Bridging Cost-sensitive and Neyman-Pearson Paradigms for Asymmetric Binary Classification

Wei Vivian Li  
Department of Biostatistics and Epidemiology  
School of Public Health  
Rutgers, The State University of New Jersey  
Piscataway, NJ 08854, USA

Xin Tong  
Department of Data Sciences and Operations  
Marshall School of Business  
University of South California  
Los Angeles, CA 90089, USA

Jingyi Jessica Li  
Department of Statistics  
University of California, Los Angeles  
Los Angeles, CA 90095, USA

Abstract
Asymmetric binary classification problems, in which the type I and II errors have unequal severity, are ubiquitous in real-world applications. To handle such asymmetry, researchers have developed the cost-sensitive and Neyman-Pearson paradigms for training classifiers to control the more severe type of classification error, say the type I error. The cost-sensitive paradigm is widely used and has straightforward implementations that do not require sample splitting; however, it demands an explicit specification of the costs of the type I and II errors, and an open question is what specification can guarantee a high-probability control on the population type I error. In contrast, the Neyman-Pearson paradigm can train classifiers to achieve a high-probability control of the population type I error, but it relies on sample splitting that reduces the effective training sample size. Since the two paradigms have complementary strengths, it is reasonable to combine their strengths for classifier construction. In this work, we for the first time study the methodological connections between the two paradigms, and we develop the TUBE-CS algorithm to bridge the two paradigms from the perspective of controlling the population type I error.

Keywords: asymmetric binary classification, cost-sensitive learning, Neyman-Pearson classification, type I error, type II error

1. Introduction
Asymmetric binary classification problems, where the consequence of misclassifying observations in one class is more severe than the other class, are ubiquitous in real-world applications. For example, in medical diagnosis, misclassifying a malignant tumor biopsy sample as benign is more severe than misclassifying a benign sample as malignant (Mazurowski et al.,
in email spam detection, removing a non-spam email leads to more severe consequences than missing a spam email (Carreras and Marquez, 2001, Zhou et al., 2014); in political conflict prediction, missing a conflict has more critical consequences than vice versa (Beck et al., 2000, Cederman and Weidmann, 2017). In addition to these examples, asymmetric binary classification problems exist in geologic studies (Horrocks et al., 2015, Fernández-Gómez et al., 2017), fraud detection (Sahin et al., 2013, Bahnsen et al., 2013), and other medical diagnosis and prognosis problems (Artan et al., 2010, Ali et al., 2016).

Throughout this article, we refer to the two classes as class 0 and class 1, and we use class 0 to represent the more important class. Accordingly, in the above examples, malignant biopsy samples, non-spam emails, and political conflict events are class 0 observations. With this encoding in asymmetric classification, the type I error, defined as the conditional probability of misclassifying a class 0 observation into class 1, demands a higher priority than the type II error, the conditional probability of misclassifying a class 1 observation into class 0. However, the asymmetric importance of type I and II errors are not reflected in common classification practices that aim to minimize the overall classification error or maximize the area under the receiver-operating characteristic curve. As a result, asymmetric classification paradigms have been developed.

To date, asymmetric classification has two major paradigms: cost-sensitive (CS) and Neyman-Pearson (NP). The CS paradigm incorporates two misclassification costs, with the type I error cost greater than the type II error cost, into its objective function so that the classifier minimizing the objective function would have the type I error smaller than the type II error. In contrast, the NP paradigm does not use misclassification costs but instead minimizes a constrained objective function, where the type II error is to be minimized subject to an upper bound on the type I error.

Desirably, the objective functions of the two paradigms have one-to-one correspondence at the population level: when both paradigms’ objective functions are defined by the population type I and II errors, the two functions’ minimizers are the same oracle classifier, whose population type I error is equal to the type I error upper bound in the NP paradigm. However, such correspondence is not always achievable at the algorithm level because the two paradigms may use different algorithms to construct practical classifiers from training data, and practical classifiers may not mimic the oracle classifier to the same extent. Hence, in practice, the connection between the two paradigms is unclear, so is the paradigm choice for a particular application. Another question is whether the two paradigms’ comparative advantages can be combined into a practical classifier’s construction.

This article addresses these questions and is structured as follows. In Sections 2 and 3, we review the CS and NP classification paradigms, respectively; in detail, for each paradigm, we explain its statistical framework, its implementation of the type I error priority, and its comparative advantages. In Section 4, we discuss two special implementations of the CS paradigm that are equivalent to the NP paradigm in constructing practical classifiers. In Section 5, we develop the TUBE algorithm for estimating the type I error upper bound—the key property of the NP paradigm—of a practical classifier constructed under the CS paradigm; the algorithm establishes a link between the two paradigms in practice. In Section 6, we propose the TUBE-CS algorithm for selecting the type I error cost parameter in the CS paradigm given a target type I error upper bound. Then we use simulation to
verify the performance of the TUBE-CS algorithm. In Section 7, we use real data studies to verify that the TUBE-CS algorithm outperforms a vanilla CS algorithm commonly used in practice. The Appendix includes proofs, a supplementary algorithm, and supplementary figures.

2. The CS classification paradigm

First, we introduce notations used throughout the paper. Let \((X,Y)\) be a random pair in which \(X \in \mathcal{X} \subset \mathbb{R}^d\) represents \(d\) features and \(Y \in \{0,1\}\) encodes a binary class label associated with \(X\). A classifier \(\phi(\cdot)\) is a map \(\phi : \mathcal{X} \to \{0,1\}\) that outputs a predicted class label given the input features \(X\). The population type I error of \(\phi(\cdot)\) is \(R_0(\phi) = \mathbb{P}(\phi(X) = 1|Y = 0)\), and the population type II error is \(R_1(\phi) = \mathbb{P}(\phi(X) = 0|Y = 1)\). With the priors, i.e., proportions of classes 0 and 1 in the population, which are denoted respectively by \(\pi_0 = \mathbb{P}(Y = 0)\) and \(\pi_1 = \mathbb{P}(Y = 1)\) (such that \(\pi_0 + \pi_1 = 1\)), the overall classification error of \(\phi(\cdot)\) is

\[
R(\phi) = \mathbb{P}(\phi(X) \neq Y) = \pi_0 R_0(\phi) + \pi_1 R_1(\phi) .
\]

(1)

We define the classical paradigm as the one that seeks a classifier to minimize \(R(\cdot)\). The classical paradigm prioritizes the type I error based on \(\pi_0\) (larger \(\pi_0\) gives the type I error a higher priority) and does not allow a user-specified upper bound on the type I error. Hence, it is unsuitable for asymmetric classification.

The CS paradigm is a natural modification of the classical paradigm for asymmetric classification. It assigns explicit misclassification costs \(c_0\) and \(c_1\) to the type I and II errors respectively (Table 1) (Margineantu, 2000, 2002, Sun et al., 2007). Then it seeks a classifier to minimize

\[
R_{CS}(\phi) = c_0 R_0(\phi) + c_1 R_1(\phi) .
\]

(2)

In certain applications, \(c_0\) and \(c_1\) can be specified in an objective manner, such as monetary and time costs (Turney, 2002). However, in most applications, users cannot concretize \(c_0\) and \(c_1\) as real-world costs. For example, it is ethically impossible to specify the cost of misdiagnosing a cancer patient as undiseased (Vidrighin and Potolea, 2008). Due to this challenge, users in practice specify \(c_0\) and \(c_1\) in a data-driven way: they vary \((c_0,c_1)\), train a classifier for each pair of costs, evaluate the classifier’s empirical type I and II errors on evaluation data, and finally choose the pair of costs so that the empirical type I error is below and closest to their target type I error upper bound \(\alpha\). While this approach is intuitive and easy to implement, it has a critical drawback—it does not inform whether the classifier trained with the chosen \((c_0,c_1)\) has the population type I error under \(\alpha\), a question the NP paradigm can answer (Section 3). Before introducing the NP paradigm, we summarize the CS paradigm’s practical implementations and their relation to the type I error control.

2.1 A review of practical implementations of the CS paradigm

We summarize practical implementations of the CS paradigm into three categories (Table 2): (a) pre-training approaches, which modify training data to reflect misclassification costs; (b)
Table 1: The misclassification cost matrix.

|                  | true class is 0 | true class is 1 |
|------------------|-----------------|-----------------|
| predicted class is 0 | 0               | $c_1$           |
| predicted class is 1 | $c_0$           | 0               |

in-training approaches, which change the internal algorithm of a classification method (e.g., logistic regression) to incorporate misclassification costs; (c) the post-training approach, which incorporates misclassification costs into the threshold on the posterior probability predicted by a trained classification method.

