Neyman-Pearson Multi-class Classification via Cost-sensitive Learning

Ye Tian
Department of Statistics
Columbia University
New York, NY 10027, USA

Yang Feng
Department of Biostatistics, School of Global Public Health
New York University
New York, NY 10003, USA

Abstract
Most existing classification methods aim to minimize the overall misclassification error rate. However, in applications, different types of errors can have different consequences. Two popular paradigms have been developed to account for this asymmetry issue: the Neyman-Pearson (NP) paradigm and the cost-sensitive (CS) paradigm. Compared to the CS paradigm, the NP paradigm does not require a specification of costs. Most previous works on the NP paradigm focused on the binary case. In this work, we study the multi-class NP problem by connecting it to the CS problem and propose two algorithms. We extend the NP oracle inequalities and consistency from the binary case to the multi-class case, showing that our two algorithms enjoy these properties under certain conditions. The simulation and real data studies demonstrate the effectiveness of our algorithms. To our knowledge, this is the first work to solve the multi-class NP problem via cost-sensitive learning techniques with theoretical guarantees. The proposed algorithms are implemented in the R package npcs on CRAN.

Keywords: multi-class classification, Neyman-Pearson paradigm, cost-sensitive learning, duality, NP oracle properties, consistency, confusion matrix, over-sampling, hypothesis testing

1. Introduction
1.1 Asymmetric Errors in Classification
Classification is one of the central tasks in machine learning, in which we try to train a classifier on training data to accurately predict the labels of test data based on predictors. In practice, we rarely achieve a perfect classifier that can correctly classify all the unknown data. There are different types of errors that a classifier can make. In binary classification with classes 1 and 2, denote the predictor vector $X \in \mathcal{X} \subseteq \mathbb{R}^p$ and the label $Y \in \{1, 2\}$. For any classifier $\phi: \mathcal{X} \rightarrow \{1, 2\}$, we usually define type-I error $R_1 = P_{X|Y=1}(\phi(X) \neq 1)$ and type-II error $R_2 = P_{X|Y=2}(\phi(X) \neq 2)$, where $P_{X|Y=k}$ represents the probability measure induced by the conditional distribution of $X$ given $Y = k$, and $k = 1$ or 2. Then the overall misclassification error can be seen as a weighted sum of type-I and type-II errors.

In many approaches to classification, classifiers are often designed to minimize the overall misclassification error. However, in many cases, different types of errors can have different
degrees of consequences, making the overall misclassification error minimization unideal in such problems. One of the most famous examples is disease diagnosis. We denote a person with severe disease as class 1 and a healthy person as class 2. Then making a type-I error, i.e., misclassifying an ill person as healthy without providing medical help, is more serious than making a type-II error, i.e., misclassifying a healthy person as ill. In such a scenario, the criterion of overall misclassification error minimization may need to be revised. Therefore, researchers developed two paradigms, the Neyman-Pearson paradigm and the cost-sensitive learning paradigm, to tackle this error asymmetry. In the following two subsections, we are going to introduce them separately.

1.2 Neyman-Pearson Paradigm

The Neyman-Pearson (NP) paradigm changes the classical classification framework by assigning different priorities to different types of errors. In binary classification, the NP paradigm seeks the classifier $\phi$, which solves the following optimization problem

$$\min_{\phi} \ P_{X|Y=2}(\phi(X) \neq 2)$$

subject to

$$P_{X|Y=1}(\phi(X) \neq 1) \leq \alpha_1,$$

(1)

with some $\alpha_1 \in [0, 1)$.

There have been many studies on the binary NP paradigm, and researchers have developed many useful tools to solve problem (1). Cannon et al. (2002) initiated the theoretical analysis of NP classification. Scott and Nowak (2005) proved theoretical properties of the empirical error minimization (ERM) approach, including so-called NP oracle inequalities and consistency. Scott (2007) proposed a new way to measure the performance under the NP paradigm. Rigollet and Tong (2011) transformed the original problem into a convex problem through some convex surrogates. They solved the new problem and proved that the optimal classifier could successfully control the type-I error in high probability. Tong (2013) tackled this problem by combining the Neyman-Pearson lemma with the kernel density estimation and came up with the so-called plug-in method, which enjoys the NP oracle inequalities. Zhao et al. (2016) extended the NP framework into the high-dimensional case via naive Bayes classifier, where the number of predictors can grow with the sample size. More recently, Tong et al. (2018) proposed an umbrella NP algorithm that can adapt to any scoring-type classifier, including linear discriminant analysis (LDA), support vector machines (SVM), and random forests. Using the order statistics and some thresholding strategy, the umbrella algorithm can provide high-probability control for all classifiers under some sample size requirements. Tong et al. (2020) further studied both parametric and non-parametric ways to adjust the classification threshold for an LDA classifier, which were proved to solve (1) with NP oracle inequalities. Scott (2019) proposed a generalized Neyman-Pearson criterion and argued that a broader class of transfer learning problems could be solved under this criterion. Li et al. (2020) first connected binary NP problems with CS problems and proposed a way to construct a CS classifier with type-I error control. Xia et al. (2021) applied the NP umbrella method proposed by Tong et al. (2018) into a social media text classification problem. Li et al. (2021) proposed a model-free feature ranking method based on the NP framework. The works we list may be incomplete. We refer interested readers to the survey paper by Tong et al. (2016) and another recent paper.
discussing the relationship between hypothesis testing and NP binary classification by Li and Tong (2020).

However, all the works mentioned above focus on the binary NP paradigm. In this paper, we consider a multi-class classification problem and develop algorithms to solve the multi-class NP problem. Suppose there are \( K \) classes (\( K \geq 2 \)), and we denote them as classes 1 to \( K \). The training sample \( \{(x_i, y_i)\}_{i=1}^n \) are i.i.d. copies of \( (X, Y) \subseteq X \times \{1, \ldots, K\} \), where \( X \subseteq \mathbb{R}^p \). Denote \( \pi^*_k = \mathbb{P}(Y = k) \) and we assume \( \pi^*_k \in (0, 1) \) for all \( k \)’s. Also denote \( \pi^* = (\pi^*_1, \ldots, \pi^*_K)^T \). To define a multi-class NP problem, it is crucial for us to extend the two types of errors in binary classification to the multi-class case. We now introduce two possible formulations.

- Mossman (1999) and Dreiseitl et al. (2000) extended binary receiver operating characteristic (ROC) to multi-class ROC by considering \( \mathbb{P}_{X|Y=k}(\phi(X) \neq k|Y = k) \) as the \( k \)-th error rate of classifier \( \phi \) for any \( k \in \{1, \ldots, K\} \). Then the NP problem can be constructed to control \( \mathbb{P}_{X|Y=k}(\phi(X) \neq k) \) for some \( k \), while minimizing a weighted sum of \( \{\mathbb{P}_{X|Y=k}(\phi(X) \neq k)\}_{k=1}^K \).

- Another way is to consider the confusion matrix \( \Gamma = [\Gamma_{rk}]_{K \times K} \), where \( \Gamma_{rk} = \mathbb{P}_{X|Y=k}(\phi(X) = r) \) for \( r \neq k \) (Edwards et al., 2004). Then we can formulate the NP problem by controlling \( \Gamma_{rk} \) while minimizing a weighted sum of \( \{\mathbb{P}_{X|Y=k}(\phi(X) = r)\}_{r,k=1}^K \).

In this paper, for ease of the readers’ understanding, we focus on the first formulation, which minimizes a weighted sum of \( \{\mathbb{P}_{X|Y=k}(\phi(X) \neq k)\}_{k=1}^K \) and controls \( \mathbb{P}_{X|Y=k}(\phi(X) \neq k) \) for \( k \in A \), where \( A \subseteq \{1, \ldots, K\} \). The confusion matrix control problem is a generalization of the first formulation and is more complicated. We will discuss it in Section 4 after a comprehensive study on the first type of extension. We formally present the Neyman-Pearson multi-class classification (NPMC) problem as

\[
\min_{\phi} \quad J(\phi) = \sum_{k=1}^K w_k \mathbb{P}_{X|Y=k}(\phi(X) \neq k) \\
\text{s.t.} \quad \mathbb{P}_{X|Y=k}(\phi(X) \neq k) \leq \alpha_k, \quad k \in A,
\]

where \( \phi : X \rightarrow \{1, \ldots, K\} \) is a classifier, \( \alpha_k \in [0, 1] \), \( w_k \geq 0 \) and \( A \subseteq \{1, \ldots, K\} \).

The formulation of (2) is closely connected to the hypothesis testing problem with a composite null hypothesis consisting of finite arguments. For example, suppose that we have collected data \( x_1, \ldots, x_n \) i.i.d. some distribution \( p_\theta \) and we would like to test \( H_0 : \theta \in \{\theta_k\}_{k=1}^K \) v.s. \( H_1 : \theta = \theta_{K+1} \). We want to maximize the statistical power, i.e., \( \mathbb{P}_{\theta_{K+1}}(\phi(x) = 1) \), while controlling the type-I error rate under level \( \alpha \) in every case, i.e., \( \max_{k=1:K} \mathbb{P}_{\theta_k}(\phi(x) = 1) \leq \alpha \). These two problems are connected and have similar formats. For instance, both of them require control over multiple errors, and there is no feasibility guarantee in general (in contrast to the binary NP problem (1) or the hypothesis testing problem with a simple \( H_0 \)). However, there are some intrinsic differences between these two problems. First, in the hypothesis testing problem, \( p_{\theta_k} \) is known, but in the NP problem (2), the distribution of \( X \) given \( Y = k \) is unknown. Second, multiple \( \theta_k \)’s belong to the same null hypothesis \( H_0 \), which is essentially a binary problem. However, in the NP problem (2), \( K \) classes are different and are associated with potentially different target control levels \( \alpha_k \)’s;
Therefore, it is a multi-class problem. More comparisons between the hypothesis testing and NP problems can be found in Li and Tong (2020). And we will provide additional discussions in Section 3.5.

Previously, there have been few works on solving the NPMC problem. Landgrebe and Duin (2005) proposed a general empirical method to solve the NPMC problem, relying on the multi-class ROC estimation. Our work tackles the NPMC problem by connecting it with the cost-sensitive learning problem (to be introduced), which is motivated by their paper. However, there are some main differences between our work and theirs. First, their algorithm requires a grid search to find the proper cost parameters. When the class number $K$ is large and we want higher accuracy, the computation cost will be too high to be affordable. Despite the efficient multi-class ROC approximation via decomposition and sensitivity analysis proposed in Landgrebe and Duin (2008), it is still somewhat restrictive without a formal connection to a cost-sensitive learning problem. Our algorithms connect the NPMC problem to cost-sensitive learning by duality and search the optimal costs in cost-sensitive learning by a direct optimization procedure, which is much more straightforward than their method. Second, there is no theoretical guarantee on their approach, while we prove the multi-class NP oracle properties and strong consistency to hold for our methods under certain conditions. Recently, Ma et al. (2020) developed regularized sub-gradient method on non-convex optimization problems, which can be applied to solve the NPMC problem with specific linear classifiers with non-convex losses. Their method is only suitable for linear classifiers with certain loss functions, while our methods are ready to be applied to any classification method. To our knowledge, our work is the first to solve the NPMC problem via cost-sensitive learning techniques with theoretical guarantees.

1.3 Cost-sensitive Learning

As we mentioned in Section 1.1, cost-sensitive learning (CS) is another way of solving the problem of asymmetric errors in classification. There are two types of cost-sensitive learning problems where the cost is associated with features or classes, respectively (Fernández et al., 2018). Here we focus on the second type, where the cost is associated with different classes. Ling and Sheng (2008) further divided methods dealing with this type of CS problem into two categories: direct and meta-learning methods. Direct methods design the algorithm structure for some specific classifiers, e.g., support vector machines (Katsumata and Takeda, 2015), $k$-nearest neighbors (Qin et al., 2013), and neural networks (Zhou and Liu, 2005). Meta-learning methods create a wrapper that converts an existing classifier into a cost-sensitive one. Instances of this type of approach include rescaling (Domingos, 1999; Zhou and Liu, 2010), thresholding (Elkan, 2001; Sheng and Ling, 2006; Tian and Zhang, 2019), and weighted-likelihood methods (Domachowski et al., 2010), among others.

Similar to the multi-class NP problem, there are also two ways to formulate the multi-class CS problem. One is to consider the per-class error rates $P_{X|Y=k}(\phi(X) \neq k|Y=k)$ for $k = 1, \ldots, K$, and the other one is to consider the confusion matrix. In this paper, we would like to connect (2) to the following cost-sensitive (CS) multi-class classification problem

$$\min_{\phi} \text{Cost}(\phi) = \sum_{k=1}^{K} \pi_k^* c_k P_{X|Y=k}(\phi(X) \neq k),$$

(3)
where $\phi : \mathcal{X} \rightarrow \{1, \ldots, K\}$, $\pi_k^* = \mathbb{P}(Y = k)$, and $\{c_k\}_{k=1}^K$ are the costs associated with each class. The relationship between the NPMC problem with the confusion matrix control and the CS problem will be discussed in Section 4.

In the following lemma, we show that CS problem (3) has an explicit solution.

**Lemma 1** Define classifier $\tilde{\phi}^* : x \mapsto \arg \max_k \{c_k \mathbb{P}_{Y|X=x}(Y = k)\}$. Then $\tilde{\phi}^*$ is the optimal classifier of (3) in the following sense: For any classifier $\phi$, $\text{Cost}(\tilde{\phi}^*) \leq \text{Cost}(\phi)$.

1.4 Multi-class NP Oracle Properties and Strong Consistency

In this section, we extend the NP oracle inequalities and the consistency proposed in Scott and Nowak (2005) to the multi-class case for problem (2). We call them the multi-class NP oracle properties and strong consistency. Classifiers with these two properties satisfied are desirable. For any classifier $\phi$, we denote $R_k(\phi) = \mathbb{P}_{X|Y=k}(\phi(X) \neq k)$.

**Multi-class NP oracle properties for the NPMC problem:**

(i) If the NPMC problem is feasible and has an optimal solution $\phi^*$, then the algorithm outputs a solution $\hat{\phi}$ which satisfies

(a) $R_k(\hat{\phi}) \leq \alpha_k + O_p(\epsilon(n))$, $\forall k \in A$;
(b) $J(\hat{\phi}) \leq J(\phi^*) + O_p(\epsilon_J(n))$,

where $\epsilon(n)$ and $\epsilon_J(n) \to 0$ as $n \to \infty$.

(ii) Denote the event that the algorithm indicates infeasibility of NPMC problem given $\{(x_i, y_i)\}_{i=1}^n$ as $\mathcal{G}_n$. If the NPMC problem is infeasible, then $\mathbb{P}(\mathcal{G}_n) \to 1$, as $n \to \infty$.

**Strong consistency for the NPMC problem:**

(i) If the NPMC problem is feasible and has an optimal solution $\phi^*$, then the algorithm outputs a solution $\hat{\phi}$ which satisfies

(a) $\lim_{n \to \infty} R_k(\hat{\phi}) \leq \alpha_k$ a.s., $\forall k \in A$;
(b) $\lim_{n \to \infty} J(\hat{\phi}) = J(\phi^*)$ a.s..

(ii) Denote the event that the algorithm indicates infeasibility of NPMC problem given $\{(x_i, y_i)\}_{i=1}^n$ as $\mathcal{G}_n$. If the NPMC problem is infeasible, then $\mathbb{P}(\lim_{n \to \infty} \mathcal{G}_n) = 1$.

It is important to remark that multi-class NP oracle properties and strong consistency can only guarantee an “approximate” control for problem (2). So our goal is to obtain a classifier $\phi$ which can control $\mathbb{P}_{X|Y=k}(\phi(X) \neq k)$ around $\alpha_k$ for all $k \in A$.

1.5 Organization

We organize the remaining part of this paper as follows. In Section 2, we develop two algorithms to solve the NPMC problem (2), which are denoted as NPMC-CX (ConveX) and NPMC-ER (Empirical Risk), respectively. In Section 3, we show that NPMC-CX enjoys multi-class NP oracle properties and strong consistency under parametric models, and NPMC-ER satisfies multi-class NP oracle properties under a broader class of models,
as long as the model can fit the data well enough. Section 4 discusses how the two proposed algorithms can be extended to solve the confusion matrix control problem. We demonstrate that our approaches are effective via simulations and real data experiments in Section 5. Section 6 summarizes our contributions and points out a few potential future research directions. All the proofs are relegated to the appendix.

1.6 Notations
Before closing the introduction part, we summarize the notations used throughout this paper. For any set $D$, $|D|$ represents its cardinality. For any real number $a$, $|a|$ denotes the maximum integer no larger than $a$. Define the non-negative half space in $\mathbb{R}^p$ as $\mathbb{R}_+^p = \{ \mathbf{x} = (x_1, \ldots, x_p)^T \in \mathbb{R}^p : \min_j x_j \geq 0 \}$. For a $p$-dimensional vector $\mathbf{x} = (x_1, \ldots, x_p)^T$, its $\ell_2$-norm is defined as $\| \mathbf{x} \|_2 = \sqrt{\sum_{j=1}^{p} x_j^2}$. For a $p \times p$ matrix $A$, $\lambda_{\max}(A)$ and $\lambda_{\min}(A)$ represent its maximum and minimum eigenvalues, respectively. We mean $A$ is positive-definite or negative-definite by writing $A \succ 0$ or $A \prec 0$, respectively. For a function $f : \mathcal{X} \rightarrow \mathbb{R}$ where $\mathcal{X}$ is some metric space, we define its sup-norm as $\|f\|_\infty = \sup_{x \in \mathcal{X}} |f(x)|$. For the empty set $\emptyset$, we define $\min_{x \in \emptyset} f(x) = +\infty$. For two non-zero real sequences $\{a_n\}_{n=1}^{\infty}$ and $\{b_n\}_{n=1}^{\infty}$, we denote $\sup_n |a_n/b_n| < \infty$ by $a_n \lesssim b_n$. For two random sequences $\{a_n\}_{n=1}^{\infty}$ and $\{b_n\}_{n=1}^{\infty}$, $a_n = \mathcal{O}_p(b_n)$ indicates that for any $\epsilon > 0$, there exists a positive constant $M$ such that $\sup_n \mathbb{P}(|a_n/b_n| > M) \leq \epsilon$. We use $\mathbb{P}$ and $\mathbb{E}$ to represent probabilities and expectations. Sometimes we add subscripts to emphasize the source of randomness. For example, $\mathbb{P}_{Y|X=x}(Y = k)$ means the probability that $Y = k$ given $X = x$. $\mathbb{E}_X$ means the expectation is taken w.r.t. the distribution of $X$. If there is no subscript, we mean the probability and expectation are calculated w.r.t. all randomness.

2. Methodology
2.1 The First Algorithm: NPMC-CX
Before formally introducing our first algorithm, we would like to derive it through heuristic calculations. For problem (2), consider its Lagrangian form as

$$F_{\lambda}(\phi) = \sum_{k \notin A} w_k \mathbb{P}_{X|Y=k}(\phi(X) \neq k) + \sum_{k \in A} (w_k + \lambda_k) \mathbb{P}_{X|Y=k}(\phi(X) \neq k) - \sum_{k \in A} \lambda_k \alpha_k$$

$$= -\sum_{k \notin A} w_k \mathbb{P}_{X|Y=k}(\phi(X) = k) - \sum_{k \in A} (w_k + \lambda_k) \mathbb{P}_{X|Y=k}(\phi(X) = k) + \sum_{k=1}^{K} w_k + \sum_{k \in A} \lambda_k (1 - \alpha_k),$$

(4)

where $\lambda = \{\lambda_k\}_{k \in A}$. Then, the dual problem of (2) can be written as

$$\max_{\lambda \in \mathbb{R}_+^{|A|}} \min_{\phi} F_{\lambda}(\phi).$$

(5)

We can see that (5) looks for a lower bound of the objective function in (2), i.e., $\max_{\lambda \in \mathbb{R}_+^{|A|}} \min_{\phi} F_{\lambda}(\phi) \leq \min_{\phi \in \mathcal{C}} \sum_{k=1}^{K} w_k \mathbb{P}_{X|Y=k}(\phi(X) \neq k)$, where $\mathcal{C}$ includes all feasible classifiers for problem (2).

We often call this fact as weak duality. In many cases, the exact equality holds, which is
called \textit{strong duality}. Under strong duality, (2) and (5) can be seen as two different ways to tackle the same problem. If one has an optimal solution, the other one has an optimal solution as well. If the original NPMC problem (2) is infeasible, then (5) must be unbounded above. If (5) is unbounded above, the NPMC problem (2) must be infeasible. Another key finding is, for given $\lambda \in \mathbb{R}_+|A|$, looking for $\phi$ that minimizes $F_\lambda(\phi)$ in (4) is actually a CS problem (3), by defining

$$c_k(\lambda, \pi^*) = \begin{cases} w_k/\pi^*_k, & k \notin A; \\ (w_k + \lambda_k)/\pi^*_k, & k \in A. \end{cases}$$

This motivates our first algorithm, where we try to solve the more trackable CS problem (5) for solving the more challenging original problem (2).

