows one replicate of the reproduced data using INNs with $T = 5$. Clearly, the sampled data approximates the testing data. We further compare the decision boundary learned via classical bagging and Rbagging. The solid lines in Figure 3 (d) are the averaged decision boundaries trained via classical bagging; clearly performance is suboptimal. The colored regions are the decision regions based on the Bayes classifier assuming the distribution of $P_{te}(Y|X = x)$ is known. The dashed lines in Figure 3 (d) are learned from Rbagging, and are closer to the Bayesian rule for the testing data.

Figure 3: (a) training data; (b) testing data; (c) reproduced samples based on INNs in Algorithm 1 with $k = 5$; (d) the dashed lines are the decision boundaries based on Rbagging; and the solid lines are the averaged decision boundaries from classic bagging; the colored region are the decision regions based on Bayes classifier.
5.2 Simulation Study without outliers

We assess the empirical performance of Rbagging in Algorithm 2 for base classifiers including logistic regression (LR) fit with maximum likelihood estimation, classification and regression trees (CART), random forest (RF), and linear discriminant analysis (LDA) via simulated experiments. We denote the above methods as Rbagging+LR, Rbagging+CART and Rbagging+RF, Rbagging+LDA, respectively. We further compare our methods with the base classifiers without domain adaptation, and two popular domain adaptation methods as the state of the art. The first method is kernel mean matching (KMM) Zhang et al. [2013]. The second method is balanced and conformal optimized prediction sets (BCOPS) Guan and Tibshirani [2019]. We also apply KMM and BCOPS with four base classifiers: LR, Bagging, RF and LDA, and denote these approaches as BCOPS+LR, BCOPS+Bagging, BCOPS+RF, BCOPS+LDA, KMM+LR, KMM+Bagging, KMM+RF, KMM+LDA, respectively. We use CART as the default classifier in Bagging. We keep the tuning parameters for each classifier the same when coupled with different data adaptation methods. For example, we fix the number of trees and number of variables to possibly split at in each node in the RF classifier for different data adaptation methods. In Rbagging, we choose $T$ as the number of iterations when the changes of proportions of classes from $D_{tr}^{(T-1)}$ to $D_{tr}^{(T)}$ is controlled by a pre-specified threshold $\varepsilon_T = 0.01$. We set $B = 500$ for both Rbagging and Bagging.

We consider three design scenarios. In each scenario, we generate the training data from two classes: $\{1\}$ and $\{2\}$ with equal proportions, and hence,

$$f_{tr}(x) = 0.5f_1(x) + 0.5f_2(x). \quad (5.1)$$

Testing data are generated with the same labels $\{1\}, \{2\}$ but with different percentages, i.e.,

$$f_{te}(x) = q_1f_1(x) + (1-q_1)f_2(x), \quad (5.2)$$

where we vary the value of $q_1$ from $(1/2, 1/3, \ldots, 1/10)$ in a decreasing order to present different magnitude of distribution shift. For each scenario, we generate training and test data with sample size 500, and set $X \in \mathbb{R}^{10}$. Testing accuracy is calculated via applying the trained classifier on the testing data. We repeat the simulation 20 times and report the mean and standard deviation of the testing accuracy.

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5.2.1 Setting I: Sparse class boundaries

We consider both $f_1$ and $f_2$ are mixture density functions. That is, for both of the training data and test data, the feature $X$ is generated conditional on the label class $Y = 1$ or 2 as follows

$$X \sim \begin{cases} \frac{1}{2}N_p(\mu_0, \Sigma) + \frac{1}{2}N_p(-\mu_0, \Sigma) & \text{if } Y = 1, \\ \frac{1}{2}N_p(\mu_1, \Sigma) + \frac{1}{2}N_p(-\mu_1, \Sigma) & \text{if } Y = 2, \end{cases}$$

where $p = 10$, $\Sigma = I_{10 \times 10}$, $\mu_0 = (2, -2, 0, \ldots, 0)^\top \in \mathbb{R}^{10}$, and $\mu_1 = (2, 2, 0, \ldots, 0)^\top \in \mathbb{R}^{10}$.

Figure 4: Simulation setting I (a)-(d): testing accuracy under different approaches.

Figure 4 illustrates the test accuracy based on different approaches. KMM methods have stable performance for different classifiers but the improvement is not significant compared with the corresponding base classifiers without considering domain adaptation. The performance of BCOPS varies under different classifiers since the algorithm highly depends on the classifier’s ability to detect domain changes. BCOPS-RF and BCOPS-Bagging significantly improve the test accuracy when $q_1 = 1/2, 1/3, 1/4, 1/5$; however the accuracy drops dramatically when the testing data are
highly unbalanced with $q_1 < 1/5$. Especially, for BCOPS-LR, the accuracy even drops below the base-line classifier. BCOPS uses a data-splitting strategy to estimate the testing data proportion, which partly explains its unstable performance. Rbagging has the highest accuracy for different classifiers and performs stably even for very unbalanced testing data sets.

5.2.2 Setting II: Rotated sparse normal

![Graphs showing testing accuracy under different approaches for different classifiers.](image)

Figure 5: Simulation setting II (a)-(d): testing accuracy under different approaches.

We consider $f_y(x)$ for $y = 1, 2$ are generated from multivariate Gaussian with the covariance matrix multiplied by a random rotation matrix, that is,

$$X \sim \begin{cases} 
N_p(\Omega_p\mu_0, \Omega_p\Sigma_0\Omega_p^T) & \text{if } Y = 1, \\
N_p(\Omega_p\mu_1, \Omega_p\Sigma_1\Omega_p^T) & \text{if } Y = 2,
\end{cases} \tag{5.4}$$

where $p = 10$, $\mu_0 = (1, 1, 1, 0, \ldots, 0)^T$, $\mu_1 = (0, 0, 0, 0, \ldots, 0)^T$, and $\Omega_p$ is a $p \times p$ rotation matrix sample according to a Haar measure; $\Omega_p$ is sampled once and kept as fixed in each replication. $\Sigma_0$ is
a block diagonal matrix with two blocks $\Sigma_0^{(1)} = \text{diag}\{\frac{3}{2}\} + \frac{1}{2}1_31_3^T$ and $\Sigma_0^{(2)} = \text{diag}\{\frac{1}{2}\} + \frac{1}{2}1_{p-3}1_{p-3}^T$; $\Sigma_1$ is also a block diagonal matrix with two blocks $\Sigma_1^{(1)} = \text{diag}\{\frac{1}{2}\} + \frac{1}{2}1_31_3^T$ and $\Sigma_1^{(2)} = \Sigma_0^{(1)}$.