Table 2: Three categories of practical implementations of the CS classification paradigm.

| category       | sub-category     | characteristics |
|----------------|------------------|-----------------|
|                |                  | change training data | change internal algorithm | require probabilistic model | require class priors |
| pre-training   | stratification   | X                |                           |                           |                  |
|                | rebalancing      |                  |                           |                           | X                 |
| in-training    | weighting        | X                |                           |                           |                  |
|                | others           |                  |                           |                           |                  |
| post-training  |                  |                  |                           |                           | X                 |

(a) **Pre-training approaches.** They consist of two sub-categories: stratification and rebalancing approaches. Stratification approaches change the proportions of the two classes in the training data such that the more important class 0 has a larger proportion in the training data than in the population (Zadrozny et al., 2003). The implementation is to either downsample the class 1 or oversample the class 0 (Margineantu, 2002, Webb and Ting, 2005, Pelayo and Dick, 2007, 2012). Stratification approaches have been applied to credit card fraud detection (Chan and Stolfo, 1998) and studied for their effects on decision-tree-based classification methods (Drummond and Holte, 2000). In contrast, the rebalancing approach does not change the training data but replaces class priors $\pi_0$ and $\pi_1$ respectively by normalized $c_0$ and $c_1$ (such that the two normalized costs add up to 1); however, it is only applicable to probabilistic classification methods, in which class priors are no longer estimated from training data but set to the specified $c_0$ and $c_1$. For example, the rebalancing approach has been implemented with the linear discriminant analysis method (function `lda` in the R package MASS (Venables and Ripley, 2002)) and the naïve Bayes method (function `naive_bayes` in the R package naivebayes (Majka, 2018)).

(b) **In-training approaches.** They change the internal algorithm of a classification method. A popular in-training approach is weighting, which assigns individual training observations with weights proportional to their misclassification costs ($c_0$ and $c_1$ for class 0 and 1 observations, respectively) during the training of a classification method. This weighting approach has been implemented with classification methods including the logistic regression (function `glm` in the R package stats (R Core Team, 2013)), the penalized logistic regression (function `glmnet` in the R package glmnet (Friedman et al., 2010)), and
the support vector machine (function \texttt{svm} in the R package \texttt{e1071} (Meyer et al., 2017)). A technical note is that, in the above three R functions, assigning an integer weight $w$ to the class 0 observations and a weight of 1 to the class 1 observations is equivalent to replicating each class 0 observation $w$ times before regular training. Unlike the weighting approach, most other in-training approaches are specific to a classification method and not generalizable. For instance, tree-based classification methods, adaptive boosting (AdaBoost), and neural networks all have special in-training approaches. Among tree-based methods, the classification and regression tree (CART) method incorporates misclassification costs into the splitting criterion used in tree growing (Breiman et al., 1984); the random forest method also implements this approach in the weighted random forest (available in the R package \texttt{randomForest}) (Chen et al., 2004); Bradford et al. discussed different pruning algorithms for decision trees to reflect asymmetric misclassification costs (Bradford et al., 1998). For AdaBoost, a variant Adacost was proposed to incorporate asymmetric misclassification costs into the weighting of data points (Fan et al., 1999); Sun et al. (2007) discussed three modifications of the weight-update formula in AdaBoost to incorporate misclassification costs. For neural networks, Kukar et al. (1998) modified the back-propagation learning algorithm to incorporate misclassification costs; Zhou and Liu (2006) proposed ensemble learning to combine multiple cost-sensitive neural network classifiers.

(c) \textbf{Post-training approach}. It requires a classification method to assign each test observation an estimated posterior probability of being in class 1. What it does is to select a threshold on the estimated probability so that each test observation is classified as 0 or 1 (Duda et al., 1973). The threshold selection depends on misclassification costs. This post-training approach has a notable difference from the previous pre-training and in-training approaches: it does not alter either the training data or the internal algorithm of a classification method. In other words, it applies to the output of a classification method without requiring access to the training data or the implementation of the classification method. An example is the MetaCost method, which constructs an ensemble classifier that implements this post-training approach (Domingos, 1999).

2.2 \textbf{Specification of misclassification costs}

In the aforementioned three categories of CS implementation approaches, users must specify the misclassification costs. However, there lacks consensus on how to specify the costs objectively. In some applications, the costs can be specified by domain experts, such as in the prediction of head injury recovery (Elder IV, 1996, Liu et al., 2016), the diagnosis of heart disease (King et al., 1995), and the classification of customer credit (Elder IV, 1996). However, in most applications, costs cannot be specified by domain experts but need to be set either arbitrarily or by some prediction criteria. For instance, many studies in medical diagnosis (Schaefer et al., 2007, Vidrighin and Potolea, 2008, Park et al., 2011, Alizadehsani et al., 2012), food safety classification (Liu et al., 2016), and climate change prediction (Lu and Wang, 2008) have used one or multiple set(s) of arbitrarily specified costs. In addition to being arbitrarily chosen, the costs may be chosen to optimize a classification accuracy measure on evaluation data. For example, Sun et al. (2007) selected the costs that led to the largest $F$ score (the harmonic mean of precision and recall) in several medical diagnose problems; Lan et al. (2010) compared the costs in terms of the
overall and class-specific misclassification errors in thyroid level prediction; Krawczyk et al. (2015) selected the costs to optimize the receiver operating characteristic (ROC) curves in breast thermogram classification.

2.3 Population type I error in CS classification

The CS classification paradigm is popular in practice due to its easy implementation. However, it remains unclear whether and to what extent this paradigm can control the population type I error, i.e., the more severe type of classification error. Here, we study a CS classifier’s performance from the perspective of controlling the population type I error. Without loss of generality, we assume \( c_0 + c_1 = 1 \) \((c_0, c_1 > 0)\) in the following text.

We denote a practical CS classifier by \( \hat{\phi}_c \), in which \( c \) is the type I error cost (i.e., \( c_0 = c \)). Suppose that one wishes to find \( c \) such that \( \hat{\phi}_c \) has the population type I error under a specified level \( \alpha \). A natural but naïve (“vanilla”) implementation of the CS paradigm is to solve

\[
\min_{\hat{\phi}_c} \hat{R}_1(\hat{\phi}_c) \text{ subject to } \hat{R}_0(\hat{\phi}_c) \leq \alpha,
\]

in which \( \hat{R}_0(\hat{\phi}_c) \) and \( \hat{R}_1(\hat{\phi}_c) \) are the empirical type I and II errors of \( \hat{\phi}_c \) on evaluation data, respectively.

We detail this vanilla implementation in Algorithm 1, which is adaptive to any CS implementation approach (pre-training, in-training, or post-training). Specifically, the training data are randomly divided into two subsets: one to train CS classifiers corresponding to candidate costs \( c_{0,1} < c_{0,2} < \cdots < c_{0,I} \); the other to evaluate the empirical type I error of each classifier. Among the \( I \) CS classifiers, the chosen one corresponds to the smallest cost such that the empirical type I error is no greater than \( \alpha \).

**Algorithm 1:** The vanilla CS implementation to control the type I error

| Input | \( S = S^0 \cup S^1 \): training data \( S^0 \) for class 0 and \( S^1 \) for class 1 | \( \alpha \): target upper bound on the type I error | \( c_{0,1} < c_{0,2} < \cdots < c_{0,I} \): candidate type I error costs |
|-------|------------------------------------------------|-------------------------------------------------|-------------------------------------------------|
| 1     | \( S^0_1, S^0_2 \leftarrow \) randomly split \( S^0 \) into two subsets | 2 for \( i \leftarrow 1 \) to \( I \) do | 3 \( \hat{\phi}_i(\cdot) = \text{CS-classifier}(S^0_1 \cup S^1, c_{0,i}) \) |
| 4     | \( r_{0,i} = \hat{R}_0(\hat{\phi}_i) \) // empirical type I error on \( S^0_2 \) | 5 end | \( i^* = \begin{cases} \min \{i : r_{0,i} \leq \alpha\} & \text{if } r_{0,i} \leq \alpha \\ I & \text{otherwise} \end{cases} \) |
| 6     | Output: \( \hat{\phi}_{\text{vanilla-CS}}(\cdot) = \hat{\phi}_{i^*}(\cdot) \) // the vanilla-CS classifier |

We use a simulation study to demonstrate that Algorithm 1 cannot guarantee to control the population type I error of its chosen classifier under \( \alpha \). In this simulation, we use the stratification approach, a type of pre-training approach, as an example to show that the population type I error of a CS classifier constructed by Algorithm 1 is not bounded by...
Figure 1: The empirical type I errors and population type I errors of CS classifiers trained by Algorithm 1. We set the target type I error upper bound $\alpha = 0.1$ and use the stratification approach combined with four classification methods: gradient boosting (GB), linear discriminant analysis (LDA), logistic regression (LR), and naïve Bayes (NB). We consider three data distributions: Gaussian, multivariate $t$, and Mixture. The violation rate of type I errors (the frequency of type I errors being greater than $\alpha = 0.1$) in each case is summarized as a percentage and marked on top of each violin plot.