To derive our first algorithm, let’s rewrite (4) as

$$F_\lambda(\phi) = -\mathbb{E}_X \left[ c_{\phi(X)}(\lambda, \pi^*) \cdot \mathbb{P}_{Y|X}(Y = \phi(X)) \right] + \sum_{k=1}^K w_k + \sum_{k \in A} \lambda_k (1 - \alpha_k).$$

Then by Lemma 1, we can define

$$\phi^*_\lambda : x \mapsto \arg \max_k \{ c_k(\lambda, \pi^*) \mathbb{P}_{Y|X}(Y = k) \} \in \arg \min_\phi F_\lambda(\phi), \quad (6)$$

$$G(\lambda) = \min_\phi F_\lambda(\phi) = F_\lambda(\phi^*_\lambda). \quad (7)$$

Therefore, on the population level, we can find $\lambda$ which maximizes $G(\lambda)$, then plug $\lambda$ in (6) to obtain the final classifier. On the other hand, due to weak duality, since the objective function in (2) is no larger than 1 when it’s feasible, we must have $\max_{\lambda \in \mathbb{R}_+|A|} G(\lambda) \leq 1$. Thus, if $\max_{\lambda \in \mathbb{R}_+|A|} G(\lambda) > 1$, the original NP problem (2) must be infeasible.

In practice, there is no access to $F_\lambda(\phi)$ and $G(\lambda)$ since we do not know the true model. We estimate $F_\lambda(\phi)$ by training data as

$$\hat{F}^{CX}_\lambda(\phi) = \frac{1}{n} \sum_{i=1}^n c_{\phi(x_i)}(\lambda, \hat{\pi}) \hat{\mathbb{P}}_{Y|X=x_i}(Y = \phi(x_i)) + \sum_{k=1}^K w_k + \sum_{k \in A} \lambda_k (1 - \alpha_k), \quad (8)$$

where

$$c_k(\lambda, \pi) = \begin{cases} w_k/\hat{\pi}_k, & k \notin A; \\ (w_k + \lambda_k)/\hat{\pi}_k, & k \in A, \end{cases}$$

and $\hat{\mathbb{P}}_{Y|X}$ is the estimated conditional probability. $\hat{\mathbb{P}}_{Y|X}$ can be obtained by fitting different models on the data, and we do not impose any conditions on it here. Here are two examples.

- For a parametric example, we may use the data to fit a multinomial logistic regression model and get the estimates of $(K-1)$ contrast coefficients $\hat{\beta}^{(k)} \in \mathbb{R}^p$. Then

$$\hat{\mathbb{P}}_{Y|X=x}(Y = k) = \frac{\exp(x^T \hat{\beta}^{(k)})}{\sum_{k'=1}^K \exp(x^T \hat{\beta}^{(k')})}$$

where $\hat{\beta}^{(K)} = 0_p$.  


For a non-parametric example, we may use the k-nearest neighbors (kNN) to obtain the estimate \( \hat{P}_{Y|X=x} \). Given such an \( x \) and the number of the nearest neighbors \( k_0 \), we can use the proportion of training observations of class \( k \) among \( k_0 \) nearest neighbors to \( x \) as an estimate \( \hat{P}_{Y|X=x}(Y = k) \). The marginal distribution of \( Y \) is estimated by the sample proportion \( \hat{\pi}_k = n_k/n \), \( n_k = \#\{i : y_i = k\} \) and \( \hat{\pi} = \{\hat{\pi}_k\}_k^{K_}\).

Similar to Lemma 1, it is easy to show that the optimal classifier that minimizes \( \tilde{F}_{\lambda}^{CX}(\phi) \) for given \( \lambda \) is
\[
\hat{\phi}_\lambda : x \mapsto \arg \max_k \{c_k(\lambda, \hat{\pi})\hat{P}_{Y|X=x}(Y = k)\} \in \arg \min_{\phi} \tilde{F}_{\lambda}^{CX}(\phi). \tag{9}
\]

Denote
\[
\tilde{G}^{CX}(\lambda) := \tilde{G}^{CX}(\lambda; \hat{P}_{Y|X}, \hat{\pi}) = \min_{\phi} \tilde{F}_{\lambda}^{CX}(\phi) = \tilde{F}_{\lambda}^{CX}(\hat{\phi}_\lambda), \tag{10}
\]
which is a well-defined function of \( \lambda \) given \( \hat{P}_{Y|X} \) and \( \hat{\pi} \). Similar to (5), we solve
\[
\max_{\lambda \in \mathbb{R}^{|A|}_+} \min_{\phi} \tilde{F}_{\lambda}^{CX}(\phi) = \max_{\lambda \in \mathbb{R}^{|A|}_+} \tilde{F}_{\lambda}^{CX}(\hat{\phi}_\lambda) = \max_{\lambda \in \mathbb{R}^{|A|}_+} \tilde{G}^{CX}(\lambda) \tag{11}
\]
to find solution \( \hat{\lambda} \), then plug it in (9) to obtain the final solution \( \hat{\phi}_\lambda \) to the original NPMC problem (2). On the other hand, considering the estimation error, if \( \max_{\lambda \in \mathbb{R}^{|A|}_+} \tilde{G}^{CX}(\lambda) > 1 \), then we conclude that the NPMC problem (2) is infeasible.

\begin{algorithm}
\caption{NPMC-CX}
\begin{algorithmic}[1]
\Input training data \( \{(x_i, y_i)\}_{i=1}^n \), target upper bounds of errors \( \alpha \), the weighting vector of objective function \( w \), the classification method \( M \) to estimate \( P_{Y|X} \)
\Output the fitted classifier \( \hat{\phi} \) or an error message
1 \( \hat{P}_{Y|X}, \hat{\pi} \leftarrow \) the estimates of \( P_{Y|X} \) (through \( M \)) and \( \pi^* \) on training data \( \{(x_i, y_i)\}_{i=1}^n \)
2 \( \hat{\lambda} \leftarrow \arg \max_{\lambda \in \mathbb{R}^{|A|}_+} \tilde{G}^{CX}(\lambda; \hat{P}_{Y|X}, \hat{\pi}) \) \tag{12}
3 \textbf{if} \( \tilde{G}^{CX}(\hat{\lambda}) \leq 1 \) \textbf{then}
4 \hspace{1em} \text{Report the NP problem as feasible and output the solution}
5 \hspace{2em} \hat{\phi}(x) = \arg \max_k \{c_k(\hat{\lambda}, \hat{\pi})\hat{P}_{Y|X=x}(Y = k)\}
6 \hspace{1em} \textbf{else}
7 \hspace{2em} \text{Report the NP problem as infeasible}
\end{algorithmic}
\end{algorithm}

Note that \( \tilde{G}^{CX}(\lambda) \) is a concave function (as we will show in Proposition 4), which implies that the optimization problem (12) is convex. Therefore we call the algorithm above NPMC-CX, which is summarized as Algorithm 1. It can be further seen that \( \tilde{G}^{CX}(\lambda) \) is also a piecewise linear function on \( \mathbb{R}^{|A|}_+ \). In practice, despite the concavity of \( \tilde{G}^{CX}(\lambda) \), the common convex optimization methods are difficult to use due to the difficulty in calculating the gradient of \( \tilde{G}^{CX}(\lambda) \) w.r.t. \( \lambda \). Instead, we implement the optimization step via direct search methods like the Hooke-Jeeves method (Hooke and Jeeves, 1961) and Nelder-Mead
method (Nelder and Mead, 1965). More implementation details will be described in Section 5.

2.2 The Second Algorithm: NPMC-ER

In Section 2.1, we came up with an estimator (8) for the Lagrangian function (4). In the literature on NP classification, a more popular estimator is built via empirical error rates on a separate data set (Landgrebe and Duin, 2005; Tong, 2013). In this section, we will develop a new algorithm, NPMC-ER, relying on a different estimator for (4) based on empirical error rates. We will compare NPMC-CX and NPMC-ER both theoretically (Section 3) and empirically (Section 5). Some take-home messages will be summarized in Section 6.

For convenience, throughout this section, we assume the training sample size to be 2n. Consider the following procedure. First, we divide the training data randomly into two parts of size n. For simplicity, denote them as \( D_1 = \{(x_i, y_i)\}_{i=1}^n \) and \( D_2 = \{(x_i, y_i)\}_{i=n+1}^{2n} \). \( D_1 \) will be used to calculate the value of \( \hat{F}^\text{ER}_\lambda (\phi) \) (to be defined), and \( D_2 \) will be used to estimate \( \hat{P}_{Y|X} \) and \( \hat{\pi} \). We estimate (4) on \( D_1 = \{(x_i, y_i)\}_{i=1}^n = \{(x_i^{(k)}, y_i^{(k)})\}_{i=1}^{n_k} \}_{k=1}^K \) by

\[
\hat{F}^\text{ER}_\lambda (\phi) = - \sum_{k \in A} w_k \cdot \frac{1}{n_k} \sum_{i=1}^{n_k} \mathbb{1}(\phi(x_i^{(k)}) = k) - \sum_{k \in A} (w_k + \lambda_k) \cdot \frac{1}{n_k} \sum_{i=1}^{n_k} \mathbb{1}(\phi(x_i^{(k)}) = k) \\
+ \sum_{k=1}^K w_k + \sum_{k \in A} \lambda_k (1 - \alpha_k),
\]

(13)

where \( \{(x_i^{(k)}, y_i^{(k)})\}_{i=1}^{n_k} \) are the observations from class \( k \) in \( D_1 \). Then similar to (11), we solve

\[
\hat{\lambda} \in \arg \max_{\lambda \in \mathbb{R}^{|A|}} \hat{F}^\text{ER}_\lambda (\phi_{\hat{\lambda}}),
\]

where \( \phi_{\hat{\lambda}} \) is defined as in (9) while \( \hat{P}_{Y|X} \) and \( \hat{\pi} \) are calculated by data in \( D_2 \). Define

\[
\hat{G}^\text{ER}(\lambda) := \hat{G}^\text{ER}(\lambda, \hat{P}_{Y|X}, \hat{\pi}) = \hat{F}^\text{ER}_\lambda (\phi_{\hat{\lambda}}).
\]

(14)

Note that in NPMC-CX, given any \( \lambda, \phi_{\hat{\lambda}} \) is a minimizer of \( \hat{F}^\text{CX}_\lambda (\phi) \) w.r.t. any classifier \( \phi \). In this case, for NPMC-ER, given \( \lambda \), we still define \( \phi_{\hat{\lambda}} \) as in (9), which is not necessarily a minimizer of \( \hat{F}^\text{ER}_\lambda (\phi) \), and \( \hat{G}^\text{ER}(\lambda) \) is not equal to \( \max_{\lambda \in \mathbb{R}^{|A|}} \min_{\phi} \hat{F}^\text{ER}_\lambda (\phi) \). The remaining steps are the same as NPMC-CX.

The reason we do not define \( \phi_{\hat{\lambda}} \) as \( \arg \min_{\phi} \hat{F}^\text{ER}_\lambda (\phi) \) is that there might be many (even infinite) minimizers, which can make the estimated model very unstable. The problem often appears when fitting models via minimizing the training error. For example, rescaling all

1. Here we randomly divide the whole data for simplicity. In practice, we recommend dividing data by class, i.e., randomly dividing samples of each class into two halves to construct \( D_1 \) and \( D_2 \). In numerical studies, we used the per-class division paradigm, which can help avoid the case that no data is sampled from specific classes when the samples from different classes are highly imbalanced. This does not affect our theoretical results.

2. This \( \hat{\lambda} \) is different from the \( \hat{\lambda} \) estimated in NPMC-CX. We ignore the superscript for simplicity.
coefficients components in logistic regression does not change the classification results and error rates.

Algorithm 2: NPMC-ER

**Input:** training data \(\{(x_i, y_i)\}_{i=1}^{2n}\), target upper bound of errors \(\alpha\), the weighting vector of objective function \(w\), a search range \(R > 0\), the classification method \(M\) to estimate \(\hat{P}_{Y|X}\)

**Output:** the fitted classifier \(\hat{\phi}\) or an error message

1. Randomly divide the whole training data (and reindex them) into \(D_1 \cup D_2 = \{(x_i, y_i)\}_{i=1}^{n} \cup \{(x_i, y_i)\}_{i=n+1}^{2n}\)
2. \(\hat{P}_{Y|X}, \hat{\pi} \leftarrow \) the estimates of \(\hat{P}_{Y|X}\) (through \(M\)) and \(\pi^*\) on \(D_2 = \{(x_i, y_i)\}_{i=n+1}^{2n}\)
3. \(\hat{\lambda} \leftarrow \arg \max_{\lambda \in \mathbb{R}_+^{|A|}, \|\lambda\|_{\infty} \leq R} \hat{G}_{ER}(\lambda; \hat{P}_{Y|X}, \hat{\pi})\), where \(\hat{G}_{ER}\) is estimated on \(D_1 = \{(x_i, y_i)\}_{i=1}^{n}\) (15)
4. **if** \(\hat{G}_{ER}(\hat{\lambda}) \leq 1\) **then**
   5. Report the NP problem as feasible and output the solution
   6. \(\phi(x) = \arg \max_k \{c_k(\hat{\lambda}, \hat{\pi})\hat{P}_{Y|X=x}(Y = k)\}\)
5. **else**
6. Report the NP problem as infeasible
7. **end**

We name the second algorithm NPMC-ER because it uses the empirical error to estimate the true error rate, and we summarize it as Algorithm 2. Similar to \(\hat{G}_{ER}(\lambda)\) defined in (10), \(\hat{G}_{ER}(\lambda)\) in (14) is also a piecewise linear function of \(\lambda\). However, it is not necessarily concave. Similar to NPMC-CX, we use the direct search method to conduct the optimization step (15) in practice. Note that since \(\hat{G}_{ER}(\lambda)\) is not necessarily concave, for technical reasons, we need to restrict the search range of the best \(\lambda\) to a bounded region. Hence compared to NPMC-CX (Algorithm 1), there is an additional argument representing the search range \(R\) in NPMC-ER (Algorithm 2). The condition on \(R\) in the theoretical analysis will be described in the next section. The empirical results are not very sensitive to the choice of \(R\), and we pick \(R = 200\) in numerical studies.

3. Theory

In this section, we will unveil the theoretical properties of the two algorithms proposed in Section 2. In Sections 3.1 and 3.2, we present the theory for NPMC-CX and NPMC-ER, respectively. In Section 3.3, we offer more discussions on the assumptions made in Sections 3.1 and 3.2. We will verify most assumptions when the logistic regression model is used as the classification method in both algorithms. In Section 3.4, the two algorithms are compared from the theoretical perspective. Lastly, in Section 3.5 after being exposed to the theory, we continue the discussion on the NPMC problem (2), which includes the connection between the hypothesis testing and NPMC problems, feasibility, and the randomization.
3.1 Analysis on NPMC-CX

In this section, suppose we estimate $P_{Y|X=x}(Y = k)$ with a parametric model where the estimated value is determined by a parameter vector $\beta \in B \subseteq \mathbb{R}^p$ and predictor $x$, where $B$ is a compact set and $p$ is fixed. Note that the value $\beta$ and its dimension $p$ do not necessarily correspond to the true model, and we do not require the true model is parametric.

As we did in the heuristic arguments in Section 2.1, the strong duality between the original NPMC problem (2) and the dual problem (5) is necessary for the algorithm to make sense. Therefore, we impose the strong duality.

**Assumption 1 (Strong duality for the NPMC problem)** It holds that

$$\min_{\phi \in \mathcal{C}} J(\phi) = \max_{\lambda \in \mathbb{R}^{|A|}} G(\lambda),$$

where $\mathcal{C}$ includes all feasible classifiers for the NPMC problem (2).

**Remark 2** Like the standard results in convex optimization problems, the strong duality implies complementary slackness. That is, when the NPMC problem (2) is feasible, for $\lambda^* = \arg \max_{\lambda \in \mathbb{R}^{|A|}} G(\lambda)$, any NP optimal solution $\phi^*$, and all $k \in A$, we have $R_k(\phi^*) - \alpha_k = 0$.

There are many sufficient conditions for strong duality in literature, e.g., Slater’s condition (Boyd and Vandenberghe, 2004). However, most of them only work for convex problems, while the original NPMC problem (2) is not necessary to be convex. The following theorem reveals that for the induced classifier from the dual CS problem (5), there is a tight relationship between its feasibility and the strong duality in the NPMC problem (2).

**Theorem 3 (Sufficient and necessary conditions for NPMC strong duality)** Suppose $X|Y = k$ are continuous random variables for all $k$’s.

(i) When the NPMC problem (2) is feasible, the strong duality holds if and only if there exists $\lambda^{(0)} = \{\lambda^{(0)}_k\}_{k \in A}$ such that $\phi^{(0)}_\lambda$ is feasible for the NPMC problem (2), i.e., $P_{X|Y=k}(\phi^{(0)}_\lambda(X) \neq k) \leq \alpha_k$ for all $k \in A$.

(ii) Suppose $P_{Y|X=x}(Y = k) \geq a > 0$ a.s. (w.r.t. the distribution of $X$) for all $k \in A$. When the NPMC problem (2) is infeasible, the strong duality holds (i.e., $\max_{\lambda \in \mathbb{R}^{|A|}} G(\lambda)$ is unbounded from above) if and only if for an arbitrary $\lambda \in \mathbb{R}^{|A|}$, $\phi^*_\lambda$ is infeasible for NPMC problem (2), i.e., $\exists$ at least one $k \in A$ such that $P_{X|Y=k}(\phi^*_\lambda(X) \neq k) > \alpha_k$.

It is well-known that no matter what the primal problem is, the Lagrangian dual function is always a concave one (Boyd and Vandenberghe, 2004), implying that $G(\lambda)$ in (7) is concave w.r.t. $\lambda$. For NPMC-CX, the empirical version $\hat{G}(\lambda)$ in (10) is a concave function as well, which makes (12) a convex optimization problem.

---

3. In $\mathbb{R}^p$ space with Euclidean distance, $B$ has to be bounded. There might be some ways of compactification to make our arguments work for unbounded $B$. For simplicity, we do not dive into the details and assume $B$ is compact in $\mathbb{R}^p$. Some compactification arguments and examples can be found in Wald (1949) and Chapter 2 of Pollard (2000).
Proposition 4 \(G(\lambda)\) and \(\tilde{G}^{CX}(\lambda)\) are concave and continuous on \(\mathbb{R}^{|A|}_+\).

To prove the NP oracle properties of NPMC-CX, we first impose the following assumptions.

**Assumption 2** \[\max_k E[\tilde{P}_{Y|X}(Y = k) - P_{Y|X}(Y = k)] \to 0 \text{ as } n \to \infty.\]

**Assumption 3** \(G(\lambda)\) is continuously twice-differentiable at \(\lambda^*\) and \(\nabla^2 G(\lambda^*) \prec 0\), where \(\lambda^* = \arg \max G(\lambda)\).

**Assumption 4** For almost all \(x\) (w.r.t. the distribution of \(X\)), the estimated conditional probability \(P_{Y|X=x}(Y = k; \beta)\) is a continuous function of coefficient \(\beta\).

**Assumption 5** Denote \(\varphi_k(x) = c_k(\lambda^*, \pi^*)P_{Y|X=x}(Y = k) - \max_{j \neq k} \{c_j(\lambda^*, \pi^*)P_{Y|X=x}(Y = j)\}\), where \(\lambda^* = \arg \max G(\lambda)\). It holds
\[
\max_{k=1:K} P_{X|Y=k}(|\varphi_k(X)| \leq t) \lesssim t^\gamma,
\]
with some \(\gamma > 0\) and a non-negative \(t\) smaller than some constant \(C \in (0, 1)\).

**Remark 5** Assumption 2 guarantees that the conditional probability can be accurately estimated. Assumption 3 is motivated by the second-order information condition used in proving MLE consistency (Wald, 1949; Van der Vaart, 2000). Assumption 5 is often called the “margin condition” in literature (Mammen and Tsybakov, 1999; Tong, 2013; Zhao et al., 2016), and it requires most data to be away from the optimal decision boundary. In many cases, it can be used to prove a faster convergence rate than \(O_p(n^{-1/2})\). In the previous binary NP classification papers like Tong (2013), Zhao et al. (2016) and Tong et al. (2020), it is not required if we are satisfied with arbitrary convergence rates. Besides, it is often imposed together with an opposite condition called “detection condition” (Tong, 2013; Zhao et al., 2016; Tong et al., 2020), which helps to estimate the optimal classification threshold accurately. Here we do not need such a detection condition, but Assumption 5 is required to hold.

Next, we show that NPMC-CX satisfies the multi-class NP oracle properties given the conditions above.

**Theorem 6 (Multi-class NP oracle properties of NPMC-CX)** NPMC-CX satisfies multi-class NP oracle properties in the following senses.

(i) When the NPMC problem (2) is feasible, if Assumptions 1-5 hold, then there exist a solution \(\phi^*\) and a constant \(C > 0\) such that
\[
\max_k P(|R_k(\tilde{\phi}) - R_k(\phi^*)| > \delta) \lesssim \exp\{-Cn\delta^{4/\gamma}\} + \delta^{-2(1+\gamma)/\gamma} \max_k E\left|\tilde{P}_{Y|X}(Y = k) - P_{Y|X}(Y = k)\right|,
\]
for any \(\delta \in (0, 1)\).
When the NPMC problem (2) is infeasible, if Assumptions 1, 2 and 4 hold, then there exists a constant $C > 0$ such that
\[
\mathbb{P}\left( |\tilde{G}^{CX}(\lambda)| \leq 1 \right) \leq \exp\{-Cn\} + \max_{k} \mathbb{E}\left| \hat{P}_{Y|X}(Y = k) - P_{Y|X}(Y = k) \right|.
\]

Remark 7 Notice that $J(\hat{\phi}) - J(\phi^*)$ is a linear combination of $\{R_k(\hat{\phi}) - R_k(\phi^*)\}_{k=1}^{K}$. Therefore, when the NPMC problem (2) is feasible, $R_k(\hat{\phi}) - \alpha_k \leq R_k(\hat{\phi}) - R_k(\phi^*) \leq O_p(\epsilon(n))$, $\forall k \in \mathcal{A}$.