As shown in Figure 5, KMM and BCOPS significantly improve the test accuracy when the testing data differ from the training data. Our proposed methods show the highest accuracy and lowest variance when $q_1$ ranges from $1/2$ to $1/10$ for different classifiers.

5.2.3 Setting III: Independent features

![Figure 6](image)

Figure 6: Simulation setting III (a)-(d): testing accuracy under different approaches.

We consider $X = (X_1, \ldots, X_p)^\top$ conditional on $Y = y \ (y = 1, 2)$ generated from different distribution classes with independent features; that is, each component $X_i$ follows

$$X_i \sim \begin{cases} N(0, 1) & \text{if } Y = 1, \\ \text{Laplace}(0, 1) & \text{if } Y = 2, \end{cases} \tag{5.5}$$

where $\text{Laplace}(0, 1)$ is the Laplace density with location parameter 0 and scale parameter 1.
As shown in Figure 6, the accuracy of KMM-RF and KMM-CART sometimes drop below the accuracy of the baseline classifiers. One possible reason of such accuracy loss is that KMM uses a Gaussian kernel which may be suboptimal for non-Gaussian data. Rbagging and BCOPS significantly increase the accuracy compared with baseline when the distribution shifts. In this setting, Rbagging+RF shows the highest accuracy.

5.3 Simulation with anomaly detection

We consider model (5.6), which accommodates anomalies in the testing data. We generate 500 training data points with half from class \( \{1\} \) and the other half from class \( \{2\} \). We set \( f_1(x), f_2(x) \) as in Section 5.2 for three different scenarios.

\[
 f_{tr}(x) = 0.5 f_1(x) + 0.5 f_2(x), \quad f_{te}(x) = q_1 f_1(x) + q_2 f_2(x) + \epsilon f_{out}(x). \tag{5.6}
\]

We also generate the testing dataset with sample size 500 for \( q_1 \) ranging from \( 0.9 \times \left( \frac{1}{2}, \frac{1}{3}, \ldots, \frac{1}{10} \right) \), \( q_2 = 0.9 - q_1 \), and \( \epsilon = 0.1 \), i.e., randomly generating 10% outliers from an alternative distribution. The outlier distribution \( f_{out}(x) \) will be specified later.

Since KMM is not able to detect the outliers, we compare our proposed method with BCOPS (Guan and Tibshirani [2019]). We apply four different classifiers with BCOPS, and denote them as BCOPS+RF, BCOPS+Bagging, BCOPS+LR, and BCOPS+LDA. We set the nominal level as \( \alpha = 0.1 \) for anomaly detection in Algorithm 3, and compare the empirical type I error and power performance. The empirical type I error is calculated as the percentage of non-outlying data points that are falsely detected, and the empirical power is calculated as the percentage of outliers detected in the testing data. We repeat the simulation 100 times and report the averaged empirical type I error and power.

We further evaluate the testing accuracy after removing the detected outliers. For fair comparison, we remove the same amount of outliers for different methods. For Rbagging, we remove 10% of testing data points with the largest \( \min_{\ell} \hat{d}_\ell(X^{te}) \), then implement Rbagging+RF, Rbagging+CART and Rbagging+LR. For BCOPS, we calculate the conformal score for each testing data point as \( \min_{\ell} c_{\ell}(X^{te}) \) where \( c_{\ell}(X^{te}) \) represents the probability of \( X^{te} \) belonging to class \( \{\ell\} \). Then we remove 10% of the testing data points with the smallest conformal score. After removing these potential outliers, we apply different classifiers: RF, Bagging with CART and LR with the estimated proportions \( \hat{q}_1, \hat{q}_2 \) in BCOPS. Testing accuracy is calculated based on the predictions on the remaining 90% testing data points. In Rbagging, we choose the number of iterations \( T \) with the pre-specified threshold \( \varepsilon_T = 0.01 \). We set \( B = 500 \) for both Rbagging and Bagging.

We repeat 20 times and report the mean and standard deviation of the testing accuracy.
5.3.1 Setting I: Sparse class boundaries with anomaly

In model (5.6), we generate $X$ from the conditional densities $f_1(x)$ and $f_2(x)$ as in (5.3). We further generate the anomaly $X_{\text{out}}$ with $f_{\text{out}}$ the density function of $N_p(\mu, \Sigma)$, where $p = 10$, $\mu = (4, 4, 0, \ldots, 0)$ and $\Sigma$ is a diagonal matrix with first two entries as 0.5 and the remaining entries as 1.

Table 1 compares the type I error and power under different approaches. Rbagging controls the type I error at the nominal level while maintaining high detection power; performance is stable under different values of $q_1$. In contrast, BCOPS has inflated type I error. The empirical power of BCOPS has a decreasing pattern as $q_1$ decreases. The low power can be explained as a sacrifice of their data-splitting procedure. After removing 10% outliers, we show the testing accuracy in Figure 7. Rbagging still has the highest accuracy under different classifiers. For BCOPS, the variance increases as $q_1$ decreases. When the testing data have a similar distribution as the training data, the accuracy of BCOPS drops below the baseline due to the extra error brought by the inaccurate estimate of the distributional changes.

![Figure 7](attachment:image.png)