$\alpha$ with high probability, even though the empirical type I error of the classifier is under $\alpha$. We implement the stratification approach with four base classification methods: logistic regression, gradient boosting, linear discriminant analysis, and naïve Bayes. We consider three data distributions, denoted as Gaussian, Multivariate $t$, and Mixture.

1. Gaussian. $\Pr(Y = 0) = 0.5$. When $Y = 0$, $X_{d \times 1} \sim N(\mu_0, \Sigma_0)$; when $Y = 1$, $X_{d \times 1} \sim N(\mu_1, \Sigma_1)$. The means are $\mu_0 = (0, 0, 0, \ldots, 0) \top$ and $\mu_1 = (1.5, 1.5, 0, \ldots, 0) \top$. The covariance matrices are $\Sigma_0 = I_d$ and $\Sigma_1$ with $1$ in diagonal entries, $0.5$ in superdiagonal and subdiagonal entries, and $0$ in the rest of entries.

2. Multivariate $t$. $\Pr(Y = 0) = 0.5$. When $Y = 1$, $X_{1:2} \sim t_3(\mu_0)$ and $X_{3:d} \sim N(0, I_{d-2})$; when $Y = 0$, $X_{1:2} \sim t_3(\mu_1)$ and $X_{3:d} \sim N(0, I_{d-2})$. The noncentrality parameters are $\mu_0 = (0, 0) \top$ and $\mu_1 = (2.5, 2.5) \top$.

3. Mixture. $\Pr(Y = 0) = 0.5$. When $Y = 0$, $X \sim \frac{1}{2}N(\mu_1, I_d) + \frac{1}{2}N(\mu_2, I_d)$; when $Y = 1$, $X \sim N(\mu_1, I_d)$. The mean parameters are $\mu_1 = (a, a, \ldots, a) \top$ and $\mu_2 = (-a, -a, \ldots, -a) \top$, where $a = 2/\sqrt{d}$. 

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For each distribution, we set $d = 30$ and simulate a training dataset with size $n_1 = 1,000$ and a large evaluation dataset with size $n_2 = 1,000,000$ (to approximate the population). In each simulation, we use Algorithm 1 (with candidate type I error costs ranging from 0.51 to 0.99 in a step size of 0.02) to train a CS classifier that has the empirical type I error under $\alpha = 0.1$. Then we approximate the population type I error of the trained classifier using the large evaluation dataset. We repeat the simulation for 200 times to calculate the violation rates of the empirical type I errors and the population type I errors, respectively. Note that the violation rate is defined as the frequency of type I errors exceeding $\alpha$. Figure 1 summarizes the results and shows that the CS classifiers constructed by Algorithm 1 fail to have population type I errors under $\alpha$ with high probability (i.e., the violation rates are large), even though these classifiers have empirical type I errors strictly$^2$ under $\alpha$.

3. The NP classification paradigm

3.1 An overview of the NP paradigm

The NP classification paradigm is another statistical framework that addresses asymmetric priorities of type I and II errors (Scott and Nowak, 2005, Scott, 2005, Rigollet and Tong, 2011). Different from the CS paradigm, the NP paradigm aims to minimize the population type II error while controlling the population type I error below a pre-specified level $\alpha$:

$$\phi^*_\alpha = \arg \min_{\phi: R_0(\phi) \leq \alpha} R_1(\phi).$$

(4)

We name $\phi^*_\alpha$ the (level-$\alpha$) NP oracle classifier. Like the misclassification costs in the CS classification objective (2), the upper bound $\alpha$ in (4) reflects users’ priorities for the type I error: a smaller $\alpha$ reflects a higher priority.

In practice, the NP oracle classifier is not achievable. Several algorithms were developed to construct data-dependent NP classifiers whose population type I error are under $\alpha$ with high probability (Zhao et al., 2016, Tong et al., 2018, 2020). Especially, Tong et al. (2018) proposed an umbrella algorithm that adapts popular classification methods (e.g., support vector machine and random forest) to construct NP classifiers. The theoretical foundation of the umbrella algorithm is given by Proposition 1 in Tong et al. (2018). For readers’ convenience, we restate this proposition as follows.

**Proposition 1.** (Tong et al., 2018). Suppose that we divide the training data into two independent parts, one with observations from both classes 0 and 1 for training a classification method to obtain a scoring function $s : \mathcal{X} \to \mathbb{R}$, and the other as a left-out class 0 sample for choosing a threshold on classification scores. Applying $s(\cdot)$ to the left-out class 0 sample of size $m$, we denote the resulting classification scores as $T_1, \ldots, T_m$, which are real-valued random variables. Then, we denote by $T_{(k)}$ the $k$-th order statistic. For a new observation $X$, we can construct a classifier $\hat{\phi}_k(X) = \mathbb{I}(s(X) > T_{(k)})$. Then

$$\mathbb{P}[R_0(\hat{\phi}_k) > \alpha] \leq \sum_{j=k}^{m} \binom{m}{j} (1 - \alpha)^j \alpha^{m-j}. \quad (5)$$

$^2$ Note that there is a 3% violation rate of empirical type I errors in the first panel of the second row of Figure 1. This is because in Algorithm 1, if all the CS classifiers have empirical type I errors larger than $\alpha$, i.e., $r_{0,l} > \alpha$, then we choose $i^* = I$. 

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That is, the probability that the population type I error of \( \hat{\phi}_k \) exceeds \( \alpha \) is under a constant that only depends on \( n, k \), and \( \alpha \). We call this probability the “violation rate” of \( \hat{\phi}_k \) and denote its upper bound by \( v(k) = \sum_{j=k}^{m} \binom{m}{j}(1 - \alpha)^j \alpha^{m-j} \). When \( T_i \)'s are continuous, this bound is tight.

According to Proposition 1, to control the violation rate at a pre-specified \( \delta \), we can construct an NP classifier \( \hat{\phi}_k^* (\cdot) = \mathbb{I}(s(\cdot) > T_{(k^*)}) \), where \( k^* = \min\{k \in \{1, \ldots, m\} : v(k) \leq \delta \} \). The minimum order is selected because among the classifiers that satisfy the type I error control, the one with the minimal type II error should be selected. The NP umbrella algorithm is summarized in Algorithm 2.

Algorithm 2: The NP umbrella algorithm

| Line | Description |
|------|-------------|
| 1 | \( S_0^0, S_2^0 \leftarrow \) randomly split class 0 data \( S^0 \) |
| 2 | \( S_2^0 = \{(x_1, y_1), \ldots, (x_m, y_m)\} (m = |S_0^0|) \) \hspace{1cm} // left-out class 0 data |
| 3 | \( k^* = \min\{k \in \{1, \ldots, m\} : \sum_{j=k}^{m} \binom{m}{j}(1 - \alpha)^j \alpha^{m-j} \leq \delta \} \) |
| 4 | \( s = \text{Classification-method}(S_0^1 \cup S^1) \) \hspace{1cm} // train a classification method to obtain a scoring function |
| 5 | \( T = \{T_1, \ldots, T_m\} \leftarrow \{s(x_1), \ldots, s(x_m)\} \) \hspace{1cm} // apply \( s \) to \( S_2^0 \) to obtain classification scores as candidate thresholds |
| 6 | \( T^{\text{sort}} = \{T(1), \ldots, T(m)\} \) \hspace{1cm} // sort candidate thresholds from the smallest to the largest |
| Output | \( \hat{\phi}_{\text{NP}}^* (\cdot) = \mathbb{I}(s(\cdot) > T_{(k^*)}) \) \hspace{1cm} // the NP classifier |

### 3.2 Population type I error in NP classification

We repeat the simulation study in Section 2.3 by replacing CS classifiers with NP classifiers constructed by Algorithm 2, and we numerically verify that the NP classifiers have their population type I errors under \( \alpha \) with high probability (i.e., the violation rates are small).