Assumption 2’ \begin{align*}
\lim_{n \to \infty} \hat{P}_{Y|X = x}(Y = k) &= P_{Y|X = x}(Y = k) \ \text{a.s. (w.r.t. the training data } \{(x_i, y_i)\}_{i=1}^{n}) \ \text{for almost everywhere } x (\text{w.r.t. the distribution of } X), \ \text{for all } k.
\end{align*}

Theorem 8 (Strong consistency of NPMC-CX) NPMC-CX satisfies strong consistency in the following senses.

(i) When the NPMC problem (2) is feasible, if Assumptions 1, 2’, 3 and 4 hold, then there exists a solution $\phi^*$, such that $\lim_{n \to \infty} R_k(\hat{\phi}) = R_k(\phi^*)$ a.s. for all $k$’s. And if $\mathbb{P}(\hat{\lambda}_k > \delta_n) \to 1$ for any vanishing sequence $\{\delta_n\}_{n=1}^{\infty} \to 0$, then $R_k(\phi^*) = \alpha_k$.

(ii) When the NPMC problem (2) is infeasible, if Assumptions 1, 2’ and 4 hold, then for any $M > 0$, $\lim_{n \to \infty} \hat{G}^{CX}(\lambda) > M$ a.s..

3.2 Analysis on NPMC-ER

One advantage of NPMC-ER over NPMC-CX is that we do not require $\hat{P}_{Y|X = x}(Y = k)$ to be parametric.

Unlike NPMC-CX, for NPMC-ER, the empirical dual function $\tilde{G}(\lambda)$ in (14) is not necessarily concave. This is caused by the “mismatch” of $\tilde{F}_\lambda(\phi)$ and $\tilde{\phi}_\lambda$. Indeed, as mentioned in Section 2.2, $\tilde{\phi}_\lambda$ is not necessarily a minimizer of $\tilde{F}_\lambda(\phi)$, which makes the dual function not a “max-min” type of function and unnecessarily concave. Despite this, the multi-class NP oracle properties still hold under similar conditions.

Theorem 9 (Multi-class NP oracle properties of NPMC-ER) NPMC-ER satisfies multi-class NP oracle properties in the following senses.

(i) When the NPMC problem (2) is feasible, if Assumptions 1, 2, 3 and 5 hold, and $R$ is sufficiently large $^4$, then there exist a solution $\phi^*$ and some constants $C, C' > 0$ such that

\[
\mathbb{P}\left( |\tilde{G}^{CX}(\lambda)| \leq 1 \right) \leq \exp\{-Cn\} + \max_{k} \mathbb{E}\left| \hat{P}_{Y|X}(Y = k) - P_{Y|X}(Y = k) \right|.
\]

\[
\epsilon(n) = n^{-5/4} + \left( \max_k \mathbb{E}\left| \hat{P}_{Y|X}(Y = k) - P_{Y|X}(Y = k) \right| \right)^{\gamma/(2\gamma(1+\gamma))} \to 0.
\]

\[
\text{Theorem 6 verifies multi-class NP oracle properties as we defined in Section 1.4.}
\]

Besides the NP oracle properties, by imposing a stronger almost sure version of Assumption 2, we can get strong consistency for NPMC-CX.

Assumption 2’ \begin{align*}
\lim_{n \to \infty} \hat{P}_{Y|X = x}(Y = k) &= P_{Y|X = x}(Y = k) \ \text{a.s. (w.r.t. the training data } \{(x_i, y_i)\}_{i=1}^{n}) \ \text{for almost everywhere } x (\text{w.r.t. the distribution of } X), \ \text{for all } k.
\end{align*}

4. Here our results hold when $R \geq \|\lambda^*\|_{\infty}$, where $\lambda^* = \arg \max G(\lambda)$.
that

$$\max_k \mathbb{P}(|R_k(\hat{\phi}) - R_k(\phi^*)| > \delta) \lesssim \exp\{-Cn\delta^{4/\gamma}\} + \delta^{-2^{\gamma}(1+\gamma)/\gamma} \max_k \mathbb{E}\left[|\hat{P}_{Y\mid X}(Y = k) - P_{Y\mid X}(Y = k)|\right],$$

for any $\delta \in [C'n^{-5/4}, 1]$.

(ii) When the NPMC problem (2) is infeasible, if Assumptions 1 and 2 hold, and $R$ is sufficiently large \(^5\), then there exists a constant $C > 0$ such that

$$\mathbb{P}\left(|\hat{G}^{ER}(\lambda)| \leq 1\right) \lesssim \exp\{-Cn\} + \max_k \mathbb{E}\left[|\hat{P}_{Y\mid X}(Y = k) - P_{Y\mid X}(Y = k)|\right].$$

Analyzing in the same way as in Remark 7, we know that Theorem 9 verifies multi-class NP oracle properties of NPMC-ER.

### 3.3 Discussions on Assumptions

In the previous two subsections, we impose a series of assumptions to show the NP oracle properties and strong consistency. Among these conditions, Assumption 1 is central and necessary to make the whole argument work. In general, since the original NPMC problem is not necessarily convex, it is challenging to demonstrate the strong duality. Theorem 3 connects the strong duality with the feasibility of solutions to the CS problem under the NPMC problem, making the strong duality condition more explicit and transparent. Assumption 2 requires the estimate $\hat{P}_{Y\mid X}$ to be close to the true conditional probability $P_{Y\mid X}$, which is often trivial to hold when the estimator is constructed with the knowledge of the true model. Assumption 4 requires the continuity of conditional probability estimator w.r.t. the coefficient.

Among these assumptions, Assumption 1 is generally hard to check. Nevertheless, thanks to Theorem 3, we might be able to demonstrate the strong duality in practice by checking the feasibility of CS solutions in the NPMC problem. Due to the space limit, we do not discuss this part in detail and leave it for future study. Assumptions 2, 2', 3, 4, and 5 can be checked given the estimated model and the underlying true model. Next, we verify them under the multinomial logistic regression model as an example.

Suppose the true conditional distribution of $Y$ given $X = \mathbf{x}$ is $P_{Y\mid X}(Y = k) = \frac{\exp((\beta_k^T\mathbf{x}))}{\sum_{j=1}^{K} \exp((\beta_j^T\mathbf{x}))}$, where $k = 1, \ldots, K$, $\beta_j^* \in \mathbb{R}^p$ and $\beta_K^* = 0$. And we estimate it by $\hat{P}_{Y\mid X}(Y = k) = \frac{\exp(\hat{\beta}_k^T\mathbf{x})}{\sum_{j=1}^{K} \exp(\hat{\beta}_j^T\mathbf{x})}$. Denote $\hat{\beta} = (\hat{\beta}_1, \ldots, \hat{\beta}_{K-1})$, which is the maximum likelihood estimator (MLE). In addition, suppose $X$ has bounded and continuously differentiable density function $f_X$ in $\mathbb{R}^p$, i.e. $f_X'$ is continuous and $\|f_X\|_\infty < \infty$.

- First let’s check Assumption 2 and 2'. By similar arguments in Wald (1949), we can prove the MLE $\hat{\beta}$ is strongly consistent to $\beta$, i.e. \(\lim_{n \to \infty} \hat{\beta} = \beta^*\) a.s., which verifies Assumption 2'. Then for any $\mathbf{x} \in \mathbb{R}^p$, \(\lim_{n \to \infty} \hat{P}_{Y\mid X = \mathbf{x}}(Y = k) = P_{Y\mid X = \mathbf{x}}(Y = k)\) a.s.. Then by dominated convergence theorem, \(\lim_{n \to \infty} \mathbb{E}_X[|\bar{P}_{Y\mid X}(Y = k) - \hat{P}_{Y\mid X}(Y = k)|]\)

---

\(^5\) Due to Assumption 1, $\sup_{\lambda \in \mathbb{R}^p} G(\lambda) = +\infty$. Here our results hold when $R$ satisfies $\sup_{\|\lambda\|_\infty \leq R} G(\lambda) > 1 + \vartheta$ for at least one $\vartheta > 0$. 

---
Next let’s verify the first part of Assumption 3, i.e. \( G(\lambda) \) is continuously twice differentiable. Denote the conditional density of \( G \) is continuous for any \( k \). We can show the twice continuous differentiability at any \( k \) with all \( \lambda_k > 0 \). To see this, consider \( \beta_j = -\beta_j^* + \beta_k^* \) for \( j \in \{1, \ldots, K\} \setminus \{k\} \), and we construct \( \{\beta_j\}_{j=k,K+1,\ldots,p} \) to be linearly independent of \( \{\beta_j\}_{j \in \{1, \ldots, K\}} \). Let \( \tilde{Z} = (\tilde{Z}_1 = \beta_1, \ldots, \tilde{Z}_p) \) for simplicity, we consider the case \( \{\beta_j\}_{j \in \{1, \ldots, K\}} \). By dominated convergence theorem, \( f_S(z) \) is continuously differentiable w.r.t. \( z \in \mathbb{R}^p \). Denote \( Z = (Z_1, \ldots, Z_{K-1}) = (\tilde{Z}_1, \ldots, \tilde{Z}_{k-1}, \tilde{Z}_{k+1}, \ldots, \tilde{Z}_K) \in \mathbb{R}^{K-1} \), which has the density \( f_Z(z) \). By dominated convergence theorem, \( f_Z(z) \) is continuously differentiable w.r.t. \( z \in \mathbb{R}^{K-1} \). Therefore,

\[
\mathbb{P}_{X|Y=k}(\phi_{X}(X) = k) = \mathbb{P}_{X|Y=k} \left( c_k(\lambda_k, \pi_k^*) \cdot \mathbb{P}_{Y|X=x}(Y = k) > \max_{j \neq k} \left[ c_j(\lambda_j, \pi_j^*) \cdot \mathbb{P}_{Y|X=x}(Y = j) \right] \right) \\
= \mathbb{P}_{X|Y=k} \left( c_k(\lambda_k, \pi_k^*) > \max_{j \neq k} \left[ c_j(\lambda_j, \pi_j^*) \cdot \exp\{\tilde{\beta}_{j}^T X\} \right] \right) \\
= \mathbb{P}_{X|Y=k} \left( \log c_k(\lambda_k, \pi_k^*) > \max_{j \neq k} \left[ \log c_j(\lambda_j, \pi_j^*) + \tilde{\beta}_{j}^T X \right] \right) \\
= \mathbb{P}_{X|Y=k} \left( \bigcap_{j \neq k} \left\{ \tilde{\beta}_{j}^T X < \log c_k(\lambda_k, \pi_k^*) - \log c_j(\lambda_j, \pi_j^*) \right\} \right) \\
= \mathbb{P}(Z_1 < z_1, \ldots, Z_{K-1} < z_{k-1}),
\]

where \( z_j(\lambda_k, \lambda_j) = \log c_k(\lambda_k, \pi_k^*) - \log c_j(\lambda_j, \pi_j^*) \) when \( j < k \), and \( z_j = \log c_k(\lambda_k, \pi_k^*) - \log c_j(\lambda_j, \pi_j^*) \) when \( j \geq k \). Next we will show \( \frac{\partial^2 \mathbb{P}(Z_1 < z_1, \ldots, Z_{K-1} < z_{k-1})}{\partial \lambda_1 \partial \lambda_2} \) exists and is continuous for any \( j_1 \) and \( j_2 \). For simplicity, we consider the case \( k \geq 3 \) and \( j_1 = 1, j_2 = 2 \). By straightforward calculations,

\[
\frac{\partial^2 \mathbb{P}(Z_1 < z_1, \ldots, Z_{K-1} < z_{k-1})}{\partial \lambda_1 \partial \lambda_2}
\]
\[
\begin{align*}
&= \int_{-\infty}^{z_3(\lambda_k, \lambda_3)} \cdots \int_{-\infty}^{z_{K-1}(\lambda_k, \lambda_{K-1})} f_Z \left( z_1(\lambda_k, \lambda_1), z_2(\lambda_k, \lambda_2), u_3, \ldots, u_{K-1} \right) du_3 \cdots du_{K-1} \\
&\quad \times \frac{\partial z_1(\lambda_k, \lambda_1)}{\partial \lambda_1} \cdot \frac{\partial z_2(\lambda_k, \lambda_2)}{\partial \lambda_2} \\
&= \int_{-\infty}^{z_3(\lambda_k, \lambda_3)} \cdots \int_{-\infty}^{z_{K-1}(\lambda_k, \lambda_{K-1})} f_Z \left( z_1(\lambda_k, \lambda_1), z_2(\lambda_k, \lambda_2), u_3, \ldots, u_{K-1} \right) du_3 \cdots du_{K-1} \\
&\quad \cdot \left[ c_1(\lambda_1, \pi_1^*) \pi_1^* \right]^{-1} \cdot \left[ c_1(\lambda_2, \pi_2^*) \pi_2^* \right]^{-1},
\end{align*}
\]

which exists and is continuous as long as \( \lambda_1 > 0 \) and \( \lambda_2 > 0 \) (avoiding the case that \( c_1(\lambda_1, \pi_1^*) = 0 \) or \( c_2(\lambda_2, \pi_2^*) = 0 \)). Similarly, we can show that \( \frac{\partial^2 \mathbb{P}(Z_1 < z_1, \ldots, Z_{K-1} < z_{K-1})}{\partial \lambda_1 \partial \lambda_2} \) exists and is continuous for any \( j_1 \) and \( j_2 \), as long as \( \lambda_j > 0 \) for all \( j \). Thus we proved the second-order continuously differentiability of \( G(\lambda) \). Besides, by Proposition 4, \( G(\lambda) \) is concave, therefore we know that \( \nabla^2 G(\lambda) \preceq 0 \). However, it is hard in general to show that \( \nabla^2 G(\lambda) \prec 0 \).

- Assumption 4 is trivial to hold by the format of \( \tilde{P}_{Y|X} \).

- Finally, let’s verify Assumption 5. Without loss of generality, suppose \( c_k^* = c_k(\lambda^*, \pi^*) > 0 \) for all \( k \)'s and \( \zeta = \left( \min_k c_k^* \right)^{-1} \). And we only check \( \mathbb{P}_{X|Y=k}(|\varphi_K(X)| \leq t) \preceq t^\gamma \) when \( t \) is smaller than some constant \( C \in (0, 1) \) and \( \gamma > 0 \). \( \mathbb{P}_{X|Y=k}(|\varphi_k(X)| \leq t) \preceq t^\gamma \) can be similarly discussed. Especially the simplest way is to change the reference level in the multinomial logistic regression model, as we did above, to verify Assumption 3. Note that

\[
|\varphi_K(X)| \leq t \\
\iff \left| c_k^* - \max_{j \leq K-1} \left\{ c_j^* e^{(\beta_j^*)^T X} \right\} \right| \leq t + t \sum_{j \leq K-1} e^{(\beta_j^*)^T X} \leq t + t(K-1) \zeta \max_{j \leq K-1} \left\{ c_j^* e^{(\beta_j^*)^T X} \right\} \\
\iff \frac{c_k^* - t}{1 + t \zeta(K-1)} \leq \max_{j \leq K-1} \left\{ c_j^* e^{(\beta_j^*)^T X} \right\} \leq \frac{c_k^* + t}{1 - t \zeta(K-1)}.
\]

Suppose \( t < (\min_k c_k^*) \wedge (\zeta(K-1))^{-1} \). Denote the density of \( (\beta_j^*)^T X \) as \( \tilde{f}_j \). It is bounded by some constant \( M > 0 \) on \( \mathbb{R} \) due to boundedness of the density of \( X \). Then the marginal probability

\[
\mathbb{P}(|\varphi_K(X)| \leq t) \leq \mathbb{P} \left( \frac{c_k^* - t}{1 + t \zeta(K-1)} \leq \max_{j \leq K-1} \left\{ c_j^* e^{(\beta_j^*)^T X} \right\} \leq \frac{c_k^* + t}{1 - t \zeta(K-1)} \right) \\
\leq \sum_{j=1}^{K-1} \mathbb{P} \left( \frac{c_k^* - t}{1 + t \zeta(K-1)} \leq c_j^* e^{(\beta_j^*)^T X} \leq \frac{c_k^* + t}{1 - t \zeta(K-1)} \right) \\
= \sum_{j=1}^{K-1} \mathbb{P} \left( \log \left( \frac{c_k^* - t}{c_j^* [1 + t \zeta(K-1)]} \right) \leq (\beta_j^*)^T X \leq \log \left( \frac{c_k^* + t}{c_j^*[1 - t \zeta(K-1)]} \right) \right)
\]
\[
\leq \sum_{j=1}^{K-1} \tilde{f}_j(\xi_{j,t}) \left[ \log \left( \frac{c_j^* + t}{c_j^*[1 - t\xi(K-1)]} \right) - \log \left( \frac{c_j^* - t}{c_j^*[1 + t\xi(K-1)]} \right) \right] \\
\leq (K-1)MC' \left| \frac{c_j^* + t}{c_j^*[1 - t\xi(K-1)]} - \frac{c_j^* - t}{c_j^*[1 + t\xi(K-1)]} \right| \\
\leq C t, 
\]

where \(C\) and \(C'\) are some positive constants and \(\xi_{j,t}\) is some constant falling between \(\log \left( \frac{c_j^* k - t c_j^*[1 + t\xi(K-1)]}{c_j^*[1 - t\xi(K-1)]} \right)\) and \(\log \left( \frac{c_j^* k + t c_j^*[1 - t\xi(K-1)]}{c_j^*[1 + t\xi(K-1)]} \right)\). Therefore, Assumption 5 holds with \(\bar{\gamma} = 1\).

### 3.4 Comparison of NPMC-CX and NPMC-ER from Theoretical Perspectives

We now summarize the difference between the two algorithms from theoretical perspectives.

- Both NPMC-CX and NPMC-ER are shown to enjoy NP oracle properties under certain conditions. In addition, NPMC-CX satisfies strong consistency if we replace Assumption 2 with its almost sure version Assumption 2'.

- However, for NPMC-CX, we assume the model used to estimate the posterior \(P_{Y|X=x}(Y = k)\) is parametric. Instead, the NP properties hold for NPMC-ER without such restrictions.

### 3.5 Discussions on NPMC Problem, Hypothesis Testing, and Randomization

In Section 1.2, we have connected the NPMC problem (2) to the hypothesis testing problem with a composite null hypothesis consisting of finite arguments and listed their similarities and differences. Here we would like to provide some additional insights. In the hypothesis testing problem, suppose that we have collected some data \(X_n = \{x_i\}_{i=1}^n \sim \text{some distribution } p_{\theta}\) and we would like to test \(H_0 : \theta \in \{\theta_k\}_{k=1}^K\) v.s. \(H_1 : \theta = \theta_{K+1}\).

We want to maximize the statistical power of the test while controlling the type-I error in every case under a target level \(\alpha\). This can be formulated as an optimization problem over a deterministic testing function \(\varphi : X_n \to \{0, 1\}\), where \(\varphi(X_n) = 0\) or \(1\) means accepting or rejecting \(H_0\), respectively. For simplicity, assume \(\{p_{\theta_k}\}_{k=1}^{K+1}\) is a family of densities under a common measure \(\mu\) (e.g. Lebesgue measure). Then the hypothesis testing problem is

\[
\max_{\varphi} \int \varphi(X_n) p_{\theta_{K+1}}(X_n) d\mu \\
\text{s.t.} \max_{k=1:K} \int \varphi(X_n) p_{\theta_k}(X_n) d\mu \leq \alpha. 
\]

In general, directly solving (16) is challenging. People usually connect it to the dual problem, where we try to find the least favorable distribution (LFD, Lehmann and Lehmann (1986)) \(\{q_k\}_{k=1}^K\) on \(\{\theta_k\}_{k=1}^K\) satisfying \(q_k \geq 0\) and \(\sum_{k=1}^{K} q_k = 1\) by solving

\[
\min_{\{q_k\}_{k=1}^K} \max_{\varphi} \int \varphi(X_n) p_{\theta_{K+1}}(X_n) d\mu 
\]
In problem (17), given any \( \{q_k\}_{k=1}^K \), the best testing function \( \varphi \) can be obtained through the NP lemma. Comparing the CS classification problem (5) with the dual of hypothesis testing problem (17), the \( \lambda_k \)'s play a similar role as the \( \{q_k\}_{k=1}^K \) does. The underlying ideas are quite similar, i.e., using strong duality to connect the primal and dual problems, then solving the dual, which leads to a primal optimal solution. Nevertheless, as we mentioned earlier in Section 1.2, the two problems have some intrinsic differences. Moreover, in the hypothesis testing problem, since \( p_\theta \) given \( \theta \) is known, in many cases, we can first guess the LFD and then verify it. However, in the NP problem, this is impossible since we do not have access to the distribution of \( X \) given \( Y = k \).