Figure 7: Simulation setting I (with anomaly) (a)-(d): testing accuracy under different approaches.
| Setting | Method     | Type I Error | Power   |
|---------|------------|--------------|---------|
|         | Rbagging   | q1/0 | 1/2  | 1/3  | 1/4  | 1/5  | 1/6  | 1/7  | 1/8  | 1/9  | 1/10 |
| Setting I | Rbagging   | type I | 0.06 | 0.06 | 0.05 | 0.05 | 0.05 | 0.05 | 0.04 | 0.05 | 0.05 |
|         | power      | type I | 1.00 | 0.99 | 1.00 | 0.99 | 1.00 | 0.99 | 0.99 | 1.00 | 1.00 |
|         | BCOPS+RF   | type I | 0.34 | 0.25 | 0.23 | 0.21 | 0.20 | 0.18 | 0.16 | 0.16 | 0.17 |
|         | power      | type I | 0.97 | 0.96 | 0.96 | 0.93 | 0.91 | 0.92 | 0.86 | 0.87 | 0.86 |
|         | BCOPS+Bagging | type I | 0.33 | 0.27 | 0.21 | 0.18 | 0.17 | 0.17 | 0.12 | 0.11 | 0.12 |
|         | power      | type I | 1.00 | 0.99 | 0.96 | 0.95 | 0.95 | 0.93 | 0.87 | 0.86 | 0.81 |
|         | BCOPS+LR   | type I | 0.33 | 0.24 | 0.22 | 0.20 | 0.20 | 0.17 | 0.16 | 0.18 | 0.16 |
|         | power      | type I | 0.99 | 0.98 | 0.99 | 0.97 | 0.95 | 0.94 | 0.92 | 0.92 | 0.89 |
|         | BCOPS+LDA  | type I | 0.34 | 0.28 | 0.22 | 0.18 | 0.17 | 0.14 | 0.15 | 0.13 | 0.15 |
|         | power      | type I | 0.99 | 0.98 | 0.97 | 0.93 | 0.94 | 0.89 | 0.92 | 0.87 | 0.88 |
| Setting II | Rbagging   | type I | 0.06 | 0.05 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 |
|         | power      | type I | 0.58 | 0.55 | 0.52 | 0.53 | 0.57 | 0.56 | 0.53 | 0.55 | 0.54 |
|         | BCOPS+RF   | type I | 0.23 | 0.21 | 0.22 | 0.23 | 0.26 | 0.23 | 0.21 | 0.21 | 0.23 |
|         | power      | type I | 0.37 | 0.36 | 0.41 | 0.41 | 0.43 | 0.35 | 0.30 | 0.39 | 0.36 |
|         | BCOPS+Bagging | type I | 0.19 | 0.19 | 0.18 | 0.16 | 0.17 | 0.18 | 0.20 | 0.18 | 0.18 |
|         | power      | type I | 0.45 | 0.46 | 0.36 | 0.33 | 0.29 | 0.35 | 0.31 | 0.30 | 0.28 |
|         | BCOPS+LR   | type I | 0.21 | 0.19 | 0.21 | 0.22 | 0.23 | 0.22 | 0.20 | 0.21 | 0.21 |
|         | power      | type I | 0.31 | 0.29 | 0.33 | 0.35 | 0.37 | 0.31 | 0.24 | 0.32 | 0.31 |
|         | BCOPS+LDA  | type I | 0.18 | 0.16 | 0.15 | 0.16 | 0.16 | 0.21 | 0.20 | 0.18 | 0.20 |
|         | power      | type I | 0.31 | 0.32 | 0.30 | 0.33 | 0.25 | 0.34 | 0.35 | 0.34 | 0.32 |
| Setting III | Rbagging   | type I | 0.05 | 0.07 | 0.08 | 0.08 | 0.08 | 0.07 | 0.07 | 0.09 | 0.08 |
|         | Power      | type I | 0.91 | 0.90 | 0.84 | 0.91 | 0.88 | 0.88 | 0.85 | 0.90 | 0.88 |
|         | BCOPS+RF   | type I | 0.67 | 0.66 | 0.69 | 0.68 | 0.70 | 0.68 | 0.71 | 0.71 | 0.69 |
|         | Power      | type I | 0.97 | 0.97 | 0.97 | 0.96 | 0.97 | 0.98 | 0.97 | 0.97 | 0.97 |
|         | BCOPS+Bagging | type I | 0.51 | 0.49 | 0.52 | 0.54 | 0.53 | 0.55 | 0.54 | 0.57 | 0.55 |
|         | Power      | type I | 0.98 | 0.91 | 0.74 | 0.57 | 0.44 | 0.44 | 0.43 | 0.39 | 0.28 |
|         | BCOPS+LR   | type I | 0.60 | 0.60 | 0.61 | 0.61 | 0.63 | 0.62 | 0.64 | 0.63 | 0.63 |
|         | Power      | type I | 0.93 | 0.92 | 0.94 | 0.92 | 0.92 | 0.94 | 0.92 | 0.94 | 0.93 |
|         | BCOPS+LDA  | type I | 0.37 | 0.46 | 0.46 | 0.49 | 0.51 | 0.53 | 0.55 | 0.53 | 0.55 |
|         | Power      | type I | 0.96 | 0.81 | 0.61 | 0.56 | 0.35 | 0.31 | 0.36 | 0.27 | 0.22 |

Table 1: Simulation setting I, II, III with anomaly: type I error and power based on different approaches.
5.3.2 Setting II: Rotated sparse normal with anomaly

Following model (5.6), we generate $X$ from $f_1(x)$ and $f_2(x)$ as in (5.4). We further generate the anomaly $X_{out}$ from $f_{out}$ the density function of $N_p(\Omega_p\mu_2,\Omega_p I_{p \times p}\Omega_p^\top)$, where $\mu_2 = (0, 0, 2, 2, 0, \ldots, 0)$ and $\Omega_p$ is the same rotation matrix defined in Setting 2(a).

![Graphs showing testing accuracy under different approaches for Rbagging+RF, BCOPS+RF, Bagging, Rbagging+CART, BCOPS+Bagging, Rbagging+LR, BCOPS+LR, LDA, Rbagging+LDA, BCOPS+LDA.]

Figure 8: Simulation setting II (with anomaly) (a)-(d): testing accuracy under different approaches.

As shown in Table 1, type I error is controlled under the nominal level for Rbagging. The power is lower compared with Setting I (with anomaly) since the outliers’ distribution $f_{out}$ is less distinguishable from $f_1$ and $f_2$. The empirical power performance of Rbagging is still stable for different $q_\ell$. BCOPS has inflated type I error, implying over sensitivity in selecting outliers; the power performance of BCOPS is unsatisfactory and unstable with respect to different classifiers and class proportions.

5.3.3 Setting III: Independent features with anomaly

In model (5.6), we generate $X$ from $f_1$ and $f_2$ as in (5.5). The anomaly $X_{out}$ are generated from $f_{out}$ the density function of $N_p(\mu_2, I_{p \times p})$, where $\mu_2 = (0, 0, 0, -3, -3, 0, 0, 0, 0)\top$ and $I_{p \times p}$ is an
identity matrix with \( p = 10 \).

Figure 9: Simulation Setting III (with anomaly) (a)-(d): testing accuracy under different approaches.

Table 1 shows the empirical type I error and power in this setting. BCOPS has a slightly higher empirical power than Rbagging. However, its corresponding type I error is significantly larger than Rbagging. After removing 10% outliers, the testing accuracy is improved for both Rbagging and BCOPS approaches. Rbagging has the highest accuracy except for the case in Rbagging-CART when the class proportion \( q_1 = 1/2 \).