In detail, from each of the three data distributions (Gaussian, Multivariate \( t \), and Mixture), we simulate a training dataset with size \( n_1 = 1,000 \) and a large evaluation dataset with size \( n_2 = 1,000,000 \) to approximate the population. In each simulation, we use Algorithm 2 to train an NP classifier with \( \alpha = 0.1 \) and \( \delta = 0.1 \), and we calculate the empirical type I error of the trained classifier using the left-out class 0 data \( S_0^0 \). Then we approximate the population type I error of the trained classifier using the large evaluation dataset. We repeat the simulation for 200 times to calculate the violation rates of the empirical type I errors and the population type I errors. Figure 2 summarizes the results and shows that the NP classifiers constructed by Algorithm 2 have population type I errors under \( \alpha \) with probability at least \( 1 - \delta \).
Figure 2: The empirical type I errors and population type I errors of NP classifiers trained by Algorithm 2. The empirical type I error of each NP classifier is computed on the left-out class 0 sample $S_0^2$ in each simulation. We set the type I error upper bound as $\alpha = 0.1$ and use four classification methods: gradient boosting (GB), linear discriminant analysis (LDA), logistic regression (LR), and naive Bayes (NB). The target violation rate is set as $\delta = 10\%$. We consider three data distributions: Gaussian, $t$, and Mixture. The violation rate of type I errors (the frequency of type I errors being greater than $\alpha = 0.1$) in each case is summarized as a percentage and marked on top of each violin plot.

4. From NP to CS: finding the type I error cost of an NP classifier

We have introduced CS and NP as two paradigms for prioritizing misclassification errors in asymmetric binary classification. It is evident that the CS objective (2) and the NP objective (4) have a one-to-one correspondence at the population level. However, it remains an unresolved question whether practical, data-dependent classifiers constructed from the same training data under the two paradigms would have a one-to-one correspondence. In this section, we establish an exact correspondence between an NP classifier and a CS classifier constructed by one of two CS implementations: the rebalancing and post-training approaches. Specifically, given an NP classifier, we can find the corresponding costs in these two CS implementations such that the resulting CS classifiers are just the NP classifier. Note that this correspondence is from NP to CS; that is, an NP classifier needs to be constructed first so that its corresponding costs can be found for the two CS implementations.
4.1 Theory

We denote by \( f_0 \) and \( f_1 \) the conditional densities of \( X|(Y=0) \) and \( X|(Y=1) \), respectively. Recall that \( \pi_0 = \mathbb{P}(Y = 0) \) and \( \pi_1 = \mathbb{P}(Y = 1) \). Then the regression function, which is the scoring function of the Bayes classifier, can be expressed as

\[
\eta(X) = \mathbb{P}(Y = 1|X) = \frac{f_1(X)\pi_1}{f_0(X)\pi_0 + f_1(X)\pi_1}.
\]

At the sample level, as in Algorithm 2, we divide the training data \( S \) into two subsets: \( S_0^1 \cup S_1^1 \): a mixture of class 0 and class 1 observations used to estimate \( \eta(\cdot) \); \( S_0^0 \): a left-out class 0 sample used to select the threshold in an NP classifier. In this context, we can estimate the scoring function \( \eta(\cdot) \) from \( S_0^0 \cup S_1^1 \) by

\[
\hat{\eta}(X) = \frac{\hat{f}_1(X)\hat{\pi}_1}{\hat{f}_0(X)\hat{\pi}_0 + \hat{f}_1(X)\hat{\pi}_1},
\]

where \( \hat{\pi}_0 \) and \( \hat{\pi}_1 \) are respectively estimates of \( \pi_0 \) and \( \pi_1 \), and \( \hat{f}_0(\cdot) \) and \( \hat{f}_1(\cdot) \) are respectively estimates of \( f_0(\cdot) \) and \( f_1(\cdot) \). Then a plug-in version of the Bayes classifier is \( \hat{\phi}_{\text{classic}}(X) = \mathbb{I}(\hat{\eta}(X) > 1/2) \), where \( \hat{\eta}(\cdot) \) is defined in (7).

Now we construct an NP classifier using \( s(\cdot) = \hat{\eta}(\cdot) \). Let \( t_{\text{NP}} = T_k^{(k^*)} \), which is found from \( S_0^0 \) by Algorithm 2. An NP classifier can then be constructed as \( \hat{\phi}_{\text{NP}}(X) = \mathbb{I}(\hat{\eta}(X) > t_{\text{NP}}) \). Next, we will show how to decide the misclassification costs corresponding to the NP classifier in two CS implementations: rebalancing and post-training.

4.1.1 Special case 1: the rebalancing approach

Recall the CS objective function

\[
c_0 R_0(\phi_{\text{CS}}) + c_1 R_1(\phi_{\text{CS}}).
\]

In the rebalancing approach, the class priors are set to the misclassification costs \( c_0 \) and \( c_1 \) instead of the two class proportions \( \hat{\pi}_0 \) and \( \hat{\pi}_1 \) in the training data. As such, the scoring function becomes

\[
\tilde{\eta}(X) = \frac{\hat{f}_1(X)c_1}{\hat{f}_0(X)c_0 + \hat{f}_1(X)c_1}.
\]

Then the CS classifier that mimics the Bayes classifier takes the form \( \hat{\phi}_{\text{CS}}^*(X) = \mathbb{I}(\tilde{\eta}(X) > 1/2) \) (Xia et al., 2020). Proposition 2 shows that, given \( \hat{\phi}_{\text{NP}} \), it is possible to construct an equivalent \( \hat{\phi}_{\text{CS}}^* \).

**Proposition 2.** Given a level-\( \alpha \) NP classifier \( \hat{\phi}_{\text{NP}}(X) = \mathbb{I}(\hat{\eta}(X) > t_{\text{NP}}) \), where \( \hat{\eta}(\cdot) \) is defined in (7) and \( 0 \leq t_{\text{NP}} \leq 1 \), if we assign a type I error cost

\[
c_0 = c_0(t_{\text{NP}}, \hat{\pi}_0) = \frac{t_{\text{NP}}\hat{\pi}_0}{(1 - t_{\text{NP}})(1 - \hat{\pi}_0) + t_{\text{NP}}\hat{\pi}_0},
\]

then the resulting CS classifier \( \hat{\phi}_{\text{CS}}^*(X) = \mathbb{I}(\tilde{\eta}(X) > 1/2) = \hat{\phi}_{\text{NP}}(X) \), where \( \tilde{\eta}(\cdot) \) is defined in (8). That is, \( R_0(\hat{\phi}_{\text{CS}}^*) \leq \alpha \) with high probability.
4.1.2 Special case 2: the post-training approach

The post-training approach constructs a CS classifier as

$$\hat{\phi}_{CS}^{pt}(X) = 1 \ I (c_1 \hat{\eta}(X) > c_0 (1 - \hat{\eta}(X)))$$

$$= 1 \ I \left( \frac{\hat{\eta}(X)}{1 - \hat{\eta}(X)} > c_0 \right)$$

$$= 1 \ I (\hat{\eta}(X) > c_0) \quad (10)$$

where the last equality holds because $c_1 = 1 - c_0$. Proposition 3, which is self-evident, shows that, given $\hat{\phi}_{NP}$, we can construct an equivalent $\hat{\phi}_{CS}^{pt}$.

**Proposition 3.** Given a level-$\alpha$ NP classifier $\hat{\phi}_{NP}(X) = 1 \ I (\hat{\eta}(X) > t_{NP})$, where the scoring function $\hat{\eta}(X) = \mathbb{P}(Y = 1 | X)$ is the estimated posterior probability either defined in (7) or constructed by other classification methods (e.g., logistic regression and random forest), if we assign a type I error cost $c_0 = t_{NP}$, then the resulting CS classifier $\hat{\phi}_{CS}^{pt}(X) = 1 \ I (\hat{\eta}(X) > c_0) = \hat{\phi}_{NP}(X)$. That is, $R_0(\hat{\phi}_{CS}^{pt}) \leq \alpha$ with high probability.

4.2 Simulation results

We perform a sanity check of Propositions 2 and 3 using simulation studies. For the rebalancing CS approach, we implement it with three classification methods: linear discriminant analysis, quadratic discriminant analysis, and naive Bayes. For the post-training CS approach, we implement it with logistic regression as an example.