Note that in both the NPMC problem (2) and the hypothesis testing problem (17), we are considering deterministic classifiers and testing functions. The family of deterministic classifiers or testing functions works well when the strong duality holds. But in some cases, especially when the distribution of \( X \) given \( Y = k \) (for the NPMC problem) and the distribution of \( X_n \) given \( \theta = \theta_k \) (for the hypothesis testing problem) are not absolutely continuous, the strong duality could break under the family of deterministic classifiers or testing functions. In this case, for the hypothesis testing problem, randomization has been shown to be a powerful method to solve the issue. For example, if we consider an enriched family of randomized testing functions \( \{\varphi : \varphi = \varphi_1 \text{ with probability } \omega \text{ and } \varphi = \varphi_2 \text{ probability } (1 - \omega) \}, 0 \leq \omega \leq 1, \varphi_1, \varphi_2 \text{ map } X_n \text{ to } \{0, 1\} \), then the strong duality will hold again, which motivates the randomization part in the NP lemma. For the NPMC problem (2), for simplicity, most of our theoretical results assume the strong duality (Assumption 1) holds. In this situation, randomization does not help. However, it may help when the strong duality breaks, in which case an enlarged family of randomized classifiers may fix the strong duality. For simplicity, we do not discuss this case in the current paper and leave it to future studies.

Similar to the hypothesis testing problem (16), the feasibility of the NPMC problem (2) is not always guaranteed. However, if the strong duality holds (which can be characterized by Theorem 3), then an unbounded dual problem (5) is equivalent to an infeasible primal problem (2). If the strong duality does not hold, then by weak duality, an unbounded dual problem (5) implies an infeasible primal problem (2).

4. Extension to Confusion Matrix Control Problem

In this section, we consider the extension of our algorithms to solve the confusion matrix control problem. For any classifier \( \phi \), we denote the component of confusion matrix at \( k \)-th row and \( r \)-th column as \( R_{kr}(\phi) = P_{X|Y=k}(\phi(X) = r) \), where \( r, k = 1, \ldots, K \). We may abuse the notations used in the previous sections, and the readers shall keep in mind that we are discussing a different version of the NP problem in this section.

---

6. Thanks to one of the reviewers for pointing out the importance of randomization.
We are interested in the following generalized Neyman-Pearson multi-class classification (GNPMC) problem:

$$\min_{\phi} \quad J(\phi) = \sum_{k=1}^{K} \sum_{r \neq k} w_{kr} \mathbb{P}_{X|Y=k}(\phi(X) = r)$$

s.t. \( \mathbb{P}_{X|Y=k}(\phi(X) = r) \leq \alpha_{kr}, \quad (k, r) \in \mathcal{A}, \) \hspace{1cm} (18)

where \( \phi : \mathcal{X} \rightarrow \{1, \ldots, K\} \) is a classifier, \( \alpha_{kr} \in (0, 1), \ w_{kr} \geq 0 \) and \( \mathcal{A} \subseteq \{(1, \ldots, K) \times \{1, \ldots, K\}\} \setminus \{(k, k) : 1 \leq k \leq K\}. \) The NPMC problem (2) we defined in Section 1 can be viewed as a simplified version of problem (18).

We want to connect (18) to the following cost-sensitive (CS) multi-class classification problem:

$$\min_{\phi} \quad \text{Cost}(\phi) = \sum_{k=1}^{K} \sum_{r \neq k} \pi^*_{kr} w_{kr} \mathbb{P}_{X|Y=k}(\phi(X) = r),$$

where \( \phi : \mathcal{X} \rightarrow \{1, \ldots, K\} \) and \( c_{kr} \geq 0. \)

Similar to Lemma 1, we can define the optimal classifier of problem (19) from the costs and conditional probabilities \( \{\mathbb{P}_{Y|X=x}(Y=k)\}_{k=1}^{K}. \)

**Lemma 10** Define classifier \( \bar{\phi}^* : x \mapsto \arg \min_{r=1:K} \left\{ \sum_{k \neq r} c_{kr} \mathbb{P}_{Y|X=x}(Y=k) \right\}. \) Then \( \bar{\phi}^* \) is the optimal classifier of (19) in the following sense: for any classifier \( \phi, \) \( \text{Cost}(\bar{\phi}^*) \leq \text{Cost}(\phi). \)

With Lemma 10 in hand, we can successfully extend our algorithms NPMC-CX and NPMC-ER to the confusion matrix control problem. Imposing similar assumptions as in the simplified case discussed in Section 3, we can prove that NPMC-CX satisfies the multi-class NP oracle properties and strong consistency, and NPMC-ER satisfies the multi-class NP oracle properties, under the generalized framework. Before getting into the details, we first extend the multi-class NP oracle properties and strong consistency described in Section 1.4 for the GNPMC problem (18).

**Multi-class NP oracle properties for the GNPMC problem:**

(i) If the GNPMC problem is feasible and has an optimal solution \( \phi^* \), then the algorithm outputs a solution \( \hat{\phi} \) which satisfies

(a) \( R_{kr}(\hat{\phi}) \leq \alpha_{kr} + O_p(\epsilon(n)), \ \forall (k, r) \in \mathcal{A}; \)

(b) \( J(\hat{\phi}) \leq J(\phi^*) + O_p(\epsilon_J(n)), \)

where \( \epsilon(n) \) and \( \epsilon_J(n) \to 0 \) as \( n \to \infty. \)

(ii) Denote the event that the algorithm indicates infeasibility of GNPMC problem given \( \{(x_t, y_t)\}_{t=1}^{n} = \mathcal{G}_n. \) If the GNPMC problem is infeasible, then \( \mathbb{P}(\mathcal{G}_n) \to 1, \) as \( n \to \infty. \)

**Strong consistency for the GNPMC problem:**

(i) If the GNPMC problem is feasible and has an optimal solution \( \phi^* \), then the algorithm outputs a solution \( \hat{\phi} \) which satisfies

(a) \( \lim_{n \to \infty} R_{kr}(\hat{\phi}) \leq \alpha_{kr}, \) a.s., \( \forall (k, r) \in \mathcal{A}; \)
(b) \( \lim_{n \to \infty} J(\phi) = J(\phi^*) \) a.s.

(ii) Denote the event that the algorithm indicates infeasibility of GNPMC problem given \( \{(x_i, y_i)\}_{i=1}^n \) as \( \mathcal{G}_n \). If the NP problem is infeasible, then \( \mathbb{P}(\lim_{n \to \infty} \mathcal{G}_n) = 1 \).

Since the intuition and most parts of the derivation for the GNPMC problem (18) are similar to those for the NPMC problem (2), we present the algorithms and the associated theory directly without deriving from sketches.

### 4.1 Two Algorithms: GNPMC-CX and GNPMC-ER

For problem (18), consider its Lagrangian form as

\[
F_\lambda(\phi) = \sum_{(k,r) \notin A} w_{kr} \mathbb{P}_{X|Y=k}(\phi(X) = r) + \sum_{(k,r) \in A} (w_{kr} + \lambda_{kr}) \mathbb{P}_{X|Y=k}(\phi(X) = r) - \sum_{(k,r) \in A} \lambda_{kr} \alpha_{kr}
\]

\[
= \sum_{r=1}^K \sum_{k \neq r} c_{kr}(\lambda, \pi^*) \mathbb{P}_{X,Y}(\phi(X) = r, Y = k) - \sum_{(k,r) \in A} \lambda_{kr} \alpha_{kr}
\]

\[
= \mathbb{E}_X \left[ \sum_{k \neq \phi(X)} c_{k \phi(X)}(\lambda, \pi^*) \mathbb{P}_{Y|X}(Y = k) \right] - \sum_{(k,r) \in A} \lambda_{kr} \alpha_{kr},
\]

where \( \lambda = \{\lambda_{kr}\}_{(k,r) \in A} \) and

\[
c_{kr}(\lambda, \pi^*) = \begin{cases} 
    w_{kr}/\pi^*_k, & (k, r) \notin A; \\
    (w_{kr} + \lambda_{kr})/\pi^*_k, & (k, r) \in A.
\end{cases}
\]

Therefore, we can define the dual problem as \( \max_{\lambda \in \mathbb{R}^{|A|}} G(\lambda) \), where \( G(\lambda) = \min_\phi F_\lambda(\phi) = F_\lambda(\phi^*_\lambda) \) and \( \phi^*_\lambda = \arg \min_{r=1:K} \{\sum_{k \neq r} c_{kr}(\lambda, \pi^*) \mathbb{P}_{Y|X}(Y = k)\} \) by Lemma 10. Define

\[
c_{kr}(\lambda, \hat{\pi}) = \begin{cases} 
    w_{kr}/\hat{\pi}_k, & (k, r) \notin A; \\
    (w_{kr} + \lambda_{kr})/\hat{\pi}_k, & (k, r) \in A.
\end{cases}
\]

Then we can extend the NPMC-CX and NPMC-ER to the algorithms GNPMC-CX and GNPMC-ER for the GNPMC problem (18) in a straightforward way.

Similar to NPMC-CX, GNPMC-CX estimates \( F_\lambda(\phi), G(\lambda), \) and \( \phi^*_\lambda \) by

\[
\hat{F}^{CX}_\lambda(\phi) = \frac{1}{n} \sum_{i=1}^n \sum_{k \neq \phi(x_i)} c_{k \phi(x_i)}(\lambda, \hat{\pi}) \mathbb{P}_{Y|X=x_i}(Y = k) - \sum_{(k,r) \in A} \lambda_{kr} \alpha_{kr},
\]

\[
\hat{G}^{CX}(\lambda) = \min_\phi \hat{F}^{CX}_\lambda(\phi) = \hat{F}^{CX}_\lambda(\phi^*_\lambda),
\]

\[
\hat{\phi}^*_\lambda : x \mapsto \arg \min_{r=1:K} \left\{ \sum_{k \neq r} c_{kr}(\lambda, \hat{\pi}) \mathbb{P}_{Y|X=x}(Y = k) \right\},
\]

respectively, where \( \mathbb{P}_{Y|X} \) is the estimated conditional probability, and \( \hat{\mathbb{P}}_{Y|X} \) can be obtained by fitting different models on the data.
For GNPMC-ER, assume the training sample size to be 2n. Similar to NPMC-ER, we divide the training data randomly into two parts of size n. For simplicity, denote them as $\mathcal{D}_1 = \{(x_i, y_i)\}_{i=1}^n = \{(x_i^{(k)}, y_i^{(k)})\}_{i=1}^{n_k} 1 \leq k \leq K$ and $\mathcal{D}_2 = \{(x_i, y_i)\}_{i=n+1}^{2n}$. Similar to NPMC-ER, GNPMC-ER estimates $\hat{F}_F^{\text{ER}}$, $G(\lambda)$, and $\phi^*_\lambda$ by

$$
\hat{F}_F^{\text{ER}}(\phi) = \sum_{(k,r) \notin \mathcal{A}} w_{kr} \cdot \frac{1}{n_k} \sum_{i=1}^{n_k} 1(\phi(x_i^{(k)}) = r) + \sum_{(k,r) \in \mathcal{A}} (w_{kr} + \lambda_{kr}) \cdot \frac{1}{n_k} \sum_{i=1}^{n_k} 1(\phi(x_i^{(k)}) = r) - \sum_{(k,r) \in \mathcal{A}} \lambda_{kr} \alpha_{kr},
$$

$$
\widehat{G}^{\text{ER}}(\lambda) := \widehat{G}^{\text{ER}}(\lambda; \hat{\mathbb{P}}_{Y|X}, \hat{\pi}) = \hat{F}_F^{\text{ER}}(\phi_\lambda),
$$

$$
\hat{\phi}_\lambda: x \mapsto \arg \min_{r=1:K} \left\{ \sum_{k \neq r} c_{kr}(\lambda, \hat{\pi}) \hat{\mathbb{P}}_{Y|X=x}(Y = k) \right\},
$$

respectively. Note that $\hat{F}_F^{\text{ER}}$ is calculated on $\mathcal{D}_1$, while $\hat{\mathbb{P}}_{Y|X}$ and $\hat{\pi}$ (hence $\hat{\phi}_\lambda$) are calculated on $\mathcal{D}_2$.

Details of the two algorithms are presented in Algorithms 3 and 4, respectively.

---

**Algorithm 3: GNPMC-CX**

**Input:** training data $\{(x_i, y_i)\}_{i=1}^n$, target upper bounds of errors $\alpha$, the weighting vector of objective function $\mathbf{w}$, the classification method $\mathcal{M}$ to estimate $\hat{\mathbb{P}}_{Y|X}$

**Output:** the fitted classifier $\hat{\phi}$ or an error message

1. $\hat{\mathbb{P}}_{Y|X}, \hat{\pi} \leftarrow$ the estimates of $\mathbb{P}_{Y|X}$ (through $\mathcal{M}$) and $\pi^*$ on training data $\{(x_i, y_i)\}_{i=1}^n$
2. $\hat{\lambda} \leftarrow \arg \max_{\lambda \in \mathbb{R}_+} \hat{G}^{\text{CX}}(\lambda; \hat{\mathbb{P}}_{Y|X}, \hat{\pi})$
3. if $\hat{G}^{\text{CX}}(\hat{\lambda}) \leq 1$ then
   4. Report the NP problem as feasible and output the solution $\hat{\phi}(x) = \arg \min_{r=1:K} \left\{ \sum_{k \neq r} c_{kr}(\lambda, \hat{\pi}) \hat{\mathbb{P}}_{Y|X=x}(Y = k) \right\}$
   5. else
   6. Report the GNPMC problem as infeasible

---

### 4.2 Theory on GNPMC-CX and GNPMC-ER

In this section, we extend the theoretical analysis in Section 3 for the NPMC problem (2) to the case of GNPMC problem (18). Some assumptions we made in Section 3 (for example, Assumptions 2 and 4) are still necessary for the GNPMC problem (18). The others, like Assumptions 1, 3, and 5, may be subject to slight changes for the GNPMC problem.

#### 4.2.1 Analysis on GNPMC-CX

Similar to the NPMC case, strong duality is the bridge between the GNPMC problem (18) and the cost-sensitive learning problem (19).
Algorithm 4: GNPMC-ER

**Input:** training data \( \{(x_i, y_i)\}_{i=1}^{2n} \), target upper bound of errors \( \alpha \), the weighting vector of objective function \( w \), a search range \( R > 0 \), the classification method \( \mathcal{M} \) to estimate \( P_{Y|X} \)

**Output:** the fitted classifier \( \hat{\phi} \) or an error message

1. Randomly divide the whole training data (and reindex them) into \( D_1 \cup D_2 = \{(x_i, y_i)\}_{i=1}^{n} \cup \{(x_i, y_i)\}_{i=n+1}^{2n} \)
2. \( \hat{P}_{Y|X}, \hat{\pi} \leftarrow \) the estimates of \( P_{Y|X} \) (through \( \mathcal{M} \)) and \( \pi^* \) on \( D_2 = \{(x_i, y_i)\}_{i=n+1}^{2n} \)
3. \( \hat{\lambda} \leftarrow \arg \max_{\lambda \in \mathbb{R}_{+}^{|A|}, \|\lambda\|_{\infty} \leq R} \hat{G}_{ER}(\lambda; \hat{P}_{Y|X}, \hat{\pi}) \), where \( \hat{G}_{ER} \) is estimated on \( D_1 = \{(x_i, y_i)\}_{i=1}^{n} \)
4. if \( \hat{G}_{ER}(\hat{\lambda}) \leq 1 \) then
5. Report the GNPMC problem as feasible and output the solution \( \hat{\phi}_{\lambda}(x) = \arg \min_{r=1:K} \left\{ \sum_{k \neq r} c_{kr}(\lambda, \hat{\pi}) \hat{P}_{Y|X=X}(Y = k) \right\} \)
6. else
7. Report the GNPMC problem as infeasible

Assumption 6 (Strong duality for the GNPMC problem) Suppose it holds that

\[
\min_{\phi \in \mathcal{E}} J(\phi) = \max_{\lambda \in \mathbb{R}_{+}^{|A|}} G(\lambda),
\]

where \( \mathcal{E} \) includes all feasible classifiers for the GNPMC problem (18).

Remark 11 The strong duality implies complementary slackness, that is, for \( \lambda^* = \arg \max_{\lambda \in \mathbb{R}_{+}^{|A|}} G(\lambda) \) and all \((k, r) \in \mathcal{A}\), we have \( \lambda^*_{kr} [R_{kr}(\hat{\phi}^*_{\lambda^*}) - \alpha_{kr}] = 0 \).

We have a sufficient and necessary characterization for strong duality as below.

Theorem 12 (Sufficient and necessary conditions for GNPMC strong duality) Suppose \( X|Y = k \) are continuous random variables for all \( k \).

(i) When the GNPMC problem (18) is feasible, the strong duality holds if and only if there exists \( \lambda = \{\lambda_{kr}\}_{(k,r) \in \mathcal{A}} \) such that \( \hat{\phi}^*_{\lambda} \) is feasible for the NP problem, i.e., \( \mathbb{P}_{X|Y=k}(\hat{\phi}^*_{\lambda}(X) = r) \leq \alpha_{kr} \) for all \((k, r) \in \mathcal{A}\).

(ii) Suppose \( \mathbb{P}_{Y=X}(Y = r) \geq a > 0 \) a.s. (w.r.t. the distribution of \( X \)) for all \( r \in \{r: (k, r) \in \mathcal{A}\} \). When the GNPMC problem (18) is infeasible, the strong duality holds (i.e., \( \max_{\lambda \in \mathbb{R}_{+}^{|A|}} G(\lambda) \) is unbounded from above) if and only if for an arbitrary \( \lambda \in \mathbb{R}_{+}^{|A|}, \phi^*_{\lambda} \) is infeasible for GNPMC problem (18), i.e., \( \exists \) at least one pair of \((k, r) \in \mathcal{A} \) such that \( \mathbb{P}_{X|Y=k}(\phi^*_{\lambda}(X) = r) > \alpha_{kr} \).

The following two assumptions are adapted from Assumptions 3 and 8 for the GNPMC problem.
Assumption 7 $G(\lambda)$ is continuously twice-differentiable at $\lambda^*$ and $\nabla^2 G(\lambda^*) < 0$, where $\lambda^* = \arg \max G(\lambda)$.

Assumption 8 Denote $\varphi_r(x) = \sum_{k \neq r} c_{kr}(\lambda^*, \pi^*) P_{Y|X=x}(Y = k) - \max_{j \neq r} \{ \sum_{k \neq j} c_{kj}(\lambda^*, \pi^*) \}$, where $\lambda^* = \arg \max G(\lambda)$. It holds
\[
\max_{k=1:K} P_{X|Y=k}(|\varphi_k(X)| \leq t) \lesssim t^{\bar{\gamma}},
\]
with some $\bar{\gamma} > 0$ and a non-negative $t$ smaller than some constant $C \in (0, 1)$.

With these conditions, we can show that the NP oracle properties hold for GNPMC-CX.

**Theorem 13 (Multi-class NP oracle properties of GNPMC-CX)** GNPMC-CX satisfies the multi-class NP oracle properties in the following senses.

(i) When the GNPMC problem (18) is feasible, if Assumptions 2, 4, 6, 7, and 8 hold, then there exist a solution $\phi^*$ and a constant $C > 0$ such that
\[
\max_{k, r: k \neq r} P(|R_{kr}(\hat{\phi}) - R_{kr}(\phi^*)| > \delta) \lesssim \exp\{-Cn\delta^{4/\bar{\gamma}}\} + \delta^{-2(1+\bar{\gamma})/\bar{\gamma}} \max_k \mathbb{E} \left| \hat{P}_{Y|X}(Y = k) - P_{Y|X}(Y = k) \right|,
\]
for any $\delta \in (0, 1)$.

(ii) When the GNPMC problem (18) is infeasible, if Assumptions 2, 4, and 6 hold, then there exists a constant $C > 0$ such that
\[
P\left(|\hat{G}^{CX}(\hat{\lambda})| \leq 1 \right) \lesssim \exp\{-Cn\} + \max_k \mathbb{E} \left| \hat{P}_{Y|X}(Y = k) - P_{Y|X}(Y = k) \right|.
\]

**Remark 14** Similar to Remark 7, when the GNPMC problem (18) is feasible, $R_{kr}(\hat{\phi}) - \alpha_{kr} \leq R_{kr}(\hat{\phi}) - R_{kr}(\phi^*) \leq O_p(\epsilon(n))$, $\forall (k, r) \in A$, $J(\hat{\phi}) - J(\phi^*) \leq O_p(\epsilon(n))$, where $\epsilon(n) = n^{-\gamma/4} + \left( \max_k \mathbb{E} \left| \hat{P}_{Y|X}(Y = k) - P_{Y|X}(Y = k) \right| \right)^{-\gamma/(2\lambda(1+\gamma))} \to 0$. Hence Theorem 13 verifies that GNPMC-CX satisfies the multi-class NP oracle properties.

Under certain conditions, we can also show that strong consistency holds for GNPMC-CX.

**Theorem 15 (Strong consistency of GNPMC-CX)** GNPMC-CX satisfies strong consistency in the following senses.

(i) When the GNPMC problem (18) is feasible, if Assumptions 2', 4, 6, 7 hold, then there exists a solution $\phi^*$, such that $\lim_{n \to \infty} R_{kr}(\hat{\phi}) = R_{kr}(\phi^*)$ a.s. for all $k$ and $r \in \{1, \ldots, K\}$. And if $P(\hat{\lambda}_{kr} > \delta_n) \to 1$ for any vanishing sequence $\{\delta_n\}_{n=1}^\infty \to 0$, then $R_{kr}(\phi^*) = \alpha_{kr}$.

(ii) When the GNPMC problem (18) is infeasible, if Assumptions 2', 4, and 6 hold, then for any $M > 0$, $\lim_{n \to \infty} \hat{G}^{CX}(\lambda) > M$ a.s.
4.2.2 Analysis on GNPMC-ER

Under certain conditions, we can verify the NP oracle properties for GNPMC-ER. As NPMC-ER, GNPMC-ER does not need the parametric assumption (Assumption 4) to satisfy NP oracle properties.