6 Real Data Analysis

In this Section, we apply our proposed method on two real data examples: breast cancer data having different tumor types and the widely used MNIST handwritten digit classification data.
6.1 Breast Cancer Data

We apply our method to the Wisconsin Breast Cancer Dataset (available at the University of California, Irvine (UCI) machine learning repository). The dataset contains nine features of tumors in 699 patients, with 241 malignant and 458 benign. Since the data are collected in different time periods, we use the data originally collected in January 1989 with sample size 367 as the training data. It includes 200 benign samples and 167 malignant samples. We use the subsequent 332 data collected from October 1989 to November 1991 as our testing data, which includes 258 benign samples and 74 malignant samples. The percentage of malignant samples in the testing data is 22.3% which is significantly lower than the percentage, 45.5%, of malignant samples in the training data. We use three baseline classifiers including RF, Bagging with CART, and logistic regression (LR), as the original classifiers without considering distribution shift. We further equip Rbagging, BCOPS and KMM with these classifiers. In Rbagging, we choose the number of iterations \( T \) with the pre-specified threshold \( \varepsilon_T = 0.01 \). We set \( B = 500 \) for both Rbagging and Bagging.

To examine the performance of Rbagging under different training sample sizes, we vary the training data via randomly sampling from the candidate training dataset with sample size \( n^{tr} = 50, 100 \) and 200 respectively. The sample size of the test dataset is \( n^{te} = 332 \). Since \( n^{te} > n^{tr} \), we first randomly sample \( n^{tr} \) data points from the test set, then use the sampled test data as the guidance in Algorithm 2. We report the test accuracy as the number of wrongly predicted data points in the whole test dataset. As shown in Table 2, Rbagging performs the best compared with other approaches, and the prediction error is stable under different sample size of the training data.

6.2 MNIST Data

We consider the MNIST handwritten digit dataset [LeCun et al., 2010]. We randomly select 500 images labeled as \( \{5\} \) and 500 images labeled as \( \{6\} \) together as the training data. For the testing data, we randomly sample 900\( q_1 \) images labeled as \( \{5\} \) and 900\( (1 - q_1) \) images labeled as \( \{6\} \) without overlap with the training set. \( q_1 \) is set in \( \{1/2, 1/5, 1/10\} \) to present different levels of heterogeneity between the training and the testing data. Then we randomly sample 100 images with labels in \( \{0, 1, 2\} \) as the new digits unobserved in the training data. We set the nominal level \( \alpha = 0.1 \) in Algorithm 3. Figure 10 evaluates the empirical type I and type II error. Clearly, compared with BCOPS, Rbagging has higher power given any fixed type I error.
| Classifier | $n^{tr} = 50$ | Rbagging | KMM | BCOPS | Original |
|------------|--------------|----------|-----|-------|----------|
| RF         | 5.00        | 9.00     | 15.00 | 13.00 |
| Bagging    | 5.00        | 10.00    | 13.00 | 14.00 |
| LDA        | 5.00        | 9.00     | 21.00 | 14.00 |
| LR         | 5.00        | 15.00    | 22.00 | 14.00 |

| Classifier | $n^{tr} = 100$ | Rbagging | KMM | BCOPS | Original |
|------------|----------------|----------|-----|-------|----------|
| RF         | 4.00          | 7.00     | 10.00 | 8.00  |
| Bagging    | 4.00          | 8.00     | 9.00  | 11.00 |
| LDA        | 4.00          | 9.00     | 15.00 | 7.00  |
| LR         | 4.00          | 15.00    | 14.00 | 7.00  |

| Classifier | $n^{tr} = 200$ | Rbagging | KMM | BCOPS | Original |
|------------|----------------|----------|-----|-------|----------|
| RF         | 4.00          | 5.00     | 5.00 | 8.00  |
| Bagging    | 4.00          | 8.00     | 6.00 | 8.00  |
| LDA        | 4.00          | 8.00     | 8.00 | 6.00  |
| LR         | 4.00          | 9.00     | 7.00 | 6.00  |

Table 2: Breast cancer dataset: number of wrongly predicted data points in the testing set under different training sample sizes.

Figure 10: Type I and Type II error for MNIST data set.
In addition, we remove 10% of the testing data points with the largest DTM for Rbagging and with the smallest conformal score for BCOPS. Then we compare the testing accuracy on the remaining data points. In Rbagging, we choose the number of iterations $T$ with the pre-specified threshold $\varepsilon_T = 0.01$. We set $B = 500$ for both Rbagging and Bagging. We use Random Forest (RF) as the baseline classifier. BCOPS-RF shows a lower accuracy due to the high error rate in detecting the outliers. For example, when $q_1 = 1/2, 1/5$, many inliers are falsely removed, the classification accuracy of BCOPS drops below the accuracy of the RF baseline classifier without considering distribution shifting.

| $q_1$ | Rbagging-RF | BCOPS-RF | RF |
|-------|-------------|-----------|----|
| 1/2   | 0.924       | 0.849     | 0.885 |
| 1/5   | 0.940       | 0.860     | 0.881 |
| 1/10  | 0.938       | 0.908     | 0.879 |

Table 3: Testing accuracy for MNIST dataset

7 Discussion

Rbagging is a promising general approach for improving classification performance when there is a distributional shift between the training and test data. Such shifts are very common in practice, and methods that fail to adjust can have very poor performance. In this article, we have focused on a particular type of distributional shift, and there are several natural next steps that are of substantial interest. The first general direction is to accommodate different types of distributional shifts. For example, instead of only allowing the label proportions to vary, one can also allow the density of the features within each class to vary. In doing this, it is important to include some commonalities between training and test sets. One possibility is represent the different feature densities with a common set of kernels, but with the weights varying not just due to variation in the label proportions but due to other unknown factors.

Another possibility, which is particularly natural for high-dimensional and geometrically structured features, is to suppose that there is some lower-dimensional structure in the data. For example, the features may tend to be concentrated close to a lower-dimensional manifold. If this lower-dimensional structure tends to be largely preserved between training and test data, then it is natural to leverage on manifold learning or other dimensionality reduction algorithms in constructing relevant distances to be used in applying an appropriate variant of the iterated nearest neighbor sampler within Rbagging.
The ideas behind Rbagging can be applied to related problems in which one wants to improve reproducibility but does not have a specific test set to focus on. If data are collected under a complex sample survey design and sampling weights are available, then Rbagging can be modified to produce bootstrap samples from the training data that are population-representative instead of representative of the test data. Alternatively, if such sampling weights are unavailable, one can develop a different version of Rbagging based on generating bootstrap samples that are designed to be highly heterogeneous across covariates groups. Ideally, this would improve generalizability to a variety of distributional shifts that may occur in future test datasets that are as of yet unobserved.