From each of the three data distributions (Gaussian, Multivariate $t$, and Mixture) in Section 2.3, we simulate a training dataset with size $n_1 = 1,000$ and a large evaluation dataset with size $n_2 = 1,000,000$. We split the training data into two subsets: $S_0^1 \cup S_1^1$: a mixture of classes 0 and 1 for obtaining the scoring function $\hat{\eta}(\cdot)$; $S_2^1$: a left-out class 0 sample for selecting the threshold $t_{NP} = T_{k^*}$ by Algorithm 2. To construct an NP classifier, we set the left-out class 0 sample size $m = |S_2^0| = 200$, the target type I error upper bound $\alpha = 0.05$, and the target violation rate $\delta = 0.1$. Based on the NP classifier, we construct the corresponding rebalancing or post-training CS classifier based on Proposition 2 or 3, respectively. Then we approximate the population type I and type II errors of these NP and CS classifiers using the large evaluation dataset. We repeated the simulation for 200 times. Figure 3 indicates that the NP classifiers and their corresponding rebalancing or post-training CS classifiers have identical population type I and type II errors, confirming each pair of NP and CS classifiers’ equivalence.

5. From CS to NP: estimating an upper bound of the population type I error of a CS classifier

Except for the rebalancing and post-training CS implementations discussed in Section 4, in general, it is infeasible to construct a CS classifier that is the same as a given NP classifier. The other direction is to evaluate a given CS classifier’s population type I error performance. We hold that it is impossible to specify $(\alpha, \delta)$, the target population type I error upper bound and the target violation rate, to train an NP classifier to be the same as the given CS classifier. However, a less ambitious goal is possible. Given a CS classifier,
Figure 3: The population type I errors ($R_0$) and type II errors ($R_1$) of NP classifiers and their corresponding rebalancing or post-training CS classifiers. We use the rebalancing approach with three classification methods: linear discriminant analysis (LDA), quadratic discriminant analysis (QDA), and naive Bayes (NB), corresponding to the first three columns. We use the post-training approach with logistic regression (the fourth column). The target violation rate is set as $\delta = 10\%$. We consider three data distributions: Gaussian, $t$, and Mixture. The violation rate of the population type I errors (i.e., the frequency of population type I errors exceeding $\alpha = 0.05$) in each case is summarized as a percentage and marked on top of each violin plot.

by considering it as fixed, we can estimate an upper bound on its population type I error using an independent class 0 sample that is not used for training. Our goal is to have the estimated upper bound (a random variable) above the classifier’s unknown population type I error (a fixed value) with high probability. We believe that estimating the population type I error upper bound will assist the interpretation and assessment of a CS classifier in practice.

In this section, we propose two algorithms to achieve this goal. We first introduce a theoretical result that motivates the design of the algorithms. Then we introduce the algorithms and present their numerical results.

5.1 Theoretical Results

Given a fixed upper bound $\alpha$ on the population type I error, the next proposition shows an upper bound on the “violation rate” of a surrogate classifier—which is constructed from a left-out class 0 sample of size $m$—of a fixed CS classifier. Note that the left-out class 0 sample is not used to train the CS classifier, and the “surrogate violation rate” is defined as the probability (over all possible left-out class 0 samples of size $m$) that the population type I error of the surrogate classifier is greater than $\alpha$. 

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Proposition 4. For a given CS classifier \( \hat{\phi}_{CS}(\cdot) = \mathbb{I}(s(\cdot) > t_{CS}) \), we consider \( s(\cdot) \) and \( t_{CS} \) as fixed. Denote by \( F \) the cumulative distribution function of \( s(X^0) \), where \( X^0 \sim X | Y = 0 \). We apply the scoring function \( \mathbb{F} \) as fixed. Denote by \( \hat{R} \) the upper bound of \( \alpha \) of a CS classifier based on Proposition 4. TUBEc is a generic algorithm applicable to all previous sections for two reasons: the classifier is the surrogate classifier, not the actual CS classifier; the randomness lies in a left-out class 0 sample not used for training, while the CS classifier is fixed. Nevertheless, Proposition 4 helps motivate algorithms to estimate an upper bound of \( R_0(\hat{\phi}_{CS}) \). Concretely, the population type I error of the surrogate classifier, \( R_0(\hat{\phi}_{k^*_2}(\cdot)) \), is always greater than \( \hat{R} \) if \( t_{CS} \geq F^{-1}(1 - \alpha) \), we can solve for \( \hat{\alpha} \) (random) of \( R_0(\hat{\phi}_{CS}) \) (fixed) such that \( \hat{\alpha} > R_0(\hat{\phi}_{CS}) \) with high probability.

5.2 The TUBE Algorithms

We propose two algorithms, TUBEc and TUBE (estimating the Type I error Upper Bound of a cost-sensitive classifier), both of which are motivated by Proposition 4. The first algorithm, TUBEc (TUBE-core), contains the core component to estimate a given CS classifier’s type I error upper bound, and it depends on the availability of a left-out class 0 sample. However, in practice it is often desirable to construct a classifier using all the available data, especially when the available sample size is small. In view of this, we further propose a second algorithm, TUBE, which is built upon TUBEc and aims to estimate a high-probability type I error upper bound of a CS classifier trained on all the available data. We will introduce TUBEc first and TUBE next.

5.2.1 The TUBEc Algorithm

The TUBEc algorithm (Algorithm 3) estimates \( F(\cdot) \) on the left-out class 0 sample using the nonparametric bootstrap procedure. TUBEc then estimates the type I error upper bound of a CS classifier based on Proposition 4. TUBEc is a generic algorithm applicable to all

Note that when we also consider the randomness of the CS classifier, \( \delta_s \) would not be a fixed number but rather depends on the random quantity \( F(t_{CS}) \), in which \( F(\cdot) \) inherits randomness from \( s(\cdot) \), and \( t_{CS} \) is possibly random too.
Algorithm 3: The TUBEc algorithm for estimating type I error upper bound

**Input:**
- $\mathbb{I}(s(\cdot) > t_{CS})$: CS classifier
- $S_0^2 = \{x_1, \ldots, x_m\}$: left-out class 0 sample
- $\delta$: pre-specified violation rate

1. $\mathcal{T} = \{T_1, \ldots, T_m\} \leftarrow \{s(x_1), \ldots, s(x_m)\}$
2. for $b \leftarrow 1$ to $B$ do
   3. $\mathcal{T}^b = \{T^b_1, \ldots, T^b_m\} \leftarrow \text{sample}(\mathcal{T}, \text{size} = m, \text{replace} = \text{true})$
      \hspace{1cm} $\{T^b_1, \ldots, T^b_m\} \leftarrow \text{sort}(\mathcal{T}^b)$
   4. if $T^b_1 > t_{CS}$ then
      5. $\hat{\alpha}_b = 1$
   6. else
      7. $k^*_{s,b} = \max\{k \in \{1, \ldots, m\} : T^b_k \leq t_{CS}\}$
      8. $\hat{F}_b(t_{CS}) = k^*_{s,b}/m$
      9. $\hat{\alpha}_b = 2 - \hat{F}_b(t_{CS}) - \left[\delta + \left(1 - \hat{F}_b(t_{CS})\right)^m\right]^{1/m}$
         \hspace{1cm} // solve for $\alpha$ based on Proposition 4
   10. end
3. end

**Output:** estimated type I error upper bound

$$\hat{\alpha} = (1 - \delta)\text{-th quantile of } \{\hat{\alpha}_b\}_{b=1}^B$$ // the TUBEc estimator

CS classifiers, which may be constructed by any of the pre-training, in-training, and post-training approaches (Table 2). Specifically, for a given classification scoring function $s(\cdot)$, a pre-determined classification score threshold $t_{CS}$, and a left-out class 0 sample $S_0^2$, TUBEc estimates the type I error upper bound of the CS classifier $\mathbb{I}(s(\cdot) > t_{CS})$. In each iteration $b$, TUBEc first obtains a bootstrap sample of the classification scores on the left-out class 0 sample, and then it estimates a type I error upper bound $\hat{\alpha}_b$. After $B$ iterations, TUBEc calculates the final estimated type I error upper bound as $\hat{\alpha} = (1 - \delta)\text{-th quantile of } \{\hat{\alpha}_b\}_{b=1}^B$.