**Theorem 16 (Multi-class NP oracle properties of GNPMC-ER)** GNPMC-ER satisfies the multi-class NP oracle properties in the following senses.

(i) When the GNPMC problem (18) is feasible, if Assumptions 2, 6, 7, and 8 hold, and $R$ is sufficiently large\(^8\), then there exist a solution $\phi^*$ and some constants $C, C' > 0$ such that

$$
\max_{k,r,k\neq r} \mathbb{P}(|R_{kr}(\hat{\phi}) - R_{kr}(\phi^*)| > \delta) \\
\lesssim \exp\{-Cn\delta^{4/\gamma}\} + \delta \cdot \frac{2^{\Lambda(1+\gamma)}}{\gamma} \max_k \mathbb{E}\left| \hat{P}_{Y|X}(Y = k) - P_{Y|X}(Y = k) \right|,
$$

for any $\delta \in [C' n^{-\gamma/4}, 1]$.

(ii) When the GNPMC problem (18) is infeasible, if Assumptions 2 and 6 hold, and $R$ is sufficiently large\(^9\), then there exists a constant $C > 0$ such that

$$
\mathbb{P}\left( |\hat{G}^{ER}(\hat{\lambda})| \leq 1 \right) \lesssim \exp\{-Cn\} + \max_k \mathbb{E}\left| \hat{P}_{Y|X}(Y = k) - P_{Y|X}(Y = k) \right|.
$$

Analyzing in the same way as in Remark 14, we know that Theorem 16 verifies multi-class NP oracle properties of GNPMC-ER.

5. Numerical Experiments

We demonstrate the effectiveness of NPMC-CX and NPMC-ER in two simulations and three real data studies. Because we focus on problem (2), our numerical studies do not include the general confusion matrix control problem discussed in Section 4.

We use R to conduct all numerical experiments. Our proposed algorithms, NPMC-CX and NPMC-ER, have been implemented in the package npcs (https://CRAN.R-project.org/package=npcs). The optimization procedure in step 2 of Algorithm 1 and step 3 of Algorithm 2 to find $\lambda$ is implemented through the function hjkb in the package dfoptim, which solves derivative-free optimization problems by Hooke-Jeeves algorithm (Hooke and Jeeves, 1961; Kelley, 1999). Various packages are used to fit different classification methods. These methods include logistic regression (logistic, package nnet), linear discriminant analysis (LDA, package MASS), k-nearest neighbors (kNN, package caret), non-parametric naïve Bayes classifier with Gaussian kernel (NNB, package naivebayes), support vector machines with RBF kernel (SVM, package e1071), and random forest (RF, package randomForest), where the corresponding abbreviations and packages are indicated in the parentheses.

---

\(^8\) Here our results hold when $R \geq \|\lambda^*\|_\infty$, where $\lambda^* = \arg \max \ G(\lambda)$.

\(^9\) Due to Assumption 6, $\sup_{\lambda \in \mathbb{R}} |G(\lambda)| = +\infty$. Here, our results hold when $R$ satisfies $\sup_{\|\lambda\|_\infty \leq R} G(\lambda) > 1 + \vartheta$ for at least one $\vartheta > 0$. 

24
\(k\)NN, the number of nearest neighbors is set to \(k = \lfloor \sqrt{n/K} \rfloor\), where \(n\) is the training sample size, and \(K\) is the number of classes. For NNB, the kernel bandwidth is selected based on Silverman’s rule of thumb (Silverman, 2018). All parameters for SVM are set to default values as suggested in package e1071. For instance, the RBF kernel has the form \(\exp\{-\gamma |u - v|\}\) with \(\gamma = 1/p\) where \(p\) is the number of variables in the data. Moreover, the constant of the regularization term in the Lagrange formulation is set to be 1. More details can be found in Meyer et al. (2019). For RF, all parameters are set to default values as suggested in package randomForest. For example, the number of trees is set to be 500, and the number of variables randomly sampled as candidates at each split is set to be \(\lfloor \sqrt{p} \rfloor\) where \(p\) is the number of variables in the data. More details are available in Liaw and Wiener (2002). In simulations, we vary the training sample size \(n\) from 1000 to 9000 with an increment of 2000, and the test sample size is fixed as 20,000. Each setting in simulations and real data studies is repeated 500 times.

5.1 Simulations

5.1.1 Case 1

Consider a three-class independent Gaussian conditional distributions \(X|Y = k \sim N(\mu_k, I_p)\), where \(p = 5\), \(\mu_1 = (-1, 2, 1, 1, 1)^T\), \(\mu_2 = (1, 1, 0, 2, 0)^T\), \(\mu_3 = (2, -1, -1, 0, 0)^T\) and \(I_p\) is the \(p\)-dimensional identity matrix. The marginal distribution of \(Y\) is \(P(Y = 1) = P(Y = 2) = 0.3\) and \(P(Y = 3) = 0.4\).

We would like to solve the following NPMC problem

\[
\begin{align*}
\min_{\phi} & \quad P_{X|Y=2}(\phi(X) \neq 2) \\
\text{s.t.} & \quad P_{X|Y=1}(\phi(X) \neq 1) \leq 0.05, \quad P_{X|Y=3}(\phi(X) \neq 3) \leq 0.01.
\end{align*}
\]

We run the proposed algorithms NPMC-CX and NPMC-ER based on four classifiers, including logistic regression, LDA, \(k\)NN, and non-parametric naïve Bayes classifier with Gaussian kernel. For comparison, we also fit vanilla classifiers as benchmarks. Box plots show the per-class error rates under each classifier and training sample size setting in Figure 1.

One can see that vanilla classifiers fail to control the error rates around specific levels. NPMC-CX and NPMC-ER equipped with four classifiers work very well by controlling the error rates around the expected control level, which matches our theoretical results in Section 3. By comparing the error rates of class 2 between NPMC methods and vanilla classifiers, we observe that to successfully control \(P_{X|Y=1}(\phi(X) \neq 1)\) and \(P_{X|Y=3}(\phi(X) \neq 3)\) around the corresponding levels, we have to pay the price by damaging the performance on class 2. When the training sample size \(n\) increases, the variance of error rates for each method tends to shrink. For NPMC-CX-LDA and NPMC-CX-NNB, when \(n\) is small, sometimes the algorithm outputs the infeasibility warning. For NPMC-CX-LDA, this might happen due to LDA’s higher sample size requirements (because we need to estimate the covariance matrix) compared to other methods like logistic regression. For NPMC-CX-NNB, this could be caused by the improper choice of bandwidth.

\[\text{To be more precise, the graphs only show the empirical error rates on the test data.}\]
Figure 1: Per-class error rates under each classifier and training sample size setting in simulation case 1. Horizontal lines in corresponding colors mark the expected control levels. For some graphs, there are additional numbers with brackets under the training sample size $n$, which indicates the number of cases that algorithms report infeasibility.

5.1.2 Case 2

In the first example, all five variables are independent Gaussian; therefore, four classifiers can estimate the posterior accurately. In this example, we consider a four-class correlated Gaussian conditional distribution, where $X|Y = k \sim N(\nu_k, \Sigma)$ for $k = 1, \ldots, 4$. And
\[ \nu_1 = (1, -2, 0, -1, 1)^T, \nu_2 = (-1, 1, -2, -1, 1)^T, \nu_3 = (2, 0, -1, 1, -1), \nu_4 = (1, 0, 1, 2, -2)^T, \]
\[ \Sigma = (0.1^{(i\neq j)})_{p \times p}, p = 5. \] The marginal distribution of \( Y \) is \( P(Y = 1) = 0.1, P(Y = 2) = 0.2, P(Y = 3) = 0.3, \) and \( P(Y = 4) = 0.4. \)

Figure 2: Per-class error rates and objective function values under each classifier and training sample size setting in simulation case 2. Horizontal lines in corresponding colors mark the expected control levels. For some graphs, there are additional numbers with brackets under the training sample size \( n \), which indicates the number of cases that algorithms report infeasibility.
The goal is to solve the following NPMC problem

$$\min_{\phi} \sum_{k=1}^{4} w_k P_{X|Y=1}(\phi(X) \neq 1)$$

s.t. $P_{X|Y=1}(\phi(X) \neq 1) \leq 0.04$, $P_{X|Y=3}(\phi(X) \neq 3) \leq 0.08$,

where $w_k = P(Y = k)$. Note that the objective function here includes errors of all four classes and is actually equal to the overall misclassification error rate $P(\phi(X) \neq Y)$.

Like case 1, we study NPMC-CX, NPMC-ER, and vanilla classifiers based on logistic regression, LDA, $k$-NN, and non-parametric naïve Bayes classifier. The results are summarized in Figure 2. It can be observed that all four vanilla classifiers failed to control the error rates around the target levels. At the same time, NPMC-CX and NPMC-ER perform much better and successfully controlled $P_{X|Y=1}(\phi(X) \neq 1)$ and $P_{X|Y=3}(\phi(X) \neq 3)$ around 0.04 and 0.08, respectively. When the training sample size $n$ increases, the variances of error rates for each method tend to shrink. When $n$ is small, except for NPMC-CX-logistic, the other NPMC methods lead to infeasibility results sometimes. An interesting phenomenon here is that although the variables are not independent, NPMC-CX-NNB and NPMC-ER-NNB still work well in controlling the error rates. Besides, NPMC-CX-$k$NN seems to be over-conservative by strictly controlling $P_{X|Y=1}(\phi(X) \neq 1)$ under level 0.04 when $n$ is large.

5.2 Real data Studies

5.2.1 Dry Bean Dataset

This dataset comes from the transformed images of 13,611 grains of 7 different registered dry beans (Koklu and Ozkan, 2020). The seven types and their corresponding sample sizes are Barbunya (1322), Bombay (522), Cali (1630), Dermosan (3546), Horoz (1928), Seker (2027), and Sira (2636). The goal is to predict the bean type correctly. There are 16 predictors of the grains in total, consisting of 12 dimensions and four shape forms. The data is available on the UCI machine learning repository (https://archive.ics.uci.edu/ml/datasets/Dry+Bean+Dataset).

For convenience, we recode the bean types into classes 1 through 7. In each replication, we randomly split the data into 10% training and 90% test data per class. Consider the following NPMC problem

$$\min_{\phi} \frac{1}{4} \left[ P_{X|Y=3}(\phi(X) \neq 3) + P_{X|Y=5}(\phi(X) \neq 5) + P_{X|Y=6}(\phi(X) \neq 6) + P_{X|Y=7}(\phi(X) \neq 7) \right]$$

s.t. $P_{X|Y=1}(\phi(X) \neq 1) \leq 0.05$, $P_{X|Y=2}(\phi(X) \neq 2) \leq 0.01$, $P_{X|Y=4}(\phi(X) \neq 4) \leq 0.03$.

We study NPMC-CX, NPMC-ER, and vanilla classifiers based on logistic regression, SVM, $k$-NN, and random forest. The performance of these methods is summarized in Figure 3. Firstly, we can see that four vanilla classifiers can only control the error rate of class 2 while failing to control the error rates of classes 1 and 4. NPMC-CX and NPMC-ER work well to control the error rates around the target levels, except for NPMC-ER-SVM and
Neyman-Pearson Multi-class Classification via Cost-sensitive Learning

NPMC-CX-RF. NPMC-ER-SVM leads to a large variance in the error rate of class 2, which might be caused by the limited sample size of class 2. Furthermore, NPMC-CX-RF fails to control the class 1 error rate. This may be caused by overfitting, because the random forest is a very complex model and the training data is used both in fitting the model and searching for $\lambda$ in Algorithm 1).

![Graphs showing per-class error rates and objective function values under each classifier for the dry bean dataset.](image)

Figure 3: Per-class error rates and objective function values under each classifier for the dry bean dataset. Horizontal lines in corresponding colors mark the expected control levels. For some graphs, there are additional numbers with brackets under the method names, which indicates the number of cases that algorithms report infeasibility.

5.2.2 Statlog (Landsat Satellite) Dataset

This dataset contains the multi-spectral values of pixels in $3 \times 3$ neighborhoods in satellite images. We aim to predict the central pixel label in each neighborhood. There are 36 predictors for each of the 6435 observations, representing the multi-spectral values. Central pixel labels and their corresponding sample sizes are red soil (1533), cotton crop (703), grey soil (1358), damp grey soil (626), soil with vegetation stubble (707), and very damp grey...
soil (1508). We recode the six classes into classes 1 to 6, respectively. In each replication, we randomly split the data into 10% training and 90% test data per class.

We consider the following NPMC problem

$$\min_{\phi} \frac{1}{6} \sum_{k=1}^{6} \mathbb{P}_{X|Y=k}(\phi(X) \neq k)$$

s.t. $\mathbb{P}_{X|Y=3}(\phi(X) \neq 3) \leq 0.15$, $\mathbb{P}_{X|Y=4}(\phi(X) \neq 4) \leq 0.2$, $\mathbb{P}_{X|Y=5}(\phi(X) \neq 5) \leq 0.1$.

As in Section 5.2.1, we explore NPMC-CX, NPMC-ER, and vanilla classifiers based on logistic regression, SVM, $k$NN, and random forest. The results are available in Figure 4. It can be seen that vanilla-logistic and vanilla-$k$NN only control $\mathbb{P}_{X|Y=3}(\phi(X) \neq 3)$ well, while vanilla-SVM and vanilla-RF successfully control $\mathbb{P}_{X|Y=3}(\phi(X) \neq 3)$ and $\mathbb{P}_{X|Y=5}(\phi(X) \neq 5)$ around the target levels. NPMC-CX and NPMC-ER successfully control all three error rates around the target levels in all cases. In addition, it is interesting that all vanilla methods over-control $\mathbb{P}_{X|Y=3}(\phi(X) \neq 3)$, which might damage the performance on other classes. NPMC-CX and NPMC-ER can fix this issue and relax this control by increasing $\mathbb{P}_{X|Y=3}(\phi(X) \neq 3)$ while still controlling other classes’ error rates around the expected levels. Thanks to this, compared to the vanilla methods, we observe that NPMC-CX and NPMC-ER can create classifiers approximately controlling the error rates around the levels without increasing the objective function value too much.

5.2.3 Dementia Dataset

Worldwide, the prevention, treatment, and precise diagnosis of subtypes of dementia is a top healthcare priority and a critical clinical focus. This dataset comes from a preliminary study based on medical and neuropathology records from participants enrolled in an NIH-funded AD research center (ADRC) at New York University. Each participant signed an IRB-approved form to donate the brain for post-mortem examination. Their clinical evaluation included an interview according to the Brief Cognitive Rating Scale, rating on the Global Deterioration Scale (GDS) (Reisberg et al., 1993), and Geriatric Depression Scale. Subjects with brain pathology, such as tumors, neocortical infarction, or diabetes, were excluded.

The selection of records that included post-mortem dementia diagnosis yielded a total of 302 observations. The original dataset includes 10 dementia subtypes. Since sample sizes of some subtypes are too small, we keep subtypes Normal (class 1) and Alzheimer’s disease (class 2), and merge the other eight subtypes into one class (class 3). And the final sample sizes of them are 103, 89, and 110, respectively. For each observation, we retrieved information from the most recent clinic visit. There are 13 predictors, including age, sex, race, education, and the nine most relevant clinical measures after list-wise deletion.

Our goal is to solve the following NPMC problem

$$\min_{\phi} \mathbb{P}_{X|Y=3}(\phi(X) \neq 3)$$

s.t. $\mathbb{P}_{X|Y=1}(\phi(X) \neq 1) \leq 0.1$, $\mathbb{P}_{X|Y=2}(\phi(X) \neq 2) \leq 0.02$.

Similar to the previous two real data studies, we fit NPMC-CX, NPMC-ER, and vanilla classifiers based on logistic regression, SVM, $k$NN, and random forest. The results are
Figure 4: Per-class error rates under each classifier for the statlog dataset. Horizontal lines in corresponding colors mark the expected control levels. For some graphs, there are additional numbers with brackets under the method names, which indicates the number of cases that algorithms report infeasibility.

available in Figure 5. It can be seen that NPMC-CX-logistic, NPMC-CX-SVM, NPMC-ER-SVM, NPMC-CX-RF, NPMC-ER-RF, and vanilla-RF approximately control the $P_{X|Y=1}(\phi(X) \neq 1)$ and $P_{X|Y=2}(\phi(X) \neq 2)$ around the target levels, while the other methods fail. Besides, NPMC-ER-logistic often fails to give a feasible solution. These issues may be due to the limited sample size.

Motivated by the over-sampling strategy often used in imbalance classification to create synthetic observations for minor classes (Feng et al., 2021), next, we try to enlarge the training dataset before running NPMC algorithms. One of the most popular over-sampling is the synthetic minority over-sampling technique (SMOTE) (Chawla et al., 2002), which creates synthetic samples via nearest neighbors. We can briefly describe the SMOTE algorithm with the number of nearest neighbors $\tilde{k}$ as follows. To enlarge the sample size of class $k$, for each class-$k$ sample $x_0$, randomly choose one of its $\tilde{k}$ nearest neighbors $x_1$ and generate a uniform random variable $u \sim \text{Unif}(0, 1)$. Then a new synthetic observation of
Figure 5: Per-class error rates under each classifier for the dementia dataset without 0.5-SMOTE. Horizontal lines in corresponding colors mark the expected control levels. For some graphs, there are additional numbers with brackets under the method names, which indicates the number of cases that algorithms report infeasibility.

class $k$ is generated as $\tilde{x} = u x_1 + (1 - u) x_0$. Compared to other over-sampling methods with replacement, SMOTE benefits from more variations and uncertainty.

In our case, we have limited observations for all classes. Therefore we need to enlarge the whole dataset instead of a single class. To make our over-sampling procedure less aggressive, we adjusted the original SMOTE algorithm and conducted a conservative version called “0.5-SMOTE” by replacing the Unif(0,1) with Unif(0,0.5). Compared to the original SMOTE, the synthetic samples generated by 0.5-SMOTE are closer to the real samples.

Next, in each of the 500 replications, we conduct 0.5-SMOTE with 5NN to generate a new training set with five times the sample size of the original data, then run NPMC and vanilla algorithms on this new training set. We summarize the results in Figure 6. Compared to the results without 0.5-SMOTE, the performance of NPMC algorithms improves significantly, and all of them successfully control the error rates around the corresponding levels. At the same time, all vanilla approaches fail to control $P_{X|Y=2}(\phi(X) \neq 2)$. It can also
Figure 6: Per-class error rates and objective function values for the dementia dataset with 0.5-SMOTE. Horizontal lines in corresponding colors mark the expected control levels. For some graphs, there are additional numbers with brackets under the method names, which indicates the number of cases that algorithms report infeasibility.

be seen that NPMC methods tend to be conservative when controlling $P_{X|Y=1}(\phi(X) \neq 1)$, which might be caused by overfitting. When the sample size is small, doing 0.5-SMOTE can help NPMC methods succeed, making our algorithms more useful in practice.

5.3 Comparison of NPMC-CX and NPMC-ER from Experimental Perspectives

From the previous numerical results, we can observe that:

- NPMC-CX works better under parametric models (e.g., logistic and LDA) by controlling the error rates well and achieving a lower objective function value compared to NPMC-ER, but can sometimes fail to control error rates under target levels for non-parametric models (e.g., $k$NN, RF, and SVM with RBF kernel).
Compared to NPMC-CX, NPMC-ER requires a larger sample size to work well due to the sample splitting in Algorithm 2, but it is more robust to different types of models. These observations match our intuition from theoretical analysis (Section 3.4) very well. Therefore, for practitioners, if some parametric model is believed to work well, we suggest using NPMC-CX. If the non-parametric model is believed to work better and the sample size is not very small, we suggest using NPMC-ER.

6. Discussions

6.1 Summary

In this paper, we connect Neyman-Pearson multi-class classification (NPMC) problems with cost-sensitive learning (CS) problems, and propose two algorithms, NPMC-CX and NPMC-ER, to solve the NPMC problem (2) via CS techniques. To the best of our knowledge, this is the first work solving NPMC problems via cost-sensitive learning with theoretical guarantees. We have presented some theoretical results, including multi-class NP oracle properties and strong consistency. Our algorithms are shown to be effective through two simulation cases and three real data studies.

We also compare NPMC-CX and NPMC-ER from both theoretical and experimental perspectives. The take-home messages can be summarized as follows.

- Both algorithms are shown to satisfy multi-class NP properties, and NPMC-CX also enjoys strong consistency. However, NPMC-CX requires the classification model to estimate $P_{Y|X=x}(Y = k)$ to be parametric, while NPMC-ER has no such restrictions.

- In practice, NPMC-CX works well for parametric models but can sometimes fail to control error rates under target levels for non-parametric models. NPMC-ER requires a larger sample size due to the data splitting but is more robust to different types of models.

- Therefore, we suggest the practitioners go with NPMC-CX when some parametric model is believed to work well. When the non-parametric model is believed to work better and there is enough training data, we suggest using NPMC-ER.

In addition, the confusion matrix control problem (i.e., GNPMC problem) (18) is discussed, and our two NPMC algorithms are extended to work for GNPMC problems. The theoretical results are also provided.

6.2 Future Research Directions

There are many interesting future avenues to explore. Here we list three of them.

(i) There are many ways to fit a CS classifier. We use (9) to fit the CS classifier in our NPMC algorithms, which sometimes is called the thresholding strategy in binary CS problems (Dmochowski et al., 2010). It might be interesting to explore other approaches and replace (9) accordingly.
(ii) The empirical results show that our algorithms require large sample sizes to succeed. In the analysis of the dementia dataset, where the training data is rather limited, we conduct a 0.5-SMOTE algorithm to enlarge the training set first, which improves the results of directly applying NPMC methods to the original data. It is interesting to conduct some theoretical analysis or explore other solutions to the issue of limited sample size.