A Appendix: Main Proofs

A.1 Proof of Lemma 3.1

Proof. Let $B_r(X^\text{te})$ be the closed ball of radius $r$ centered at $X^\text{te}$, i.e., $B_r(X^\text{te}) = \{Z \in \mathbb{R}^p : \|Z - X^\text{te}\| \leq r\}$, for some metric $\| \cdot \|$ defined on $\mathbb{R}^p$. We first consider a point $X^\text{te} \in D_{\text{te}}$ such that for any $r > 0$,

$$
\mathbb{P}_{tr}(B_r(X^\text{te})) = \mathbb{P}_{tr}(Z \in B_r(X^\text{te}), Z \sim f_{tr}(z)) = \int_{B_r(X^\text{te})} f_{tr}(z)dz = \sum_{\ell=1}^{L} \int_{B_r(X^\text{te})} p_\ell f_\ell(z)dz \\
\geq \sum_{\ell,q \neq 0} \int_{B_r(X^\text{te})} p_\ell f_\ell(z)dz \geq \min_{\ell,q \neq 0} \left\{ \frac{p_\ell}{q_\ell} \right\} \sum_{\ell,q \neq 0} \int_{B_r(X^\text{te})} q_\ell f_\ell(z)dz \\
= \min_{\ell,q \neq 0} \left\{ \frac{p_\ell}{q_\ell} \right\} \int_{B_r(X^\text{te})} f_{te}(z)dz > 0. \tag{A.1}
$$

Then, for any $r > 0$, given $X^\text{te} \sim f_{te}$, we have

$$
\mathbb{P}_{tr}(\min_{i \in \{1,\ldots,n\}} \{\|X_i - X^\text{te}\| \geq r\}) = \prod_{i=1}^{n} \mathbb{P}(\|X_i - X^\text{te}\| \geq r, X_i \in D_{tr}) = \prod_{i=1}^{n} (1 - \mathbb{P}_{tr}(B_r(X^\text{te}))) \\
= [1 - \mathbb{P}_{tr}(B_r(X^\text{te}))]^n \to 0.
$$

Denote the points that do not satisfy (A.1) as $\tilde{X}$. Consider a point $\tilde{X} \in \tilde{X}$, that is, there exists some $\tilde{r}$, such that $\int_{B_{\tilde{r}}(\tilde{X})} f_{te}(z)dz = 0$. There exists a rational point $a_{\tilde{X}}$, s.t $a_{\tilde{X}} \in B_{\tilde{r}/2}(\tilde{X})$. Consequently, there exists a small sphere $B_{\tilde{r}/2}(a_{\tilde{X}})$, s.t $B_{\tilde{r}/2}(a_{\tilde{X}}) \subset B_{\tilde{r}}(\tilde{X})$, and $\int_{B_{\tilde{r}/2}(a_{\tilde{X}})} f_{te}(z)dz = 0$. Also, $\tilde{X} \in B_{\tilde{r}/2}(a_{\tilde{X}})$. Since $a_{\tilde{X}}$ is countable, there is at most a countable set of such spheres that contain the entire $\tilde{X}$. Therefore, $\tilde{X} \subset \cup_{\tilde{X} \in \tilde{X}} B_{\tilde{r}/2}(a_{\tilde{X}})$. Then we have $\mathbb{P}(\tilde{X}) = 0$. \hfill \Box

A.2 Proof of Theorem 3.2

We start with the simple case that

$$
f_{tr}(x) = p_1 f_1(x) + (1 - p_1) f_2(x) \quad \text{and} \quad f_{te}(x) = f_1(x). \tag{A.2}
$$
That is, the training data contain two classes, while the testing data only contain one class. To simplify notation, for any \( X^{te} \sim f_{te}(x) \), define its nearest neighbor in \( D^{br,(t)}_{tr} \) as \( X(1) \), and the corresponding label of \( X(1) \) is \( Y(1) \). Denote \( P^{(t)}_{te}(Y(1) = 1) \) as the probability that for \( X \sim f_{te} \), its nearest neighbor in \( D^{br,(t)}_{tr} \) is labeled as class 1. Here we use the unified symbol \( D^{(t)}_{tr} \) to represent \( D^{br,(t)}_{tr} \) for \( b = 1, \ldots, B \). Then we show that \( P^{(t)}_{te}(Y(1) = 1) \) approaches to 1 as \( t \) increases.

**Lemma A.1.** Assume \( f_{tr}(x) \) and \( f_{te}(x) \) hold as (A.2). \( \lim_{t \to \infty} P^{(t)}_{te}(Y(1) = 1) = 1. \)

**Proof.** For simplicity, define \( p^{(t)} := P^{(1)}_{te}(Y(1) = 1) = \mathbb{E} 1_{\{Y(1)=1\}} = \mathbb{E} \{ \mathbb{E} (1_{\{Y(1)=1\}}|X^{te} = x) \} \)

\[
\begin{align*}
p^{(1)} &= \mathbb{E} \mathbb{P}(Y(1) = 1|X^{te} = x) = \mathbb{E} \frac{p_1 f_1(X(1))}{p_1 f_1(X(1)) + (1 - p_1) f_2(X(1))} \\
&= \mathbb{E}_{x\sim f_{te}} \frac{p_1 f_1(x)}{p_1 f_1(x) + (1 - p_1) f_2(x)} = \mathbb{E}_{x\sim f_{te}} \frac{p_1}{p_1 + (1 - p_1) f_2(x)/f_1(x)} > p_1,
\end{align*}
\]

where the expectation is with respect to both of \( X^{te} \sim f_{te}(x) \) and \( (X(1), Y(1)) \) in \( D_{tr} \); the fifth equality is due to \( X(1) \to X^{te} \) with probability 1 by Lemma 3.1, and the Lipschitz property of \( \frac{p_1 f_1(x)}{p_1 f_1(x) + (1 - p_1) f_2(x)} \); and the inequality “>” is based on Jensen’s.

Based on Algorithm 2, we have samples \( D^{(t)}_{tr} \), and \( \mathbb{P}(Y = 1, Y \in D^{(t)}_{tr}) = P^{(1)}_{te}(Y(1) = 1) \). That is, \( X \) in \( D^{(1)}_{tr} \) follows the density function

\[
f^{(1)}(x) = p^{(1)} f_1(x) + (1 - p^{(1)}) f_2(x),
\]

with \( p^{(1)} > p_1 \) proved in (A.3). Follow the same line, at the \( t \)-th iteration, we have \( p^{(t)} > p^{(t-1)} \). On the other hand, since \( p^{(t)} \) is bounded by 1, as \( p^{(t)} \to 1 \) with \( t \) increasing, we have

\[
\lim_{t \to \infty} P^{(t+1)}_{te}(Y(1) = 1) = \lim_{t \to \infty} \mathbb{E} \mathbb{P}(Y(1) = 1|X^{te} = x) = \lim_{t \to \infty} \mathbb{E} \frac{p^{(t)} f_1(x)}{p^{(t)} f_1(x) + (1 - p^{(t)}) f_2(x)} = 1.
\]

Therefore, \( \mathbb{P}(Y = 1, Y \in D^{(T)}_{tr}) = \lim_{t \to \infty} P^{(t)}_{te}(Y(1) = 1) = 1 \), and \( f^{(T)} = f_1(x) = f_{te}(x). \)

Next, we consider

\[
f_{tr}(x) = p_1 f_1(x) + (1 - p_1) f_2(x), \quad \text{and} \quad f_{te}(x) = q_1 f_1(x) + (1 - q_1) f_2(x),
\]

where \( 0 < p_1 \leq 1 \), and \( 0 \leq q_1 \leq 1 \).