We apply the TUBEc algorithm to multiple simulation settings to estimate the type I error upper bound of CS classifiers. We consider two classification methods, logistic regression and gradient boosting, combined with the stratification approach for constructing CS classifiers. For each classification method, we consider three left-out sample sizes ($|S_0^2| = m$): 50, 100, and 200, and we set the type I error cost $c_0$ to 0.7. The simulated data are drawn from the three distributions used in previous simulations, Gaussian, Multivariate $t$, and Mixture (Section 2.3). We set the desired violation rate to $\delta = 0.1$ for all settings. In each setting, we first train a CS classifier on a training sample of size 500 and then apply the TUBEc algorithm to 100 independent left-out class 0 samples to estimate the type I error upper bound of the CS classifier. We repeat this simulation experiment three times for every combination of a classification method, a left-out sample size, and a data distribution.

We compare the TUBEc estimator with the empirical estimator $\hat{\alpha}^{\text{emp}}$ defined as the empirical type I error of the CS classifier on the left-out sample. Moreover, to demonstrate the necessity of the bootstrap procedure in the TUBEc algorithm, we consider a plug-in estimator defined directly based on Proposition 4. Concretely, instead of using estimates
\(\hat{\alpha}_1, \ldots, \hat{\alpha}_B\) based on the bootstrapped class 0 scores \(T^1, \ldots, T^B\), we define the plug-in estimator \(\hat{\alpha}_{\text{plug-in}} = 2 - \hat{F}(t_{CS}) - [\delta + (1 - \hat{F}(t_{CS}))^n]^{1/m}\), where \(\hat{F}(t_{CS})\) is estimated from \(T\), the left-out class 0 scores. Figure 4 shows the distribution of the difference between each estimator and the population type I error of the given CS classifier under each simulation setting. We expect that the distributions corresponding to a good estimator should have probabilities close to \(\delta = 10\%\) for negative differences, indicating that the estimator is greater than the population type I error with high probability. Among the three estimators (empirical, plug-in, and TUBEc), only the TUBEc estimator achieves this property.

5.2.2 The TUBE Algorithm

The TUBEc algorithm estimates a type I error upper bound for a CS classifier whose training sample does not include the left-out class 0 sample. However, in real applications, it is often desirable or even necessary to train a CS classifier using the whole sample \(S\), since a larger training sample size in general leads to better classification performance. Therefore, we further propose TUBE (Algorithm 4) as a modified version of the TUBEc algorithm to estimate the type I error upper bound of a CS classifier constructed using \(S\). The central strategy is to adjust up the empirical type I error computed on \(S\) by the difference between the TUBEc estimate and this empirical type I error. Note that the TUBEc estimate is only calculable when a separate left-out class 0 sample is available; however, as we have used up all the available observations, we cannot calculate this difference but have to mimic it by an average of the differences evaluated by random partitioning of \(S\), in which each partition leads to (1) a mixed class sample for training a CS classifier and calculating the empirical type I error and (2) a left-out class 0 sample for calculating the TUBEc estimate.

**Algorithm 4:** The TUBE algorithm for estimating type I error upper bound

| Input | \(S = S^0 \cup S^1\): training sample \((S^0 \text{ for class } 0 \text{ and } S^1 \text{ for class } 1)\) |
|---|---|
| \(c_0\): type I error cost | \(\delta\): pre-specified violation rate |
| 1 | \(\mathbb{I}(s(\cdot) > t_{CS}) = \text{CS-classifier}(S, c_0)\) |
| 2 | \(\hat{\alpha} = \text{empirical type I error of } \mathbb{I}(s(\cdot) > t_{CS}) \text{ on } S \) // on training sample |
| 3 | for \(b_1 \leftarrow 1 \text{ to } B_1\) do |
| 4 | \(S^0_{b_1}, S^1_{b_1} \leftarrow \text{randomly split class } 0 \text{ sample } S^0\) |
| 5 | \(S_{b_1} = S^1 \cup S^0_{b_1}\) // training data for CS classifier |
| 6 | \(\mathbb{I}(s_{b_1}(\cdot) > t_{CS,b_1}) = \text{CS-classifier}(S_{b_1}, c_0)\) |
| 7 | \(\hat{\alpha}_{b_1}^{\text{TUBE}_c} = \text{TUBEc}(\mathbb{I}(s_{b_1}(\cdot) > t_{CS,b_1}), S^0_{b_1}, \delta)\) // the TUBEc estimator |
| 8 | \(\hat{\alpha}_{b_1} = \text{empirical type I error of } \mathbb{I}(s_{b_1}(x) > t_{CS,b_1}) \text{ on } S_{b_1}\) |
| 9 | end |
| 10 | \(\hat{\alpha}^{\text{TUBE}} = \hat{\alpha} + \frac{1}{B_1} \sum_{b_1=1}^{B_1} (\hat{\alpha}_{b_1}^{\text{TUBE}_c} - \hat{\alpha}_{b_1})\) // the TUBE estimator |

**Output:** \(\hat{\alpha}^{\text{TUBE}}\)

In Figure 5, using training samples generated from the Gaussian distribution (Section 2.3), we construct CS classifiers using the stratification approach with two classification methods: gradient boosting and logistic regression. Given these CS classifiers, we compare the TUBE estimator \(\hat{\alpha}^{\text{TUBE}}\) (with \(\delta = .1\)) with the empirical estimator \(\hat{\alpha}^{\text{emp}}\), which is de-
Figure 4: Performance of the TUBEc estimator ($\hat{\alpha}^{\text{TUBEc}}$), the empirical estimator ($\hat{\alpha}^{\text{emp}}$), and the plug-in estimator ($\hat{\alpha}^{\text{plug-in}}$). The simulated data are drawn from three distributions: (a) Gaussian, (b) Multivariate $t$, and (c) Mixture. We use the stratification approach with two classification methods, gradient boosting (GB) and logistic regression (LR), to construct CS classifiers. The boxplots show the distributions of the difference between the estimated type I error upper bound ($\hat{\alpha}$) and the actual population type I error of the given CS classifier ($R_0$) (approximated on a large sample of size $10^6$). The violate rate (percentage of simulations in which $R_0 > \hat{\alpha}$) is labeled on the top of each boxplot. The left-out class 0 sample size is labeled on the right of each row. The horizontal axis indicates the three experiments as replications of each simulation setting.
fined as the empirical type I error of a CS classifier on the training sample. (Results for the Multivariate t and Mixture distributions are in Figure A1 in the Appendix). Granted, \( \hat{\alpha}_{\text{TUBE}} \) is not guaranteed to dominate the true type I error of a CS classifier with at least \( 1 - \delta \) probability. Still, Figure 5 shows that \( \hat{\alpha}_{\text{TUBE}} \) is a high-probability upper bound on the true type I error. Empirically, we observe that the actual violation rate (i.e., the probability that \( \hat{\alpha}_{\text{TUBE}} \) is below the true type I error) is below \( 1.5\delta \) in all cases, and it falls under \( \delta \) when the training sample size is large. In contrast, \( \hat{\alpha}_{\text{emp}} \) fails to be a high-probability upper bound, as expected.

**Figure 5:** Performance of the TUBE estimator (\( \hat{\alpha}_{\text{TUBE}} \); blue) and the empirical estimator (\( \hat{\alpha}_{\text{emp}} \); yellow). Data are generated from the Gaussian distribution (Section 2.3). We use the stratification approach with two classification methods, gradient boosting (GB) and logistic regression (LR), to construct CS classifiers. The boxplots show the distributions of the difference between the estimated type I error upper bound (\( \hat{\alpha} \)) and the actual population type I error of the given CS classifier (\( R_0 \)) (approximated on a large sample of size \( 10^6 \)). The horizontal axis denotes the type I error cost (\( c_0 = 0.7, 0.8, \text{or} 0.9 \)). The training sample size (250, 500, or 1000) is labeled on the top of each column. The violation rate (percentage of simulations in which \( R_0 > \hat{\alpha} \)) is labeled on the top of each boxplot.

6. TUBE-assisted CS classification for type I error control

In this section, we introduce a TUBE-assisted algorithm for selecting the type I error cost \( c_0 \) in CS classification so that the resulting CS classifier has its population type I error under a target upper bound \( \alpha \) with high probability. Note that the TUBE algorithm (Algorithm 4) provides an estimated high-probability upper bound on the population type I errors of CS classifiers constructed with a given cost \( c_0 \). Hence, if we have a target type I error upper bound \( \alpha \), we can supply candidate type I error costs into the TUBE algorithm and evaluate their corresponding TUBE estimates; then, we can compare these TUBE estimates with \( \alpha \) and pick the smallest type I error cost whose TUBE estimate is under \( \alpha \). We refer to this TUBE-assisted algorithm by TUBE-CS and describe it in Algorithm 5.