(iii) Li et al. (2020) first studied the methodological relationship between the binary NP paradigm and CS paradigm, and constructed a CS classifier with type-I error controls. In this paper, we focus on the multi-class NP paradigm and construct a multi-class NP classifier via CS learning, which can be viewed as the inverse to Li et al. (2020). It is interesting to study the other direction in the multi-class cases: developing multi-class CS classifiers with specific error controls.

Acknowledgements

We thank the Editor Professor Gabor Lugosi and an anonymous reviewer for their insightful comments, which greatly improved a prior version of the paper. This research was partially supported by NIH Grant 1R21AG074205-01, a grant from the New York University School of Global Public Health, NYU University Research Challenge Fund, and through the NYU IT High Performance Computing resources, services, and staff expertise.

References

O. Bousquet. Concentration inequalities for sub-additive functions using the entropy method. In *Stochastic inequalities and applications*, pages 213–247. Springer, 2003.

S. Boyd and L. Vandenberghe. *Convex optimization*. Cambridge university press, 2004.

A. Cannon, J. Howse, D. Hush, and C. Scovel. Learning with the Neyman-Pearson and min-max criteria. *Los Alamos National Laboratory, Tech. Rep. LA-UR*, pages 02–2951, 2002.

N. V. Chawla, K. W. Bowyer, L. O. Hall, and W. P. Kegelmeyer. SMOTE: synthetic minority over-sampling technique. *Journal of artificial intelligence research*, 16:321–357, 2002.

J. P. Dmochowski, P. Sajda, and L. C. Parra. Maximum likelihood in cost-sensitive learning: Model specification, approximations, and upper bounds. *Journal of Machine Learning Research*, 11(12), 2010.

P. Domingos. Metacost: A general method for making classifiers cost-sensitive. In *Proceedings of the fifth ACM SIGKDD international conference on Knowledge discovery and data mining*, pages 155–164, 1999.

S. Dreiseitl, L. Ohno-Machado, and M. Binder. Comparing three-class diagnostic tests by three-way roc analysis. *Medical Decision Making*, 20(3):323–331, 2000.
D. C. Edwards, C. E. Metz, and M. A. Kupinski. Ideal observers and optimal roc hyper-surfaces in n-class classification. *IEEE Transactions on Medical Imaging*, 23(7):891–895, 2004.

C. Elkan. The foundations of cost-sensitive learning. In *International joint conference on artificial intelligence*, volume 17, pages 973–978. Lawrence Erlbaum Associates Ltd, 2001.

Y. Feng, M. Zhou, and X. Tong. Imbalanced classification: A paradigm-based review. *Statistical Analysis and Data Mining: The ASA Data Science Journal*, pages 1–24, 2021. doi: https://doi.org/10.1002/sam.11538.

A. Fernández, S. García, M. Galar, R. C. Prati, B. Krawczyk, and F. Herrera. Cost-sensitive learning. In *Learning from Imbalanced Data Sets*, pages 63–78. Springer, 2018.

R. Hooke and T. A. Jeeves. “Direct search” solution of numerical and statistical problems. *Journal of the ACM (JACM)*, 8(2):212–229, 1961.

S. Katsumata and A. Takeda. Robust cost sensitive support vector machine. In *Artificial intelligence and statistics*, pages 434–443. PMLR, 2015.

C. T. Kelley. *Iterative methods for optimization*. SIAM, 1999.

M. Koklu and I. A. Ozkan. Multiclass classification of dry beans using computer vision and machine learning techniques. *Computers and Electronics in Agriculture*, 174:105507, 2020.

V. Koltchinskii. *Oracle inequalities in empirical risk minimization and sparse recovery problems: École D’Été de Probabilités de Saint-Flour XXXVIII-2008*, volume 2033. Springer Science & Business Media, 2011.

T. Landgrebe and R. Duin. On Neyman-Pearson optimisation for multiclass classifiers. In *Proceedings 16th Annual Symposium of the Pattern Recognition Association of South Africa. PRASA*, pages 165–170, 2005.

T. C. Landgrebe and R. P. Duin. Efficient multiclass roc approximation by decomposition via confusion matrix perturbation analysis. *IEEE transactions on pattern analysis and machine intelligence*, 30(5):810–822, 2008.

E. L. Lehmann and E. Lehmann. *Testing statistical hypotheses*, volume 2. Springer, 1986.

J. J. Li and X. Tong. Statistical hypothesis testing versus machine learning binary classification: Distinctions and guidelines. *Patterns*, 1(7):100115, 2020.

J. J. Li, Y. E. Chen, and X. Tong. A flexible model-free prediction-based framework for feature ranking. *Journal of Machine Learning Research*, 22(124):1–54, 2021.

W. V. Li, X. Tong, and J. J. Li. Bridging cost-sensitive and Neyman-Pearson paradigms for asymmetric binary classification. *arXiv preprint arXiv:2012.14951*, 2020.

A. Liaw and M. Wiener. Classification and regression by randomforest. *R News*, 2(3):18–22, 2002. URL https://CRAN.R-project.org/doc/Rnews/
C. X. Ling and V. S. Sheng. Cost-sensitive learning and the class imbalance problem. *Encyclopedia of machine learning*, 2011:231–235, 2008.

R. Ma, Q. Lin, and T. Yang. Quadratically regularized subgradient methods for weakly convex optimization with weakly convex constraints. In *International Conference on Machine Learning*, pages 6554–6564. PMLR, 2020.

E. Mammen and A. B. Tsybakov. Smooth discrimination analysis. *The Annals of Statistics*, 27(6):1808–1829, 1999.

D. Meyer, E. Dimitriadou, K. Hornik, A. Weingessel, and F. Leisch. e1071: Misc Functions of the Department of Statistics, Probability Theory Group (Formerly: E1071), TU Wien, 2019. URL https://CRAN.R-project.org/package=e1071. R package version 1.7-3.

D. Mossman. Three-way rocs. *Medical Decision Making*, 19(1):78–89, 1999.

J. A. Nelder and R. Mead. A simplex method for function minimization. *The computer journal*, 7(4):308–313, 1965.

D. Pollard. Asymptopia: an exposition of statistical asymptotic theory. *URL http://www.stat.yale.edu/pollard/Books/Asymptopia*, 2000.

Z. Qin, A. T. Wang, C. Zhang, and S. Zhang. Cost-sensitive classification with k-nearest neighbors. In *International Conference on Knowledge Science, Engineering and Management*, pages 112–131. Springer, 2013.

B. Reisberg, S. H. Ferris, and S. G. Sclan. Empirical evaluation of the global deterioration scale for staging alzheimer’s disease. *American Journal of Psychiatry*, 150(4):680–a, 1993.

P. Rigollet and X. Tong. Neyman-Pearson classification, convexity and stochastic constraints. *Journal of Machine Learning Research*, 12:2831–2855, 2011.

C. Scott. Performance measures for Neyman–Pearson classification. *IEEE Transactions on Information Theory*, 53(8):2852–2863, 2007.

C. Scott. A generalized Neyman-Pearson criterion for optimal domain adaptation. In *Algorithmic Learning Theory*, pages 738–761. PMLR, 2019.

C. Scott and R. Nowak. A Neyman-Pearson approach to statistical learning. *IEEE Transactions on Information Theory*, 51(11):3806–3819, 2005.

S. Shalev-Shwartz and S. Ben-David. *Understanding machine learning: From theory to algorithms*. Cambridge university press, 2014.

V. S. Sheng and C. X. Ling. Thresholding for making classifiers cost-sensitive. In *AAAI*, volume 6, pages 476–481, 2006.

B. W. Silverman. *Density estimation for statistics and data analysis*. Routledge, 2018.

Y. Tian and W. Zhang. THORS: An efficient approach for making classifiers cost-sensitive. *IEEE Access*, 7:97704–97718, 2019.
X. Tong. A plug-in approach to Neyman-Pearson classification. *Journal of Machine Learning Research*, 14(1):3011–3040, 2013.

X. Tong, Y. Feng, and A. Zhao. A survey on Neyman-Pearson classification and suggestions for future research. *Wiley Interdisciplinary Reviews: Computational Statistics*, 8(2):64–81, 2016.

X. Tong, Y. Feng, and J. J. Li. Neyman-Pearson classification algorithms and np receiver operating characteristics. *Science advances*, 4(2):eaa01659, 2018.

X. Tong, L. Xia, J. Wang, and Y. Feng. Neyman-Pearson classification: parametrics and sample size requirement. *Journal of Machine Learning Research*, 21(12):1–48, 2020.

A. W. Van der Vaart. *Asymptotic statistics*, volume 3. Cambridge university press, 2000.

A. Wald. Note on the consistency of the maximum likelihood estimate. *The Annals of Mathematical Statistics*, 20(4):595–601, 1949.

L. Xia, R. Zhao, Y. Wu, and X. Tong. Intentional control of type I error over unconscious data distortion: A Neyman–Pearson approach to text classification. *Journal of the American Statistical Association*, 116(533):68–81, 2021.

A. Zhao, Y. Feng, L. Wang, and X. Tong. Neyman-Pearson classification under high-dimensional settings. *Journal of Machine Learning Research*, 17(1):7469–7507, 2016.

Z.-H. Zhou and X.-Y. Liu. Training cost-sensitive neural networks with methods addressing the class imbalance problem. *IEEE Transactions on knowledge and data engineering*, 18(1):63–77, 2005.

Z.-H. Zhou and X.-Y. Liu. On multi-class cost-sensitive learning. *Computational Intelligence*, 26(3):232–257, 2010.

**Appendix A. Technical Lemmas and Propositions**

**Lemma 17** Consider Algorithm 1 (NPMC-CX). Under Assumptions 3 and 4, for any bounded $\Lambda \subseteq \mathbb{R}^{|A|}$, we have

$$\mathbb{P}\left(\sup_{\lambda \in \Lambda} |\hat{F}_{\lambda}(\hat{\phi}_{\lambda}) - F_{\lambda}(\phi^*_\lambda)| > \sqrt{\delta} \lor \delta\right) \lesssim \exp\{-n(\delta \lor \delta^2)\} + \delta^{-1} \max_k \mathbb{E}\left|\hat{P}_{Y|X}(Y = k) - P_{Y|X}(Y = k)\right|,$$

for any $\delta > 0$.

**Proposition 18** Consider Algorithm 1 (NPMC-CX). Suppose Assumptions 3 and 4 hold. If NP problem (2) is feasible and Assumption 1 holds, then

$$\mathbb{P}(\|\hat{\lambda} - \lambda^*\|_2 > \delta) \lesssim \exp\{-Cn\delta^4\} + \delta^{-2} \max_k \mathbb{E}\left|\hat{P}_{Y|X}(Y = k) - P_{Y|X}(Y = k)\right|,$$

for any $\delta \in (0, 1)$, where $\lambda^* = \arg\max_{\lambda \in \mathbb{R}^p} G(\lambda)$. 38
Lemma 19 Consider Algorithm 1 (NPMC-CX). Suppose Assumptions 2', 3, 4 hold. For any bounded set $\Lambda \subseteq \mathbb{R}^{|A|}$, $\lim_{n \to \infty} \sup_{\lambda \in \Lambda} |\hat{F}_\lambda(\hat{\phi}_\lambda) - F_\lambda(\hat{\phi}_\lambda)| = 0$ a.s..

Lemma 20 Consider Algorithm 1 (NPMC-CX). Suppose Assumptions 2', 3, 4 hold. For any bounded set $\Lambda \subseteq \mathbb{R}^{|A|}$, $\lim_{n \to \infty} \sup_{\lambda \in \Lambda} |\hat{F}_\lambda(\hat{\phi}_\lambda) - F_\lambda(\phi^*_\lambda)| = 0$ a.s..

Lemma 21 Consider Algorithm 2 (NPMC-ER). We define $F_\lambda(\phi)$ as in (13). Under Assumptions 1 and 3, for any bounded set $\Lambda \subseteq \mathbb{R}^{|A|}$, $\sup_{\lambda \in \Lambda} |\hat{F}_\lambda(\hat{\phi}_\lambda) - F_\lambda(\phi^*_\lambda)| = 0$ a.s., if $C' \sqrt{\frac{1}{n}} \leq \delta < 1$ with some constant $C' > 0$.

Appendix B. Proofs

We mean “without loss of generality” by writing “WLOG”.

B.1 Proof of Lemmas

B.1.1 Proof of Lemma 1

We can easily write the cost function of any classifier $\phi$ as

$$\text{Cost}(\phi) = \sum_{k=1}^{K} \pi^*_k c_k - \mathbb{E}[c_Y 1(\phi(X) = Y)]$$

$$= \sum_{k=1}^{K} \pi^*_k c_k - \mathbb{E}_X \left\{ \mathbb{E}_{Y|X}[c_Y 1(\phi(X) = Y)] \right\}$$

$$= \sum_{k=1}^{K} \pi^*_k c_k - \mathbb{E}_X \left\{ \sum_{k=1}^{K} [1(\phi(X) = k) \cdot c_k \mathbb{P}_{Y|X}(Y = k)] \right\}.$$ 

By the last expression and the definition of $\phi^*$, we have $\text{Cost}(\phi) \geq \text{Cost}(\phi^*)$ for any $\phi$.

B.1.2 Proof of Lemma 10

Similar to the proof of Lemma 1, let’s first simplify the cost function of any classifier $\phi$ as

$$\text{Cost}(\phi) = \mathbb{E}\left[ \sum_{r \neq Y} c_{Y,r} 1(\phi(X) = r) \right]$$

$$= \mathbb{E}_X \left\{ \mathbb{E}_{Y|X}[\sum_{r \neq Y} c_{Y,r} 1(\phi(X) = r)] \right\}$$

$$= \mathbb{E}_X \left\{ \sum_{k=1}^{K} \sum_{r \neq k} [1(\phi(X) = r) \cdot c_k \mathbb{P}_{Y|X}(Y = k)] \right\}.$$ 

Therefore by the definition of $\phi^*$, we have $\text{Cost}(\phi) \geq \text{Cost}(\phi^*)$ for any $\phi$. 39
B.1.3 Proof of Lemma 17
First, we prove that for any compact sets $\Lambda \subseteq \mathbb{R}_{+}^{d}$, $B \subseteq \mathbb{R}^{p}$ and $\Pi \subseteq \mathbb{R}_{+}^{K}$, it holds

\[
\sup_{\lambda \in \Lambda} \sup_{\beta \in B} \sup_{\pi \in \Pi} \left\| \frac{1}{n} \sum_{i=1}^{n} c_{\hat{\phi}(x_{i})}(\lambda, \pi) \mathbb{P}_{Y|x=x_{i}}(Y = \hat{\phi}(x_{i}; \beta, \lambda, \pi); \beta) - \mathbb{E} \left[ c_{\hat{\phi}(X)}(\lambda, \pi) \mathbb{P}_{Y|X}(Y = \hat{\phi}(X; \beta, \lambda, \pi); \beta) \right] \right\| \lesssim \sqrt{\delta} \lor \delta,
\]

with probability at least $1 - \exp\{ -Cn\delta \}$, where $C$ is a positive constant. Here $\hat{\phi}(x; \beta, \lambda, \pi) = \arg \max_{\pi} \{ c_{k}(\lambda, \pi) \mathbb{P}_{Y|x=x} (Y = k; \beta) \}$.

Let $g(x; \beta, \lambda, \pi) = \max_{\pi} \{ c_{k}(\lambda, \pi) \mathbb{P}_{Y|x=x} (Y = k; \beta) \} - \mathbb{E} \left[ \max_{\pi} \{ c_{k}(\lambda, \pi) \mathbb{P}_{Y|x=x} (Y = k; \beta) \} \right]$. Then $\mathbb{E} \hat{\phi}(X) = 0$ and $\sup_{\lambda \in \Lambda} \sup_{\beta \in B} \sup_{\pi \in \Pi} \| \hat{\phi} \|_{\infty} < \infty$. There exists $\sigma > 0$ such that $\sup_{\lambda \in \Lambda} \sup_{\beta \in B} \sup_{\pi \in \Pi} \| \hat{\phi} \|_{\infty} \geq \sum_{i=1}^{n} \mathbb{E} [ \hat{\phi}(X_{i}) ]^{2}$. Then (20) holds due to Theorem 7.3 in Bousquet (2003).

Next, we will show that

\[
\mathbb{P} \left( \sup_{\lambda \in \Lambda} |F_{X}(\hat{\phi}) - F_{X}(\phi^{*})| > \delta \right) \lesssim \delta^{-1} \sup_{k} \mathbb{P} \left[ \mathbb{P}_{Y|X}(Y = k) - \mathbb{P}_{Y|X}(Y = k) > \exp\{ -Cn\delta^{2} \} \right].
\]

By the proof of Lemma 20, combined with Markov inequality and union bounds,

\[
\mathbb{P} \left( \sup_{\lambda \in \Lambda} |F_{X}(\hat{\phi}) - F_{X}(\phi^{*})| > \delta \right) \leq \sum_{k=1}^{K} \mathbb{P} \left( \mathbb{E}_{X} |\mathbb{P}_{Y|X}(Y = k) - \mathbb{P}_{Y|X}(Y = k)| > \frac{\delta}{2CK} \right) + \sum_{k=1}^{K} \mathbb{P} \left( |\hat{\pi}_{k} - \pi_{k}| > \frac{\delta}{2CK} \right) 
\]

\[
\lesssim \delta^{-1} \max_{k} \mathbb{E} \left[ \mathbb{P}_{Y|X}(Y = k) - \mathbb{P}_{Y|X}(Y = k) \right] + \exp\{ -Cn\delta^{2} \}.
\]

Finally, combining (20) and (21), we get the desired conclusion, which completes the proof of Lemma 17.

B.1.4 Proof of Lemma 19
Denote $\theta = (\beta, \lambda, \pi)^{T}$, $U(x; \theta) = c_{\hat{\phi}(x)} \mathbb{P}_{Y|x=x}(Y = \hat{\phi}(x; \theta); \beta) - \mathbb{E} \left[ c_{\hat{\phi}(X)} \mathbb{P}_{Y|X}(Y = \hat{\phi}(X; \theta); \beta) \right]$, and $\hat{\phi}(x; \beta, \lambda, \pi) = \arg \max_{\pi} \{ c_{k}(\lambda, \pi) \mathbb{P}_{Y|x=x} (Y = k; \beta) \}$. First, we prove that for any compact sets $\Lambda \subseteq \mathbb{R}_{+}^{d}$, $B \subseteq \mathbb{R}^{p}$ and $\Pi \subseteq \mathbb{R}_{+}^{K}$, it holds

\[
\lim_{n \to \infty} \sup_{\lambda \in \Lambda} \sup_{\beta \in B} \sup_{\pi \in \Pi} \left| \frac{1}{n} \sum_{i=1}^{n} U(x_{i}; \theta) \right| = 0, \quad a.s.,
\]

We follow the proof idea of Theorem 5.14 in Van der Vaart (2000), which was first stated in Wald (1949). We first check the following two conditions:
(i) $U(x; \theta)$ is a continuous function of $\theta = (\beta, \lambda, \pi)$ for a.s. $x$ w.r.t. the distribution of $X$.

(ii) There is a function $m(x)$ satisfying

$$\sup_{\lambda \in \Lambda} \sup_{\beta \in B} \sup_{\pi \in \Pi} |c_{\hat{\phi}(x)}(\lambda, \pi)P_{Y|X=x}(Y = \hat{\phi}(x; \beta, \lambda, \pi); \beta)| \leq m(x), \mathbb{E}m(x) < \infty.$$ 

First, (ii) is trivial according to the fact that $P_{Y|X=x}(Y = \hat{\phi}(x; \beta, \lambda, \pi); \beta)$ is bounded. For (i), note that $U(x; \theta)$ can be written as a maximum of $K$ continuous functions of $\theta$ by the definition of $\hat{\phi}$, then the continuity of the maximum follows.