**Lemma A.2.** \( \lim_{t \to \infty} P^{(t)}_{te}(Y(1) = 1) = q_1. \)
Proof. For simplicity, define $p^{(t)} = \mathbb{P}^{(t)}_{te}(Y_1 = 1)$. Without loss of generality, suppose $p_1 < q_1$. Then we have

$$
\mathbb{P}^{(1)}_{te}(Y_1 = 1) = \mathbb{E}1_{Y_1 = 1} = \mathbb{E}_{x \sim f_{te}} \{ \mathbb{E}(1_{Y_1 = 1}|X^{te} = x) \} = \mathbb{E}_{x \sim f_{te}} \mathbb{P}(Y_1 = 1|X^{te} = x) = \mathbb{E}_{x \sim f_{te}} \frac{p_1 f_1(X^{(1)})}{p_1 f_1(X^{(1)}) + (1 - p_1)f_2(X^{(1)})} \tag{A.4}
$$

where the first expectation is with respect to both $X^{te} \sim f_{te}(x)$ and $(X^{(1)}, Y_1) \in \mathcal{D}_{tr}$; equation (A.4) is due to $X^{(1)} \rightarrow X^{te}$ with probability 1 by Lemma 3.1 and the Lipschitz property of $\frac{p_1 f_1(x)}{p_1 f_1(x) + (1 - p_1)f_2(x)}$; the inequality in (A.5) is due to the fact that $\psi(z) = \frac{q_1 + (1 - q_1)z}{p_1 + (1 - p_1)z}$ is convex, and applying Jensen's inequality.

Denote the sampling data as $\mathcal{D}^{(1)}_{tr}$, and for $(X_i, Y_i) \in \mathcal{D}^{(1)}_{tr}$, denote the conditional density of $X_i$ given $Y_i = \ell$ for $\ell = 1, 2$, as $f^{(1)}(x|Y_i = \ell)$. Then by Algorithm 2, we have $f^{(1)}(x|Y = 1) = f_1(x)$ and $f^{(1)}(x|Y = 2) = f_2(x)$. Then the marginal distribution of $X_i$ in $\mathcal{D}^{(1)}_{tr}$, i.e., $f^{(1)}(x)$ has the expression

$$
f^{(1)}(x) = \mathbb{P}^{(1)}_{te}(Y_1 = 1)f^{(1)}(x|Y = 1) + \mathbb{P}^{(1)}_{te}(Y_1 = 2)f^{(1)}(x|Y = 2) = p_1^{(1)} f_1(x) + (1 - p_1^{(1)}) f_2(x),
$$

with $p_1^{(1)} > p_1$.

Next, we show that $p_1^{(t)}$ increases as $t$ increases when $p_1^{(t)} < q_1$, then converges to $q_1$ as $t \rightarrow \infty$. At the $t$-th iteration, denote the sampled data as $\mathcal{D}^{(t)}_{tr}$. For any $(X_i, Y_i) \in \mathcal{D}^{(t)}_{tr}$, the prior distribution of $Y_i$ is $\mathbb{P}(Y_i = 1) = \mathbb{P}^{(t)}_{te}(Y_1 = 1) := p_1^{(t)}$, then the marginal distribution of $X_i$ can be written as

$$
f^{(t)}(x) = p_1^{(t)} f_1(x) + (1 - p_1^{(t)}) f_2(x).
$$
If \( p_1 < p_1^{(t)} < q_1 \), then using the above strategy but replacing \( D_{tr} \) and \( f_{tr} \) by \( D_{tr}^{(t)} \) and \( f^{(t)} \), at the \((t + 1)\)–th iteration, we have \( p_1^{(t+1)} > p_1^{(t)} \).

If \( p_1^{(t)} > q_1 \), then at the \((t + 1)\)-th iteration, for any test data \( X^{te} \), its nearest neighbor at \( D_{tr}^{(t)} \) is denoted as \( X_{(1)} \), and the corresponding label of \( X_{(1)} \) is \( Y_{(1)} \).

\[
P_{te}^{(t+1)}(Y_{(1)} = 1) = E_{x \sim f_{te}} P(Y_{(1)} = 1 | X^{te} = x) = E_{x \sim f_{te}} \frac{p_1^{(t)} f_1^{(t)}(X_{(1)})}{p_1^{(t)} f_1(X_{(1)}) + (1 - p_1^{(t)}) f_2(X_{(1)})}
\]

\[
= E_{x \sim f_{te}} \frac{p_1^{(t)} f_1(x)}{p_1^{(t)} f_1(x) + (1 - p_1^{(t)}) f_2(x)}
\]

\[
= p_1^{(t)} \int \frac{f_1^{(t)}(x) f_{te}(x)}{p_1^{(t)} f_1(x) + (1 - p_1^{(t)}) f_2(x)} dx
\]

\[
= p_1^{(t)} \int \frac{q_1 f_1(x) + (1 - q_1) f_2(x)}{p_1^{(t)} f_1(x) + (1 - p_1^{(t)}) f_2(x)} f_1(x) dx
\]

\[
= p_1^{(t)} E_{x \sim f_1} \frac{q_1 f_1(x) + (1 - q_1) f_2(x)}{p_1^{(t)} f_1(x) + (1 - p_1^{(t)}) f_2(x)}
\]

\[
< p_1^{(t)} \frac{q_1 + (1 - q_1) E_{x \sim f_1} \frac{f_2(x)}{f_1(x)}}{p_1^{(t)} + (1 - p_1^{(t)}) E_{x \sim f_1} \frac{f_2(x)}{f_1(x)}}
\]

\[
= p_1^{(t)},
\]

where (A.7) is due to Jensen’s inequality and the function \( \psi(z) = \frac{q_1 + (1 - q_1) z}{p_1^{(t)} + (1 - p_1^{(t)}) z} \) is concave when \( p > q_1 \).

Therefore, whenever \( p_1^{(t)} > q_1 \), in the next iteration, the proportion \( p_1^{(t+1)} \) will decrease.