To evaluate TUBE-CS, we compare it with three algorithms: the TUBEc-assisted algorithm (TUBEc-CS; Algorithm A1 in Appendix), the vanilla CS implementation (Algorithm 1), and the NP umbrella algorithm (Algorithm 2). Note that TUBEc-CS is similar to TUBE-CS in that it replaces TUBE estimates with TUBEc estimates. Since TUBE-c re-
quires a left-out class 0 sample, TUBEc-CS requires sample splitting, unlike TUBE-CS. We have shown that the vanilla CS implementation cannot construct CS classifiers with population type I errors under $\alpha$ with high probability (Section 2.3), and here we use it as a negative control. The NP umbrella algorithm is designed exactly for this type I error control purpose; however, it requires sample splitting for constructing NP classifiers. All the four algorithms—TUBE-CS, TUBEc-CS, vanilla-CS, and NP—construct classifiers given a classification method, a target type I error upper bound $\alpha$, and a pre-specified violation rate $\delta$. The goal is to evaluate whether their constructed classifiers have population type I errors under $\alpha$ with a high probability close to $1 - \delta$.

**Algorithm 5: TUBE-assisted CS implementation (TUBE-CS)**

```plaintext
Input : $\mathcal{S} = \mathcal{S}^0 \cup \mathcal{S}^1$: training data ($\mathcal{S}^0$ for class 0 and $\mathcal{S}^1$ for class 1)
\alpha: target upper bound on the type I error
c_{0,1} < c_{0,2} < \cdots < c_{0,I}$: candidate type I error costs
$\delta$: pre-specified violation rate

1 for $i \leftarrow 1$ to $I$ do
    2 $\hat{\alpha}_i = \text{TUBE}(\mathcal{S}, c_{0,i}, \delta)$
3 end
4 $i^* = \min\{i : \hat{\alpha}_i \leq \alpha\}$

Output: $\hat{\phi}^{\text{TUBE-CS}}(.) = \text{CS-classifier}(\mathcal{S}, c_{0,i^*})$ \hspace{1cm} // the TUBE-CS classifier
```

To compare the four algorithms, we design a simulation study with $\alpha = 0.05$ and $\delta = 0.1$. We pair each algorithm with four classification methods: logistic regression, naïve Bayes, gradient boosting, and random forest. We simulate data from the Gaussian distribution (Section 2.3) with $d = 30$. In each simulation, we generate a training sample with size $n_1 = 1,000$ and a large evaluation sample with size $n_2 = 1,000,000$ (to approximate the population). We use the stratification approach to construct CS classifiers.

Figure 6 shows the comparison results. As expected, the NP umbrella algorithm is the only one whose constructed classifiers have population type I errors under $\alpha$ with more than $1 - \delta$ probability in every setting. The TUBE-CS and TUBEc-CS algorithms have achieved desirable type I error control with logistic regression, naïve Bayes, and random forest, but not with gradient boosting. The vanilla-CS algorithm cannot construct classifiers with desirable type I error control, regardless of the classification method.

Regarding the type II error, classifiers constructed by the TUBE-CS algorithm generally have smaller population type II errors than those of the classifiers constructed by the NP umbrella algorithm. This advantage comes from the fact that the TUBE-CS algorithm trains scoring functions in classifiers using all the training data, while the NP umbrella algorithm leaves out a portion of the class 0 sample from the training of scoring functions. Unlike the TUBE-CS algorithm, the TUBEc-CS algorithm tends to be too conservative in controlling the type I error and thus does not outperform the NP umbrella algorithm in terms of the type II error. Together, these results suggest that the NP umbrella algorithm should always be preferred if a strict high-probability control on the type I error is desired. However, when such a strict control can be loosened a bit and the training sample size is...
Figure 6: Comparison of four algorithms: vanilla-CS (“vanilla”), TUBE-CS (“TUBE”), TUBEc-CS (“TUBEc”), and NP umbrella (“NP”) algorithms. The population type I and II errors (approximated on the large evaluation sample) are shown as boxplots for four classification methods: (a) logistic regression, (b) naïve Bayes, (c) gradient boosting, and (d) random forest. The violation rate (percentage of simulations in which the population type I error exceeds $\alpha = 0.05$) is labeled on the top of each boxplot.

moderate or small, the TUBE-CS algorithm is preferred because it delivers smaller type II errors thanks to better scoring functions trained on all available data.

7. Comparison of vanilla-CS and TUBE-CS algorithms on real datasets

In this section, we compare the vanilla-CS and TUBE-CS algorithms on four real datasets from the UCI Machine Learning Repository (Dua and Graff, 2017). A summary of these four datasets is in Table 3. The Diabetes dataset (generated by the National Institute of Diabetes and Digestive and Kidney Diseases) allows the training of a classifier to predict whether a patient has diabetes from his/her diagnostic measurements; the more severe type of classification error is the misprediction of a diabetes patient as undiseased. The Thyroid dataset (generated by the Garavan Institute) allows the training of a classifier to predict whether a subject has the euthyroid sick syndrome; the more severe type of classification error is the misprediction of a euthyroid sick patient as undiseased. The Breast cancer dataset allows the training of a classifier to predict the state (benign or malignant) of a mammographic mass lesion, so as to help physicians decide whether to perform a biopsy on the lesion or just schedule a short-term follow-up examination; the more severe type of classification error is the misprediction of a malignant lesion as benign. The Marketing dataset of a Portuguese banking institution allows the training of a classifier to predict if a
client will subscribe (yes or no) to a term deposit based on the information gathered in a phone call; the more severe type of classification error is missing a potential subscriber.

Table 3: Description of four real datasets. For each dataset, the sample size (n), the proportion of class 0 observations (n₀/n), the number of features (d), and the class encodings are listed.

| dataset     | n   | n₀/n | d  | class 0          | class 1        |
|-------------|-----|------|----|------------------|----------------|
| Diabetes    | 768 | 0.35 | 8  | diabetes         | negative       |
| Thyroid     | 3090| 0.09 | 18 | euthyroid sick   | negative       |
| Breast cancer | 960 | 0.46 | 5  | malignant        | benign         |
| Marketing   | 4119| 0.11 | 18 | yes              | no             |

For each real dataset, we randomly split the data into two subsets of equal size, one used as the training sample for constructing CS classifiers by the vanilla-CS or the TUBE-CS algorithm, and the other used as the evaluation sample for calculating the type I and II errors. When implementing the vanilla-CS and TUBE-CS algorithms, we use the logistic regression as the classification method and the stratification approach as the CS implementation. We set the target type I error upper bound to \( \alpha = 0.05 \) and the violation rate to \( \delta = 10\% \), and we repeat the random splitting for 50 times. Since we do not have a large evaluation set to approximate the population in these real datasets, we cannot assess the violation rates of CS classifiers' population type I errors. However, using the empirical type I errors on the evaluation sample as a proxy, we can see that the TUBE-CS classifiers clearly have better control of type I error than the vanilla-CS classifiers do on all the four datasets (Figure 7).

These results suggest that the TUBE-CS algorithm is a useful tool for choosing the type I error cost \( c_0 \) in CS classification, when users have a target type I error upper bound in mind. Moreover, the TUBE algorithm offers a way to estimate an upper bound on the type I error of a CS classifier constructed with a cost \( c_0 \), thus improving the interpretability of CS classifiers.

8. Conclusions

In this article, we discuss two classification paradigms, CS and NNP, for prioritizing misclassification errors in asymmetric binary classification problems. Our work, for the first time, discusses the methodological connections between the two paradigms. We identify two special cases in which we can construct a CS classifier that is identical to a given NP classifier. For a given CS classifier, using a left-out class 0 sample, the TUBEc algorithm delivers a numerically validated estimate of a high-probability upper bound on the population type I error of the CS classifier. Moreover, the TUBE algorithm, which uses only the training data and a pre-specified type I error cost (without having access to an actual CS classifier), delivers a less accurate but still reasonable estimate of the upper bound. The TUBE algorithm is valuable when the overall class 0 (usually the more severe state) sample size is small. Powered by the TUBE algorithm, the TUBE-CS algorithm offers a substitute for the NP umbrella algorithm for constructing classifiers so that the classifiers have population type I errors under a pre-specified upper bound \( \alpha \) with high probability.
Figure 7: Comparison of the vanilla-CS (“vanilla”) and TUBE-CS (“TUBE”) algorithms on the four real datasets (Table 3): (a) Diabetes, (b) Thyroid, (c) Breast cancer, (d) and Marketing. The type I errors are calculated on evaluation data across 50 random splits, each of which divides each dataset into two halves for training and evaluation. Boxplots are shown for the type I errors and the type I error costs ($c_0$) of the classifiers constructed by each algorithm.