Define $W(x; r, \theta) = \sup_{\|\theta'\|_2 \leq r} U(x; \theta')$. By the continuity of $U(x; \theta)$ w.r.t. $\theta$, $W(x; r, \theta)$ is continuous w.r.t. $r$. In addition, by dominated convergence theorem,

$$\lim_{r \to 0} \mathbb{E}[W(X; r, \theta)] = \mathbb{E}\left[\lim_{r \to 0} W(X; r, \theta)\right] = 0.$$ 

Then for any $\theta \in B \otimes \Lambda \otimes \Pi$, any $\epsilon > 0$, $\exists r_\epsilon(\theta)$, such that $\mathbb{E}[W(X; r_\epsilon(\theta), \theta)] \leq \epsilon$. Because $B \otimes \Lambda \otimes \Pi$ is compact, there exists a finite subcover of $\bigcup_{\theta \in B \otimes \Lambda \otimes \Pi} B_{r_\epsilon}(\theta)$, which we denoted as $\bigcup_{l=1}^{L} B_{r_l}(\theta)$. Then

$$\sup_{\theta \in B \otimes \Lambda \otimes \Pi} \frac{1}{n} \sum_{i=1}^{n} U(x_i; \theta) \leq \sup_{l=1, \ldots, L} \frac{1}{n} \sum_{i=1}^{n} W(x_i; r_l, \theta) \overset{a.s.}{\rightarrow} \sup_{l=1, \ldots, L} \mathbb{E}[W(X; r_l, \theta)] \leq \epsilon.$$

Constructing a vanishing series $\{\epsilon_r\}_{r=1}^{\infty} \rightarrow 0$ leads to

$$\mathbb{P}\left(\lim_{n \to \infty} \sup_{\theta \in B \otimes \Lambda \otimes \Pi} \frac{1}{n} \sum_{i=1}^{n} U(x_i; \theta) \leq 0\right) = \lim_{r \to \infty} \mathbb{P}\left(\lim_{n \to \infty} \sup_{\theta \in B \otimes \Lambda \otimes \Pi} \frac{1}{n} \sum_{i=1}^{n} U(x_i; \theta) \leq \epsilon_r\right) = 1. \tag{24}$$

On the other hand, we can show $\mathbb{P}\left(\liminf_{n \to \infty} \inf_{\theta \in B \otimes \Lambda \otimes \Pi} \frac{1}{n} \sum_{i=1}^{n} U(x_i; \theta) \geq 0\right) = 1$ in the same way, which combines with (24) implies (23). Therefore, by plugging $\beta = \hat{\beta}$ and $\pi = \hat{\pi}$ in (23), we have

$$\lim_{n \to \infty} \left|\hat{F}_\lambda(\hat{\phi}_\lambda) - \mathbb{E}_X \left[c_{\hat{\phi}_\lambda(X)}(\lambda, \pi)\hat{P}_{Y|X}(Y = \hat{\phi}_\lambda(X))\right]\right| = 0, \text{ a.s..} \tag{25}$$

Next we want to show

$$\lim_{n \to \infty} \sup_{\lambda \in \Lambda} \mathbb{E}_X \left[c_{\hat{\phi}_\lambda(X)}(\lambda, \pi)\hat{P}_{Y|X}(Y = \hat{\phi}_\lambda(X)) - c_{\hat{\phi}_\lambda(X)}(\lambda, \pi)P_{Y|X}(Y = \hat{\phi}_\lambda(X))\right] = 0, \text{ a.s..} \tag{26}$$

Note that the left-hand side is no larger than

$$\lim_{n \to \infty} \max_{k} \mathbb{E}_X \left[\hat{P}_{Y|X}(Y = k) - P_{Y|X}(Y = k)\right]\cdot \max_{k} c_k + 2 \lim_{n \to \infty} \sup_{\lambda \in \Lambda} \max_{k} |c_k(\lambda, \hat{\pi}) - c_k(\lambda, \pi)| = 0,$$

a.s., which is derived by Assumption 2’ with dominated convergence theorem combined with the strong consistency of $\hat{\pi}$. Combining (25) and (26), we finish the proof of Lemma 19.
B.1.5 Proof of Lemma 20

\[
\lim_{n \to \infty} \sup_{\lambda \in \Lambda} |F_n(\hat{\phi}_\lambda) - F_n(\phi^*_\lambda)| = \lim_{n \to \infty} \sup_{\lambda \in \Lambda} \left| \mathbb{E}_X \left[ c_{\phi^*_\lambda}(\lambda, \pi^*) \mathbb{P}_{Y|X}(Y = \phi^*_\lambda(X)) - c_{\phi^*_\lambda}(\lambda, \pi^*) \mathbb{P}_{Y|X}(Y = \hat{\phi}_\lambda(X)) \right] \right|
\leq \lim_{n \to \infty} \sum_{k=1}^{K} \left| \mathbb{E}_X \left[ \mathbb{P}_{Y|X}(Y = k) - \mathbb{P}_{Y|X}(Y = \hat{k}) \right] \cdot \sup_{\lambda \in \Lambda} \max_k c_k + \sup_{\lambda \in \Lambda} \left| c_k(\lambda, \hat{\pi}) - c_k(\lambda, \pi^*) \right| \right|
= 0,
\]
a.s., where the last equation holds because of Assumption 2' and the strong consistency of \( \hat{\pi} \). It suffices to verify the intermediate inequality. For any \( X = x \) and \( \lambda \in \Lambda \), denote \( k = \hat{k}(x) = \hat{\phi}_\lambda(x) \), \( k^* = \hat{k}^*(x) = \phi^*_\lambda(x) \). Then by the definition of \( \hat{\phi}_\lambda \) and \( \phi^*_\lambda \),

\[
0 \leq \mathbb{E}_X \left[ c_{\phi^*_\lambda}(\lambda, \pi^*) \mathbb{P}_{Y|X=x}(Y = \phi^*_\lambda(x)) - c_{\phi^*_\lambda}(\lambda, \pi^*) \mathbb{P}_{Y|X=x}(Y = \hat{\phi}_\lambda(x)) \right]
\leq \mathbb{E}_X \left[ \mathbb{P}_{Y|X=x}(Y = k^*) c_{k^*}(\lambda, \pi^*) - \mathbb{P}_{Y|X=x}(Y = \hat{k}) c_{\hat{k}}(\lambda, \hat{\pi}) \right]
+ \mathbb{E}_X \left[ \mathbb{P}_{Y|X=x}(Y = k^*) c_{k^*}(\lambda, \pi^*) - \mathbb{P}_{Y|X=x}(Y = \hat{k}) c_{\hat{k}}(\lambda, \pi^*) \right]
+ \mathbb{E}_X \left[ \mathbb{P}_{Y|X=x}(Y = \hat{k}) c_{\hat{k}}(\lambda, \pi^*) - \mathbb{P}_{Y|X=x}(Y = \hat{k}) c_{\hat{k}}(\lambda, \pi^*) \right]
\leq 2 \sum_{k=1}^{K} \left| \mathbb{P}_{Y|X=x}(Y = k) c_{k}(\lambda, \pi) - \mathbb{P}_{Y|X=x}(Y = k) c_{k}(\lambda, \pi^*) \right|
\leq 2 \sum_{k=1}^{K} \left| \mathbb{P}_{Y|X=x}(Y = k) c_{k}(\lambda, \pi) - \mathbb{P}_{Y|X=x}(Y = k) c_{k}(\lambda, \pi^*) \right|
\]  

where we used the fact that \( \mathbb{P}_{Y|X=x}(Y = k^*) c_{k^*}(\lambda, \pi^*) - \mathbb{P}_{Y|X=x}(Y = \hat{k}) c_{\hat{k}}(\lambda, \pi) \leq 0 \). Taking the supremum w.r.t. \( \lambda \) and the limit \( n \to \infty \) leads to the desired conclusion.

B.1.6 Proof of Lemma 21

Let’s fix \( D_2 \) and \( n_k \) first. Denote \( \hat{R}_k(\hat{\phi}_\lambda) = n_k^{-1} \sum_{i=1}^{n_k} \mathbb{1}(\hat{\phi}(x_i^{(k)}) = k) = n_k^{-1} \sum_{i=1}^{n_k} \mathbb{1}(g(\hat{\lambda})(x_i^{(k)}) > 0) \), where \( g(\hat{\lambda})(x) = c_k(\lambda, \hat{\pi}) \mathbb{P}_{Y|X=x}(Y = k) - \max_{j \neq k} \left[ c_j(\lambda, \hat{\pi}) \mathbb{P}_{Y|X=x}(Y = j) \right] \). Given any \( D_2 \), we claim that the VC dimension of \( A_k = \{ \mathbb{1}(g(\hat{\lambda})(x) > 0) : \lambda \succeq 0 \} \) is finite for any \( k \).

The proof is straightforward. Recall that given \( D_2 \) and \( \lambda \),

\[
c_k(\lambda, \pi) = \begin{cases} 
   w_k/\hat{\pi}_k, & k \notin A; \\
   (w_k + \lambda_k)/\hat{\pi}_k, & k \in A.
\end{cases}
\]

For \( k \in A \), \( g(\hat{\lambda})(x) = (w_k + \lambda_k)/\hat{\pi}_k \cdot \mathbb{P}_{Y|X=x}(Y = k) - \max_{j \notin A} \left[ (w_j + \lambda_j)/\hat{\pi}_j \cdot \mathbb{P}_{Y|X=x}(Y = j) \right] \). Note that

\[
\{ x : g(\hat{\lambda})(x) > 0 \} = \bigcap_{j \in A \setminus \{ k \}} \{ x : (w_j + \lambda_j)/\hat{\pi}_j \cdot \mathbb{P}_{Y|X=x}(Y = j) < (w_k + \lambda_k)/\hat{\pi}_k \cdot \mathbb{P}_{Y|X=x}(Y = k) \}.
\]
\[ \bigcap_{j \notin A} \{ x : w_j / \pi_j \cdot \hat{P}_{Y|X=x}(Y = j) < (w_k + \lambda_k) / \pi_k \cdot \hat{P}_{Y|X=x}(Y = k) \}, \]

where each of \( \{ x : (w_j + \lambda_j) / \pi_j \cdot \hat{P}_{Y|X=x}(Y = j) < (w_k + \lambda_k) / \pi_k \cdot \hat{P}_{Y|X=x}(Y = k) \} \) belongs to the classification result of a linear classifier with parameter \( \lambda_j \) if we see \( \{ \hat{P}_{Y|X=x}(Y = j) \} \) as the predictors. Denote \( s_{\lambda_j}(x) = 1((w_j + \lambda_j) / \pi_j \cdot \hat{P}_{Y|X=x}(Y = j) < (w_k + \lambda_k) / \pi_k \cdot \hat{P}_{Y|X=x}(Y = k)) \) and \( \tilde{s}_{\lambda_j}(x) = 1(w_j / \pi_j \cdot \hat{P}_{Y|X=x}(Y = j) < (w_k + \lambda_k) / \pi_k \cdot \hat{P}_{Y|X=x}(Y = k)) \).

For any \( \tilde{n} \) data points \( \{ x_1, \ldots, x_{\tilde{n}} \} \), denote \( \{ \{ s_{\lambda_j}(x_i) \} \}_{i=1}^{\tilde{n}} : \lambda_j \geq 0 \} \) as \( S_j(\{ x_i \}_{i=1}^{\tilde{n}}) \) for \( j \notin A \), \( \{ \{ \tilde{s}_{\lambda_j}(x_i) \} \}_{i=1}^{\tilde{n}} : \lambda_j \geq 0 \} \) as \( \tilde{S}_j(\{ x_i \}_{i=1}^{\tilde{n}}) \), which include all possible classification result of \( \{ x_i \}_{i=1}^{\tilde{n}} \) for all possible \( \lambda_j \) values. Since linear classifiers have finite VC dimension \( d_k \), by Sauer’s lemma, when \( \tilde{n} \geq d_k \), \( |S_j(\{ x_i \}_{i=1}^{\tilde{n}})| \leq C \tilde{n}^{d_k} \), \( |\tilde{S}_j(\{ x_i \}_{i=1}^{\tilde{n}})| \leq C \tilde{n}^{d_k} \). And it’s easy to see that \( |S_k(\{ x_i \}_{i=1}^{\tilde{n}})| = 2^{\tilde{n}} > C \tilde{n}^{d_k} \) as \( \tilde{n} \) is larger than some constant, which is contradicted. Therefore VC(\( A_k \)) must be finite. The same arguments hold with \( k \notin A \).

Then the \( \epsilon \)-covering number of \( G_k(\Lambda) = \{ \{ \tilde{s}_{\lambda_j}(x_i) \} : \lambda_j \in \Lambda \} \) w.r.t. \( \ell^2_{\Lambda_k} \)-norm satisfies \( N(\epsilon, G_k, \ell^2_{\Lambda_k}) \leq (C / \epsilon)^V \), where \( V \) is a universal constant for any \( k \). By Lemma 26.2 in Shalev-Shwartz and Ben-David (2014),

\[
E \left[ \sup_{\lambda \in \Lambda} |\hat{R}_k(\hat{\phi}_\lambda) - R_k(\hat{\phi}_\lambda)| \right| D_2, n_k \] \leq 2E \text{Rad}_n(G_k(\Lambda)),
\]

where Rademacher complexity \( \text{Rad}_n(A) = n^{-1}E_{\sigma} \sup_{a \in A} |\sigma^T a| \) and \( \sigma = (\sigma_1, \ldots, \sigma_n)^T \) where each of \( \sigma_i \) independently follows \text{Unif} \((-1, 1)) \). Denote \( n_k = \# \{ i = 1, \ldots, n : y_i = k \} \). Then by applying Dudley’s entropy integral (Theorem 3.1 in Koltchinskii (2011)), for any \( \{ x_1^{(k)}, \ldots, x_n^{(k)} \} \), we get

\[
\text{Rad}_n(G_k(\Lambda)) \leq \int_0^{1/2} \frac{\log N(\epsilon, G_k, \ell^2_{\Lambda_k})}{n_k} \, de \leq n_k^{-1/2} \int_0^{1/2} \sqrt{\log(C / \epsilon)} \, de \leq \sqrt{\frac{1}{n_k}},
\]

leading to

\[
E \left[ \sup_{\lambda \in \Lambda} |\hat{R}_k(\hat{\phi}_\lambda) - R_k(\hat{\phi}_\lambda)| \right| D_2, n_k \] \leq \sqrt{\frac{1}{n_k}}.
\]

Then by the bounded difference inequality,

\[
P \left( \sup_{\lambda \in \Lambda} |\hat{R}_k(\hat{\phi}_\lambda) - R_k(\hat{\phi}_\lambda)| > \delta + Cn_k^{-1/2} \right| D_2, n_k \) \leq \exp(-Cn_k\delta^2),
\]

Thus,

\[
P \left( \sup_{\lambda \in \Lambda} |\hat{R}_k(\hat{\phi}_\lambda) - R_k(\hat{\phi}_\lambda)| > \delta + Cn_k^{-1/2} \right| D_2 \) \leq E \left[ P \left( \sup_{\lambda \in \Lambda} |\hat{R}_k(\hat{\phi}_\lambda) - R_k(\hat{\phi}_\lambda)| > \delta + Cn_k^{-1/2} \right| D_2, n_k \geq \frac{1}{2} n \pi_k^* \right] \right| D_2 \right] + P \left( n_k < \frac{1}{2} n \pi_k^* \right)
\]
\[ \lesssim \exp\{-Cn\delta^2\}, \]

where the constants are not related to \( D_2 \). By taking the expectation w.r.t. \( D_2 \), we get

\[ P \left( \sup_{\lambda \in \Lambda} |\hat{R}_k(\hat{\phi}) - R_k(\hat{\phi})| > \delta + Cn^{-1/2} \right) \lesssim \exp\{-Cn\delta^2\} \]

Since \( \hat{F}_\lambda(\hat{\phi}_\lambda) - F_\lambda(\hat{\phi}_\lambda) \) is a linear combination of \( \hat{R}_k(\hat{\phi}) - R_k(\hat{\phi}) \) with different \( k \)'s, by union bounds, we have

\[ P \left( \sup_{\lambda \in \Lambda} |\hat{F}_\lambda(\hat{\phi}_\lambda) - F_\lambda(\hat{\phi}_\lambda)| > \delta + Cn^{-1/2} \right) \lesssim \exp\{-Cn\delta^2\}. \tag{28} \]

Applying similar arguments in (22), we get

\[ P \left( \sup_{\lambda \in \Lambda} |F_\lambda(\hat{\phi}_\lambda) - F_\lambda(\hat{\phi}_\lambda)| > \delta + Cn^{-1/2} \right) \lesssim \delta^{-1} \max_k E|\hat{F}_Y|X(Y = k) - P_{Y|X}(Y = k)| + \exp\{-Cn\delta^2\}. \tag{29} \]

Combine (28) and (29), we obtain

\[ P \left( \sup_{\lambda \in \Lambda} |\hat{F}_\lambda(\hat{\phi}_\lambda) - F_\lambda(\hat{\phi}_\lambda)| > \delta \right) \lesssim \delta^{-1} \max_k E|\hat{F}_Y|X(Y = k) - P_{Y|X}(Y = k)| + \exp\{-Cn\delta^2\}. \]

when \( \delta \geq C'n^{-1/2} \) for some constant \( C' > 0 \).

### B.2 Proof of Propositions

#### B.2.1 Proof of Proposition 4

Because \( G(\lambda) = \min_{\phi} F_\lambda(\phi) \) and \( F_\lambda(\phi) \) is an affine function in \( \lambda \), by definition \( G(\lambda) \) is concave. Similarly, by definition, \( \hat{G}(\lambda) = \min_{\phi} \hat{F}_\lambda(\phi) \), where \( \hat{F}_\lambda(\phi) \) is an affine function in \( \lambda \). Therefore \( \hat{G}(\lambda) \) is concave as well, which completes our proof.

#### B.2.2 Proof of Proposition 18

By the proof of Theorem 8, for any \( \delta > 0 \), similar to (34) and (35), we can obtain

\[ P(\|\hat{\lambda} - \lambda^*\|_2 > \delta) \leq P \left( \sup_{\lambda \in B_{2\delta}(\lambda^*)} \hat{G}(\lambda) \geq \hat{G}(\lambda^*) \right) + P \left( \sup_{\lambda \in B_{2\delta}(\lambda^*)} G(\lambda) \geq \hat{G}(\lambda^*) \right) \]

\[ \leq P \left( \sup_{\lambda \in B_{2\delta}(\lambda^*)} |\hat{G}(\lambda) - G(\lambda)| \geq -\frac{1}{8} \delta^2 \lambda_{\max}(\nabla^2 G(\lambda^*)) \right) \]

\[ + P \left( \sup_{\lambda \in B_{2\delta}(\lambda^*)} |\hat{G}(\lambda) - G(\lambda)| \geq \frac{1}{8} \inf_{\lambda \in B_{2\delta}(\lambda^*)} t^{-1}_\lambda \delta^2 \lambda_{\max}(\nabla^2 G(\lambda^*)) \right) \]

\[ \leq 2P \left( \sup_{\lambda \in B_{2\delta}(\lambda^*)} |\hat{G}(\lambda) - G(\lambda)| \geq -\frac{1}{8} \delta^2 \lambda_{\max}(\nabla^2 G(\lambda^*)) \right) \]
\[
\zeta \geq \exp\{-Cn\delta^4\} + \delta^2 \max_k \mathbb{E}\left|\hat{\beta}_{Y|X}(Y = k) - \beta_{Y|X}(Y = k)\right|,
\]

where the last inequality comes from Lemma 17 and the second last inequality comes from the fact \(t\alpha > 1\) for any \(\lambda \notin \hat{B}_{2\delta}(\lambda^*)\).

### B.3 Proof of Theorems

#### B.3.1 Proof of Theorem 3

(i) When the strong duality holds, it’s trivial to see that the classifier \(\phi_{\lambda^*}\), which is induced from the solution \(\lambda^*\) in (5) satisfies all the constraints in NP problem (2). This proves the “only if” part. In the following, we will prove the “if” part by assuming such an \(\lambda^{(0)}\) exists.

WLOG, suppose \(P_{X|Y=k}(\phi_{\lambda^{(0)}}(X) \neq k) < \alpha_k\) for all \(k \in \mathcal{A}\). In fact, if some constraints hold with equality, then we can directly jump into Step 2. It is because in each step, we either tune the corresponding \(\lambda\) value to make the constraint hold with equality or shrink the \(\lambda\) to zero. We can treat these classes in \(\mathcal{A}\) for which the constraint holds with equality at the beginning in the same way as the classes for which the constraint holds with equality after tuning in Step 1.

(1) **Step 1:** Let \(\lambda_k = t\lambda^{(0)}_k + (t-1)w_k\) with \(t \in \left[\max_{k \in \mathcal{A}}\{w_k(w_k + \lambda^{(0)}_k)^{-1}\}, 1\right]\), for all \(k \in \mathcal{A}\). As \(t\) decreases from 1, \(P_{X|Y=k}(\phi_{\lambda}(X) \neq k)\) is non-decreasing for all \(k \in \mathcal{A}\). To see this, note that \(\{x : \phi_{\lambda}(X) = k, \phi_{\lambda^{(0)}}(X) = k_2\}\) does not change with \(t\) for any \(k_1, k_2 \in \mathcal{A}\), while event \(\{x : \phi_{\lambda}(X) \in \mathcal{A}, \phi_{\lambda^{(0)}}(X) \notin \mathcal{A}\}\) is non-decreasing in \(t\). Let’s assume one of \(P_{X|Y=k}(\phi_{\lambda}(X) \neq k) - \alpha_k\) will reach zero before \(t\) hits \(\max_k\{w_k(w_k + \lambda^{(0)}_k)^{-1}\}\) for now, and we will revisit the case that \(P_{X|Y=k}(\phi_{\lambda}(X) \neq k) < \alpha_k\) when \(t = \max_k\{w_k(w_k + \lambda^{(0)}_k)^{-1}\}\) by the end of the proof. Denote \(t^{(0)}\) as the maximum \(t\) such that at least one of equations \(P_{X|Y=k}(\phi_{\lambda}(X) \neq k) - \alpha_k\) does not hold. WLOG, suppose \(P_{X|Y=1}(\phi_{\lambda^{(1)}}(X) \neq 1) = \alpha_1\) and \(P_{X|Y=k}(\phi_{\lambda^{(1)}}(X) \neq k) < \alpha_k\) when \(k \in \mathcal{A}\setminus\{1\}\), where \(\lambda^{(1)}_k = t^{(0)}\lambda^{(0)}_k + (t^{(0)} - 1)w_k\).