If \( \lim_{t \to \infty} p_1^{(t)} = q_1 \), then

\[
\lim_{t \to \infty} p_1^{(t+1)} := \lim_{t \to \infty} P_{te}^{(t+1)}(Y_{(1)} = 1) = E_{x \sim f_{te}} \frac{p_1^{(t)} f_1(x)}{p_1^{(t)} f_1(x) + (1 - p_1^{(t)}) f_2(x)}
\]

\[
= \lim_{t \to \infty} p_1^{(t)} E_{x \sim f_1} \frac{q_1 f_1(t) + (1 - q_1) f_1(t)}{p_1^{(t)} f_1(x) + (1 - p_1^{(t)}) f_2(x)}
\]

\[
= \lim_{t \to \infty} p_1^{(t)} = q_1.
\]

Therefore, \( \lim_{t \to \infty} P_{te}^{(t+1)}(Y_{(1)} = 1) = q_1 \). On the other hand, according to our sampling procedure, in \( D_{tr}^{(T)} \), the conditional density of \( X_i | Y_i = \ell \) is \( f^{(T)}(x | Y = \ell) = f_{\ell} \) for \( \ell = 1, 2 \). Hence the marginal density of \( X_i \) in \( D_{tr}^{(T)} \) is \( f^{(T)}(x) = q_1 f_1(x) + (1 - q_1) f_2(x) \).
A.3 Proof of Theorem 3.3

Proof. We now adapt the proof of Theorem 2 in Cannings and Samworth [2017] to our case. Define \( \eta(x) = \mathbb{P}(Y_{te} = 1 | X_{te} = x) \), then the joint density of \((X, Y)\) for testing set is \( f(x, y) = f_{te}(x) \eta(x) + f_{te}(x)(1 - \eta(x)) \). Then we have

\[
R(C_n^{RB}) - R(C_{Bayes}) = \int \left[ 2\eta(x) - 1 \mathbb{1}_{\{\nu_n(x) < 1/2\}} - \mathbb{1}_{\{\eta(x) < 1/2\}} \right] f_{te}(x) dx
\]

\[
= \int \left[ 2\eta(x) - 1 \mathbb{1}_{\{\nu_n(x) \geq 1/2\}} \mathbb{1}_{\{\eta(x) < 1/2\}} + 2\eta(x) - 1 \mathbb{1}_{\{\nu_n(x) < \alpha\}} \mathbb{1}_{\{\eta(x) \geq 1/2\}} \right] f_{te}(x) dx
\]

\[
\leq \int \left[ 2\eta(x) - 1 \nu_n(x) \mathbb{1}_{\{\eta(x) < 1/2\}} + 2\eta(x) - 1 \mathbb{1}_{\{\nu_n(x) \geq 1/2\}} \right] f_{te}(x) dx
\]

Note that \( \mathbb{E}R(C_n^{RB}) - R(C_{Bayes}) = \mathbb{E}\{R(C_n^{RB})\} - R(C_{Bayes}) \), where \( \mathbb{E} \) is the expectation conditional on the observations \( \mathcal{D}_{tr}, \mathcal{D}_{te} \). Conditioning on \( \mathcal{D}_{tr}, \mathcal{D}_{te} \), \( \xi_1, \ldots, \xi_B \) are i.i.d., so that \( C_n^{\xi_b} \) for \( b = 1, \ldots, B \) are i.i.d. Therefore,

\[
\mathbb{E}\{R(C_n^{RB})\} - R(C_{Bayes}) = \mathbb{E}\left\{ \int \left[ 2\eta(x) - 1 \mathbb{1}_{\{\nu_n(x) < 1/2\}} \mathbb{1}_{\{\eta(x) = 1\}} \right] f_{te}(x) dx \right\}
\]

\[
\leq 2\mathbb{E}\left\{ \int \left[ 2\eta(x) - 1 \mathbb{1}_{\{\nu_n(x) \geq 1/2\}} \mathbb{1}_{\{\eta(x) = 1\}} \right] f_{te}(x) dx \right\}
\]

Then we have \( \mathbb{E}R(C_n^{RB}) - R(C_{Bayes}) = \mathbb{E}\{R(C_n^{RB})\} - R(C_{Bayes}) \leq 2\mathbb{E}\{R(C_n^{\xi_1})\} - R(C_{Bayes}) \). \( \square \)

A.4 Proof of Theorem 3.5

Proof. Conditional on \( \mathcal{D}_{tr}, \mathcal{D}_{te} \), \( \xi_1, \ldots, \xi_B \) are i.i.d. For any pair \((X, Y)\) with \( \mathbb{P}(Y = \ell) = q_\ell \) and \( f(X = x | Y = \ell) = f_\ell(x) \), the test error of the ensemble classifier can be written as

\[
\mathbb{E}\{R(C_n^{RB})\} = q_1 \int_{\mathbb{R}^p} \mathbb{1}_{\{C_n^{RB}(x) = 2\}} f_1(x) dx + q_2 \int_{\mathbb{R}^p} \mathbb{1}_{\{C_n^{RB}(x) = 1\}} f_2(x) dx
\]

\[
= q_1 \int_{\mathbb{R}^p} \mathbb{P}\{\Lambda_n(x) < \frac{1}{2}\} f_1(x) dx + q_2 \int_{\mathbb{R}^p} \mathbb{P}\{\Lambda_n(x) \geq \frac{1}{2}\} f_2(x) dx
\]

where the final equality follows by Fubini’s theorem. Let \( U_b := \mathbb{1}_{\{C_n^{\xi_b}(x) = 1\}} \) for \( b = 1, \ldots, B \). Then, conditional on \( \mu_n(x) = \theta \in [0, 1] \), the random variables \( U_1, \ldots, U_B \) are independent, each having
a Bernoulli(θ) distribution. Denote \( L_{\mu_n,1} \) and \( L_{\mu_n,2} \) as the distribution function of \( \mu_n(X)|Y = 1 \) and \( \mu_n(X)|Y = 2 \) respectively. That is, \( L_{\mu_n,\ell} \) is short for \( L_{\mu_n,\ell}(t | (D_{tr}, D_{te}), Y = \ell) \) for \( \ell = 1, 2 \) respectively. Then we have

\[
\int_{\mathbb{R}} P\{\Lambda_n(x) < \frac{1}{2}\} f_1(x) dx = \int_{[0,1]} \mathbb{P}\{\frac{1}{B} \sum_{b=1}^{B} U_b < 1/2 | \mu(X) = \theta\} dL_{\mu_n,1}(\theta) = \int_{[0,1]} \mathbb{P}(T < B/2) dL_{\mu_n,1}(\theta),
\]

where \( T \) denotes a random variable following Binomial distribution with parameters \( B, \theta \); that is, \( T \sim \text{Bin}(B, \theta) \). Similarly, we can write

\[
\int_{\mathbb{R}} P\{\Lambda_n(x) \geq \frac{1}{2}\} f_2(x) dx = 1 - \int_{[0,1]} \mathbb{P}(T < B/2) dL_{\mu_n,2}(\theta).
\]