The TUBE-CS algorithm is preferable when the high-probability requirement is not strict or the minimum class 0 sample size required by the NP umbrella algorithm is not met.

9. Code availability

The source code for the statistical analysis in this work is available at https://github.com/Vivianstats/TUBE.
Appendix 1. Supplementary Text

Proof of Proposition 2

Proof. When the type I error cost \( c_0 \) takes the form

\[
c_0 = \frac{t_{\text{NP}} \hat{\pi}_0}{(1 - \hat{\pi}_0)(1 - t_{\text{NP}}) + t_{\text{NP}} \hat{\pi}_0},
\]

in view of our assumption \( c_0 + c_1 = 1 \), we have \( \forall X \in \mathcal{X}, \)

\[
\hat{\eta}(X) > \frac{1}{2} \iff \frac{\hat{f}_1(X)}{f_0(X)} > \frac{c_0}{1 - c_0} \iff \frac{\hat{f}_1(X)}{f_0(X)} > \frac{t_{\text{NP}} \hat{\pi}_0}{(1 - \hat{\pi}_0)(1 - t_{\text{NP}}) + t_{\text{NP}} \hat{\pi}_0} \iff \frac{\hat{f}_1(X)}{f_0(X)} > \frac{t_{\text{NP}} \hat{\pi}_0}{(1 - \hat{\pi}_0)(1 - t_{\text{NP}})} \iff \hat{\eta}(X) > t_{\text{NP}}.
\]

Therefore, the rebalancing CS classifier \( \hat{\phi}_{\text{CS}}(X) = \mathbb{I}(\hat{\eta}(X) > 1/2) \) is the same as the NP classifier \( \hat{\phi}_{\text{NP}}(X) = \mathbb{I}(\hat{\eta}(X) > t_{\text{NP}}). \) \( \square \)

Proof of Proposition 4

Proof. We consider the type I errors of the CS classifier \( \hat{\phi}_{\text{CS}}(\cdot) = \mathbb{I}(s(\cdot) > t_{\text{CS}}) \) and the surrogate classifier \( \hat{\phi}_{k^*_s}(\cdot) = \mathbb{I}(s(\cdot) > T_{(k^*_s)}) \). Given that \( \hat{\phi}_{\text{CS}} \) is fixed, its population type I error is a fixed value

\[
R_0(\hat{\phi}_{\text{CS}}) = 1 - F(t_{\text{CS}}),
\]

while the population type I error of \( \hat{\phi}_{k^*_s} \) is a random variable

\[
R_0(\hat{\phi}_{k^*_s}) = 1 - F(T_{(k^*_s)})
\]

due to the randomness of \( T_{(k^*_s)} \).

Under the assumption that \( T_{(1)} \leq t_{\text{CS}} \), we have \( T_{(k^*_s)} \leq t_{\text{CS}} \), and hence \( R_0(\hat{\phi}_{k^*_s}) \geq R_0(\hat{\phi}_{\text{CS}}) \). In other words, the population type I error of the CS classifier is no greater than the population type I error of the surrogate classifier.
Next, we calculate the probability (regarding measure $\mathbb{P}_m$) that the population type I error of the surrogate classifier $\hat{\phi}_{k^*_s}$ exceeds $\alpha$:

$$
\mathbb{P}_m(R_0(\hat{\phi}_{k^*_s}) > \alpha) = \mathbb{P}_m(1 - F(T_{(k^*_s)}) > \alpha) \\
= \mathbb{P}_m(T_{(k^*_s)} < F^{-1}(1 - \alpha)) \\
= \sum_{k=1}^{m} \mathbb{P}_m(T_{(k)} < F^{-1}(1 - \alpha), k^*_s = k) \\
= \sum_{k=1}^{m-1} \mathbb{P}_m(T_{(k)} < F^{-1}(1 - \alpha), T_{(k)} \leq t_{CS}, T_{(k+1)} > t_{CS}) \\
+ \mathbb{P}_m(T_{(m)} < F^{-1}(1 - \alpha), T_{(m)} \leq t_{CS}) .
$$

If $t_{CS} < F^{-1}(1 - \alpha)$,

$$
\mathbb{P}_m(R_0(\hat{\phi}_{k^*_s}) > \alpha) = \sum_{k=1}^{m-1} \mathbb{P}_m(T_{(k)} \leq t_{CS}, T_{(k+1)} > t_{CS}) + \mathbb{P}_m(T_{(m)} \leq t_{CS}) = 1.
$$

If $t_{CS} \geq F^{-1}(1 - \alpha)$,

$$
\mathbb{P}_m(R_0(\hat{\phi}_{k^*_s}) > \alpha) = \sum_{k=1}^{m-1} \mathbb{P}_m(T_{(k)} < F^{-1}(1 - \alpha), T_{(k+1)} > t_{CS}) + \mathbb{P}_m(T_{(m)} < F^{-1}(1 - \alpha)) \\
= \sum_{k=1}^{m-1} \binom{m}{k} \mathbb{P}_m(T_1 < F^{-1}(1 - \alpha), \ldots, T_k < F^{-1}(1 - \alpha), T_{k+1} > t_{CS}, \ldots, T_{m-1} > t_{CS}) \mathbb{P}_m(T_1 < F^{-1}(1 - \alpha), \ldots, T_m < F^{-1}(1 - \alpha)) \\
\leq \sum_{k=1}^{m} \binom{m}{k} (1 - \alpha)^k (1 - F(t_{CS}))^{m-k} \\
= (1 - \alpha + u)^m - u^m.
$$

In summary,

$$
\mathbb{P}_m(R_0(\hat{\phi}_{k^*_s}) > \alpha) \begin{cases}
0 & \text{if } t_{CS} < F^{-1}(1 - \alpha) \\
1 & \text{if } t_{CS} \geq F^{-1}(1 - \alpha)
\end{cases}
$$

In other words, when $t_{CS} < F^{-1}(1 - \alpha)$, the type I error of $\hat{\phi}_{k^*_s}$ exceeds $\alpha$ with probability 1; when $t_{CS} \geq F^{-1}(1 - \alpha)$, the type I error of $\hat{\phi}_{k^*_s}$ exceeds $\alpha$ with probability no larger than $
\delta_s = (2 - \alpha - F(t_{CS}))^m - (1 - F(t_{CS}))^m .
$\hfill \Box

Algorithm A1
Algorithm A1: TUBEc-assisted CS classification (TUBEc-CS)

**Input**: $S = S^0 \cup S^1$: training data ($S^0$ for class 0 and $S^1$ for class 1)  
$\alpha$: target upper bound on the type I error  
$c_{0,1} < c_{0,2} < \cdots < c_{0,I}$: candidate type I error costs  
$\delta$: violation rate

1. $S^0_1, S^0_2 \leftarrow$ randomly split class 0 data $S^0$
2. for $i \leftarrow 1$ to $I$ do
   3. $\hat{\phi}_i(\cdot) = \text{CS-classifier}(S^1 \cup S^0_1, c_{0,i})$
   4. $\hat{\alpha}^c_i = \text{TUBEc}(\hat{\phi}_i(\cdot), S^0_2, \delta)$
5. end
6. $i^{*c} = \min \{i : \hat{\alpha}^c_i \leq \alpha\}$

**Output**: $\hat{\phi}^\text{TUBEc-CS}(\cdot) = \hat{\phi}_{i^{*c}}(\cdot)$  // the TUBE-CS classifier
Appendix 2: Supplementary Figures

Figure A1: Performance of the TUBE estimator ($\hat{\alpha}^{\text{TUBE}}$; blue) and the empirical estimator ($\hat{\alpha}^{\text{emp}}$; yellow). Data are generated from (a) the Multivariate $t$ distribution and (b) the Mixture distribution (Section 2.3). We use the stratification approach with two classification methods, gradient boosting (GB) and logistic regression (LR), to construct CS classifiers. The boxplots show the distributions of the difference between the estimated type I error upper bound ($\hat{\alpha}$) and the actual population type I error of the given CS classifier ($R_0$) (approximated on a large sample of size $10^6$). The horizontal axis denotes the type I error cost ($c_0 = 0.7, 0.8, \text{or } 0.9$). The training sample size (250, 500, or 1000) is labeled on the top of each column. The violation rate (percentage of simulations in which $R_0 > \hat{\alpha}$) is labeled on the top of each boxplot.
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