Therefore,

\[
\mathbb{E}\{R(C_n^{RB})\} = q_2 + \int_{[0,1]} \mathbb{P}(T < B/2) dL_{\mu_n,2}(\theta).
\]

Then we aim to show that

\[
\int_{[0,1]} \{\mathbb{P}(T < B/2) - 1_{\theta < 1/2}\} d(q_1 L_{n,1}(\theta) - q_2 L_{n,2}(\theta)) = \gamma_n,
\]

where \( \gamma_n = (1/2 - (B/2 - [B/2]))\{q_1 g_{n,1}(1/2) - q_2 g_{n,2}(1/2)\} + \frac{1}{8}\{q_1 \hat{g}_{n,1}(1/2) - q_2 \hat{g}_{n,2}(1/2)\} \). The proof of (A.9) requires a one-term Edgeworth expansion to the binomial distribution function; refer to the proofs of Theorem 1 in Cannings and Samworth [2017].

### A.5 Proof of Theorem 4.1

We first introduce a Lemma to bound the difference between \( d_\ell(x) \) and \( \hat{d}_\ell(x) \).

**Lemma 1.** Suppose Assumptions A2 and A3 hold, with \( \delta \) specified in Assumption A2 (b). Denote the support of \( \mathbb{P}_\ell \) and \( \mathbb{P}_0 \) as \( S_\ell \) and \( S_0 \) respectively. Under Assumption A3, with probability at least \( 1 - \delta \), for any \( x \in S_\ell \cup S_0 \),

\[
\sup_x |d_\ell(x) - \hat{d}_\ell(x)| \leq C \beta_n(x) (\beta_n(x) + \sqrt{m_\ell}).
\]

Defining the event \( \mathcal{E}_\ell = \{\sup_x |d_\ell(x) - \hat{d}_\ell(x)| \leq C \beta_n(x) (\beta_n(x) + \sqrt{m_\ell})\} \), Lemma 1 guarantees that the event \( \mathcal{E}_\ell \) holds with high probability, that is, \( \hat{d}_\ell \) is a consistent estimate of \( d_\ell \) for all \( x \) in \( S_\ell \cup S_0 \). The proof of Lemma 1 refers to Theorem 3.5 in Gu et al. [2019].
Proof. We first prove Theorem 4.1 (a). Under $H_0$, for any $X^{te} \in D_{te}$, denote the corresponding label as $Y^{te}$. Suppose $Y^{te} = \ell$, i.e., $\ell$ is the true label of $X^{te}$

\[
\mathbb{P}(T(X^{te}) > c \mid Y^{te} = \ell) = \mathbb{P}\left(\left(\hat{d}_1(X^{te}) > c_1 \right) \cap \cdots \cap (\hat{d}_L(X^{te}) > c_L) \mid Y^{te} = \ell\right)
\leq \mathbb{P}(\hat{d}_\ell(X^{te}) > c_\ell \mid Y^{te} = \ell)
= \mathbb{P}(d_\ell(X^{te}) > c_\ell - (\hat{d}_\ell(X^{te}) - d_\ell(X^{te})) \mid Y^{te} = \ell)
\leq \mathbb{P}(d_\ell(X^{te}) > c_\ell - (\hat{d}_\ell(X^{te}) - d_\ell(X^{te})) \mid Y^{te} = \ell, \mathcal{E}_\ell) \mathbb{P}(\mathcal{E}_\ell) + \mathbb{P}(\mathcal{E}_\ell^c)
\leq \mathbb{P}(d_\ell(X^{te}) > c_\ell - C\beta_n(\beta_n + \sqrt{m_\ell}) \mid Y^{te} = \ell)(1 - \delta) + \delta \leq \alpha + o(1),
\]

where the last step is based on Lemma 1 and $\beta_n(\beta_n + \sqrt{m_\ell}) = o(c_\ell)$ as $n_\ell \to \infty$.

We next provide an upper bound for $\mathbb{P}(\hat{d}_\ell(X^{te}) \leq c_\ell \mid Y^{te} \notin \{1, \ldots, L\})$. It is sufficient to prove

\[
\inf_{X^{te} \sim \text{out}} d_\ell(X^{te}) > c_\ell + C\beta_n(\beta_n + \sqrt{m_\ell}) \text{ under event } \mathcal{E}. \text{ Note that}
\inf_{X^{te} \sim \text{out}} d_\ell(X^{te}) = \inf_{X^{te} \sim \text{out}} \frac{1}{m_\ell} \int_{0}^{m_\ell} r_{\ell, t}(X^{te}) dt
\geq \inf_{X^{te} \sim \text{out}} \frac{1}{m_\ell} \int_{\ell}^{m_\ell} r_{\ell, t}(X^{te}) dt \geq \frac{m_\ell - \ell}{m_\ell} M > c_\ell + C\beta_n(\beta_n + \sqrt{m_\ell}),
\]

where the last step is due to Assumption A2 (a). Therefore,

\[
\mathbb{P}(\hat{d}_\ell(X^{te}) < c_\ell \mid Y^{te} \notin \{1, \ldots, L\}) \leq \mathbb{P}(\hat{d}_\ell(X^{te}) < c_\ell | E_\ell, Y^{te} \notin \{1, \ldots, L\}) \mathbb{P}(E_\ell) + \mathbb{P}(E_\ell^c)
\leq \mathbb{P}(\hat{d}_\ell(X^{te}) < c_\ell | E_\ell, Y^{te} \notin \{1, \ldots, L\}) \mathbb{P}(E_\ell) + \mathbb{P}(E_\ell^c)
\leq \mathbb{P}(d_\ell(X^{te}) - C\beta_n(\beta_n + \sqrt{m_\ell}) < c_\ell | E_\ell, Y^{te} \notin \{1, \ldots, L\}) \mathbb{P}(E_\ell) + \mathbb{P}(E_\ell^c)
\leq \mathbb{P}(E_\ell^c) \leq \delta.
\]

Then we have

\[
\mathbb{P}(T(X^{te}) > c \mid Y^{te} \notin \{1, \ldots, L\}) \geq 1 - \sum_{\ell=1}^{L} \mathbb{P}(\hat{d}_\ell(X^{te}) \leq c_\ell \mid Y^{te} \notin \{1, \ldots, L\}) \geq 1 - L\delta.
\]

\[\square\]
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