(2) **Step 2:** Let \(\lambda_k = t\lambda^{(1)}_k + (t-1)w_k\) with \(t \in \left[\max_{k \in \mathcal{A}\setminus\{1\}}\{w_k(w_k + \lambda^{(1)}_k)^{-1}\}, 1\right]\), for all \(k \in \mathcal{A}\setminus\{1\}\). We would like \(\lambda_1\) to satisfy

\[
P_{X|Y=1}(\phi_{\lambda}(X) \neq 1) \\
= P_{X|Y=1}\left(\frac{\lambda_1 + w_1}{\pi_1}P_{Y|X}(Y = 1) < \max\left\{\max_{k \in \mathcal{A}\setminus\{1\}}\left[\frac{\lambda_k + w_k}{\pi_k}P_{Y|X}(Y = k)\right]\right\}\right) \\
= \alpha_1.
\]

Therefore we can solve \(\lambda_1 = \lambda_1(t)\) from (30) as an increasing function of \(t\). Note that when \(t = 1, \lambda_1 = \lambda^{(1)}_1\). Similar to Step 1, as \(t\) decreases from 1, it can be shown that \(P_{X|Y=k}(\phi_{\lambda}(X) \neq k)\) are non-decreasing for all \(k \in \mathcal{A}\setminus\{1\}\). Again, we assume one of \(P_{X|Y=k}(\phi_{\lambda}(X) \neq k) - \alpha_k\) will be zero before \(t\) hits \(\max_{k \in \mathcal{A}\setminus\{1\}}\{w_k(w_k + \lambda^{(1)}_k)^{-1}\}\), and denote \(t^{(1)}\) as the maximum \(t\) such that at least one of equations \(P_{X|Y=k}(\phi_{\lambda}(X) \neq k) - \alpha_k = 0\) holds. WLOG, suppose \(P_{X|Y=1}(\phi_{\lambda^{(2)}}(X) \neq 1) = \alpha_1, P_{X|Y=2}(\phi_{\lambda^{(2)}}(X) \neq 2) = \alpha_2\) and
However, by definition, $\Pr_{X|Y=k}(\phi^*_\lambda(X) \neq k) < \alpha_k$ when $k \in \mathcal{A}\backslash\{1, 2\}$, where $\lambda^{(2)}_k = t(1)\lambda^{(1)}_k + (t(1) - 1)w_k$, $\lambda^{(1)}_1 = \lambda_1(t(1))$.

(3) Step 3: Let $\lambda_k = t\lambda^{(2)}_k + (t - 1)w_k$ with $t \in \left[\max_{k \in \mathcal{A}\backslash\{1, 2\}}\{w_k(w_k + \lambda^{(1)}_k)^{-1}\}, 1\right]$, for all $k \in \mathcal{A}\backslash\{1, 2\}$.

Continue this process, until the final classifier $\phi^*_\lambda$ corresponding to the final $\lambda$ satisfies all constraints with equality. That is, in the final step, we obtain $\tilde{\lambda}$ such that $\Pr_{X|Y=k}(\phi^*_\tilde{\lambda}(X) \neq k) = \alpha_k$ for all $k \in \mathcal{A}$. Define Lagrangian dual function $L(\lambda, \phi) = \sum_{k \in \mathcal{A}} \lambda_k[\Pr_{X|Y=k}(\phi(X) \neq k) - \alpha_k] + \sum_{k=1}^K w_k\Pr_{X|Y=k}(\phi(X) \neq k)$. Then $\phi^*_\lambda$ is feasible in NP problem,

$$L(\tilde{\lambda}, \phi^*_\lambda) = \inf_{\phi} L(\lambda, \phi)$$

$$= \sum_{k=1}^{K} w_k\Pr_{X|Y=k}(\phi^*_\lambda(X) \neq k)$$

$$\geq \sum_{k=1}^{K} w_k\Pr_{X|Y=k}(\phi^*(X) \neq k)$$

$$= \inf_{\lambda \in \mathbb{R}^{|\mathcal{A}|}_+} \sup_{\phi} L(\lambda, \phi).$$

Therefore $\sup_{\lambda \in \mathbb{R}^{|\mathcal{A}|}_+} \inf_{\phi} L(\lambda, \phi) = \inf_{\phi} \sup_{\lambda \in \mathbb{R}^{|\mathcal{A}|}_+} L(\lambda, \phi)$, which implies the strong duality.

The last thing left is to discuss the issue we mentioned in Step 1, i.e. what happens if $\Pr_{X|Y=k}(\phi^*_\lambda(X) \neq k) < \alpha_k$ when $t = \max_{k \in \mathcal{A}\backslash\{1\}}\{w_k(w_k + \lambda^{(0)}_k)^{-1}\}$. At this time, at least one $\lambda_k$ will be zero. WLOG, suppose $\lambda_1 = 0$ while the other $\lambda_k > 0$. Let $\lambda_k(t) = t\lambda_k + (t - 1)w_k$, where $t \in \left[\max_{k \in \mathcal{A}\backslash\{1\}}\{w_k(w_k + \lambda^{(0)}_k)^{-1}\}, 1\right]$, for $k \in \mathcal{A}\backslash\{1\}$. Again, it can be shown that as $t$ decreases from 1, $\Pr_{X|Y=k}(\phi^*_\lambda(X) \neq k)$ are non-decreasing for all $k \in \mathcal{A}$. Then we will either find some $t$ such that $\Pr_{X|Y=k}(\phi^*_\lambda(X) \neq k) = \alpha_k$ holds for some $k \in \mathcal{A}\backslash\{1\}$, or get $\Pr_{X|Y=k}(\phi^*_\lambda(X) \neq k) < \alpha_k$ for all $k$ when $t = \max_{k \in \mathcal{A}\backslash\{1\}}\{w_k(w_k + \lambda^{(0)}_k)^{-1}\}$. Repeating the process will lead to two results. One is that we get $\Pr_{X|Y=k}(\phi^*_\lambda(X) \neq k) = \alpha_k$ holds for at least one $k$ with some $\lambda$. The other one is we get $\Pr_{X|Y=k}(\phi^*_0(X) \neq k) < \alpha_k$ for all $k \in \mathcal{A}$. In the first case, we can continue the steps above to finally get some $\lambda''$ such that $\Pr_{X|Y=k}(\phi^*_\lambda''(X) \neq k) < \alpha_k$ if and only if $\lambda''_k = 0$. This implies

$$\sup_{\lambda \in \mathbb{R}^{|\mathcal{A}|}_+} \inf_{\phi} L(\lambda, \phi) = L(\lambda'', \phi^*_\lambda'')$$

$$\geq \sum_{k=1}^{K} w_k\Pr_{X|Y=k}(\phi^*_\lambda''(X) \neq k)$$

$$\geq \sum_{k=1}^{K} w_k\Pr_{X|Y=k}(\phi^*(X) \neq k)$$
By the condition, there exists $\phi^*_\lambda$ such that $\phi^*_\lambda$ is feasible for NP problem, then by (i) the NP problem should be feasible as well, which is a contradiction. Therefore the “only if” part holds. Next we will prove the “if” part, where we assume that for any $\lambda \in \mathbb{R}^{[A]}_+$, $\exists$ at least one $k \in A$ such that $R_k(\phi^*_\lambda) = \mathbb{P}_{X|Y \rightarrow k}(\phi^*_\lambda(X) \neq k) > \alpha_k$.

Define the cost
\[ c_k = c_k(\lambda) = \begin{cases} \frac{w_k}{\pi_k^*}, & k \notin A; \\ \frac{(w_k + \lambda_k)}{\pi_k^*}, & k \in A. \end{cases} \]

(i) Step 1: We arbitrarily pick one $\lambda \in \mathbb{R}^{[A]}_+$. Suppose $R_{k_1}(\phi^*_\lambda) > \alpha_{k_1}$ for some $k_1$. Due to the assumption that $\min_{k \in A} \mathbb{P}_{Y|X = x}(Y = k) \geq a > 0$ for a.s. $x$ w.r.t. $\mathbb{P}_X$, if we increase $\lambda_{k_1}$ and keep other $\lambda_k$’s fixed, then $R_{k_1}(\phi^*_\lambda)$ will decrease and finally equal $\alpha_{k_1}$. Denote the current $\lambda$ as $\lambda^{[1]}$.

(ii) Step 2: By the condition, there exists $k_2 \in A \setminus \{k_1\}$ such that $R_{k_2}(\phi^*_\lambda^{[1]}) > \alpha_{k_2}$, $R_{k_1}(\phi^*_\lambda^{[1]}) = \alpha_{k_1}$. Next, we increase $\lambda_{k_2}^{[1]}(1)$ and $\lambda_{k_1}^{[1]}(1)$ at the same time, to decrease $R_{k_2}(\phi^*_\lambda^{[1]})$ while keeping $R_{k_1}(\phi^*_\lambda^{[1]}) = \alpha_{k_1}$. Here we cannot increase $\lambda_{k_2}^{[1]}$ only and leave all the other $\lambda_k^{[1]}$’s unchanged, otherwise we must have $R_{k_1}(\phi^*_\lambda^{[1]}) > \alpha_{k_1}$. Consider all the possible $(\lambda_{k_2}, \lambda_{k_1})$’s which belongs to $Q = \{(\lambda_{k_2}, \lambda_{k_1}) \in \mathbb{R}^2 : \lambda_{k_2} \geq \lambda_{k_1}^{(1)}, \lambda_{k_1} \geq \lambda_{k_1}^{(1)}, R_{k_2}(\phi^*_\lambda^{[1]}) = \alpha_{k_2}, R_{k_1}(\phi^*_\lambda^{[1]}) = \alpha_{k_1} \}$ with $\lambda$ satisfying $\hat{\lambda}_{k_1} = \lambda_{k_1}, \hat{\lambda}_{k_2} = \lambda_{k_2}, \tilde{\lambda}_k = \lambda_{k_1}^{(1)}$ for other $k \neq k_1, k_2$. If $Q = \emptyset$, then we can arbitrarily pick a pair of $(\lambda_{k_2}, \lambda_{k_1})$ in $Q$, denote the corresponding $\lambda$ as $\lambda^{[2]}$, and proceed with Step 3. If $Q = \emptyset$, then for any $\lambda$ with $\lambda_k = \lambda_k^{(1)}$ for $k \in A \setminus \{k_1, k_2\}$ and $R_{k_2}(\phi^*_\lambda^{[1]}) = \alpha_{k_2}$, we must have $R_{k_1}(\phi^*_\lambda^{[1]}) > \alpha_{k_1}$, no matter what $\lambda_{k_1}$ is. Taking one such $\lambda$ such that $R_{k_1}(\phi^*_\lambda^{[1]}) = 1$ for all $k \neq k_1, k_2$ 11, increasing $\lambda_{k_1}$ to $\tilde{\lambda}_{k_1}$, $\lambda_{k_2}$ to $\tilde{\lambda}_{k_2}$ while keeping other $\lambda_k$ fixed, we denote the new $\lambda$ as $\lambda$. We require such a $\lambda$ to satisfy $R_{k_2}(\phi^*_\lambda) = \alpha_{k_2}$. Then due to the absolute continuity of $X|Y = k$ for any $k$, we must have $G(\lambda(t)) = F(\phi^*_\lambda) = \sum_{k \in A} \mathbb{P}_{X|Y \rightarrow k}(\phi^*_\lambda(X) \neq k) + \sum_{k \in A} (w_k + \tilde{\lambda}_k) \mathbb{P}_{X|Y \rightarrow k}(\phi^*_\lambda(X) \neq k) - \sum_{k \in A} \tilde{\lambda}_k \alpha_k \\
\geq C + (w_{k_1} + \tilde{\lambda}_{k_1}) [R_{k_1}(\phi^*_\lambda) - \alpha_{k_1}]$

11. This is possible due to the assumption that $\min_{k \in A} \mathbb{P}_{Y|X = x}(Y = k) \geq a > 0$. In fact, any $\lambda$ satisfying $\min_{k = k_1, k_2} c_k(\lambda, \pi^*) > \max_{k \neq k_1, k_2} c_k(\lambda, \pi^*)(1 - a)$ would work.
as $t \to +\infty$, where $C$ is a constant which does not depend on $t$.

(3) Step 3: We can continue the procedure described in Step 2, and it will finally terminate with an unbounded $G(\bar{\lambda}(t))$ as $t \to +\infty$. Otherwise, we will have $R_k(\phi) \leq \alpha_k$ holds with some classifier $\phi$ for all $k \in A$, which is contradicted. This completes our proof.

B.3.2 Proof of Theorem 6

Part (i) of the proof of Theorem 6 is the same as part (i) of the proof of Theorem 9. So we just sketch the main procedure here and omit the details. First, we need to derive

$$
\mathbb{P}\left( \|\hat{\lambda} - \lambda^*\|_2 > \delta \right) \leq \mathbb{P}\left( \sup_{\lambda \in \mathbb{B}_{2\delta}(\lambda^*)} |\hat{G}(\lambda) - \hat{G}(\lambda^*)| \geq \delta \right) + \mathbb{P}\left( \sup_{\lambda \in \mathbb{B}_{2\delta}(\lambda^*)} |\hat{G}(\lambda) - \hat{G}(\lambda^*)| \geq 0 \right)
$$

$$
\leq 2\mathbb{P}\left( \sup_{\lambda \in \mathbb{B}_{2\delta}(\lambda^*)} |\hat{G}(\lambda) - G(\lambda)| \geq -\frac{1}{8}\delta^2\max_{\lambda \in \Lambda} (\nabla^2 G(\lambda^*)) \right) \lesssim \exp\{-Cn\delta^4\} + \delta^{-2}\max_{k} \mathbb{E}\left[ \left| \hat{P}_{Y|X}(Y = k) - P_{Y|X}(Y = k) \right| \right],
$$

for any $\delta \in (0, 1)$, where the last step is due to Lemma 17. This part can be done by following part (i) in the proof of Theorem 8. Next, we follow (36) in the proof of Theorem 9 to get the desired bound.

For part (ii), by recalling part (ii) in the proof of Theorem 8 and letting $M = 1$, there exists a compact set $\Lambda \subseteq \mathbb{R}^{\lvert A \rvert}_{+}$, such that $\sup_{\lambda \in \Lambda} G(\lambda) > 2$. Therefore,

$$
\mathbb{P}\left( \sup_{\lambda \in \mathbb{R}^{\lvert A \rvert}_{+}} |\hat{G}(\lambda)| = 1 \right) \geq \mathbb{P}\left( \sup_{\lambda \in \Lambda} |G(\lambda) - \hat{G}(\lambda)| \leq 1, \sup_{\lambda \in \Lambda} G(\lambda) > 2 \right)
$$

$$
= \mathbb{P}\left( \sup_{\lambda \in \Lambda} |G(\lambda) - \hat{G}(\lambda)| \leq 1 \right)
$$

$$
\geq 1 - C \left( \max_{k} \mathbb{E}\left[ \hat{P}_{Y|X}(Y = k) - P_{Y|X}(Y = k) \right] \right) + \exp\{-Cn\},
$$

which completes the proof.

B.3.3 Proof of Theorem 8

(i) By Lemmas 19 and 20, for any bounded set $\Lambda \subseteq \mathbb{R}^{\lvert A \rvert}_{+}$,

$$
\lim_{n \to \infty} \sup_{\lambda \in \Lambda} |\hat{G}(\lambda) - G(\lambda)| = 0, a.s.. \quad (32)
$$
Due to Assumption 3, for any sufficiently small $\delta_0 > 0$, when $\lambda \in \bar{B}_{2\delta_0}(\lambda^*), \nabla^2 G(\lambda) \preceq \frac{1}{4} \nabla^2 G(\lambda^*) < 0$. Then by Taylor expansion,

$$G(\lambda) - G(\lambda^*) = \nabla G(\lambda^*)^T (\lambda - \lambda^*) + \frac{1}{2} (\lambda - \lambda^*)^T \nabla^2 G(\lambda^*) (\lambda - \lambda^*)$$

$$\leq \frac{1}{4} (\lambda - \lambda^*)^T \lambda_{\text{max}}(\nabla^2 G(\lambda^*)) (\lambda - \lambda^*),$$

where $t_\lambda \in (0, 1)$. For $\lambda \in \bar{B}_{2\delta_0}(\lambda^*) \setminus \bar{B}_{\delta_0}(\lambda^*)$, $G(\lambda) - G(\lambda^*) \leq \frac{1}{4} \delta_0^2 \lambda_{\text{max}}(\nabla^2 G(\lambda^*))$. Therefore, for any $\lambda \notin \bar{B}_{2\delta_0}(\lambda^*)$, $\exists t_\lambda \in (0, 1)$ such that $(1 - t_\lambda)\lambda^* + t_\lambda \lambda \in \bar{B}_{2\delta_0}(\lambda^*) \setminus \bar{B}_{\delta_0}(\lambda^*)$, which combines with concavity leading to

$$(1 - t_\lambda)G(\lambda^*) + t_\lambda G(\lambda) \leq G((1 - t_\lambda)\lambda^* + t_\lambda \lambda) \leq G(\lambda^*) + \frac{1}{4} \delta_0^2 \lambda_{\text{max}}(\nabla^2 G(\lambda^*)).$$

It follows that $G(\lambda) \leq G(\lambda^*) + \frac{1}{4} \delta_0^2 \lambda_{\text{max}}(\nabla^2 G(\lambda^*))$ for any $\lambda \notin \bar{B}_{2\delta_0}(\lambda^*)$. Besides,

$$\mathbb{P}\left( \limsup_{n \to \infty} \sup_{\lambda \in \bar{B}_{2\delta_0}(\lambda^*) \setminus \bar{B}_{\delta_0}(\lambda^*)} \sup_{\lambda \in \bar{B}_{2\delta_0}(\lambda^*)} \hat{G}(\lambda) - \hat{G}(\lambda^*) \geq 0 \right)$$

$$\leq \mathbb{P}\left( \sup_{\lambda \in \bar{B}_{2\delta_0}(\lambda^*) \setminus \bar{B}_{\delta_0}(\lambda^*)} G(\lambda) + 2 \limsup_{n \to \infty} \sup_{\lambda \in \bar{B}_{2\delta_0}(\lambda^*)} |\hat{G}(\lambda) - G(\lambda)| \geq G(\lambda^*) \right)$$

$$\leq \mathbb{P}\left( \limsup_{n \to \infty} \sup_{\lambda \in \bar{B}_{2\delta_0}(\lambda^*)} |\hat{G}(\lambda) - G(\lambda)| \geq -\frac{1}{8} \delta_0^2 \lambda_{\text{max}}(\nabla^2 G(\lambda^*)) \right)$$

$$= 0. \quad (34)$$

Similarly, for any $\lambda \notin \bar{B}_{2\delta_0}(\lambda^*)$, $\exists t_\lambda \in (0, 1)$ such that $(1 - t_\lambda)\lambda^* + t_\lambda \lambda \in \bar{B}_{2\delta_0}(\lambda^*) \setminus \bar{B}_{\delta_0}(\lambda^*)$. Combining this fact and (33) with the concavity of $\hat{G}(\lambda)$, it implies that

$$(1 - t_\lambda)\hat{G}(\lambda^*) + t_\lambda \hat{G}(\lambda) \leq \hat{G}((1 - t_\lambda)\lambda^* + t_\lambda \lambda)$$

$$\leq G((1 - t_\lambda)\lambda^* + t_\lambda \lambda) + \sup_{\lambda \in \bar{B}_{2\delta_0}(\lambda^*)} |\hat{G}(\lambda) - G(\lambda)|$$

$$\leq G(\lambda^*) - \frac{1}{4} \delta_0^2 \lambda_{\text{max}}(\nabla^2 G(\lambda^*)) + \sup_{\lambda \in \bar{B}_{2\delta_0}(\lambda^*)} |\hat{G}(\lambda) - G(\lambda)|$$

$$\leq \hat{G}(\lambda^*) - \frac{1}{4} \delta_0^2 \lambda_{\text{max}}(\nabla^2 G(\lambda^*)) + 2 \sup_{\lambda \in \bar{B}_{2\delta_0}(\lambda^*)} |\hat{G}(\lambda) - G(\lambda)|,$$

implying

$$\hat{G}(\lambda) \leq \hat{G}(\lambda^*) + t_\lambda^{-1} \left[ \frac{1}{4} \delta_0^2 \lambda_{\text{max}}(\nabla^2 G(\lambda^*)) + 2 \sup_{\lambda \in \bar{B}_{2\delta_0}(\lambda^*)} |\hat{G}(\lambda) - G(\lambda)| \right].$$

Therefore,

$$\mathbb{P}\left( \limsup_{n \to \infty} \sup_{\lambda \notin \bar{B}_{2\delta_0}(\lambda^*)} |\hat{G}(\lambda) - \hat{G}(\lambda^*)| \geq 0 \right)$$

49
\[ P \left( \limsup_{n \to \infty} \sup_{\lambda \notin B_{2 \epsilon_0}(\lambda^*)} \left\{ t_{\lambda}^{-1} \left[ \frac{1}{4} \delta_0^2 \lambda_{\max}(\nabla^2 G(\lambda)) + 2 \sup_{\lambda \in B_{2 \epsilon_0}(\lambda^*)} |\hat{G}(\lambda) - G(\lambda)| \right] \right\} \geq 0 \right) \leq P \left( \sup_{\lambda \notin B_{2 \epsilon_0}(\lambda^*)} \left\{ t_{\lambda}^{-1} \left[ \frac{1}{4} \delta_0^2 \lambda_{\max}(\nabla^2 G(\lambda)) + 2 \limsup_{n \to \infty} \sup_{\lambda \in B_{2 \epsilon_0}(\lambda^*)} |\hat{G}(\lambda) - G(\lambda)| \right] \right\} \geq 0 \right) \leq P \left( \sup_{\lambda \notin B_{2 \epsilon_0}(\lambda^*)} \left\{ t_{\lambda}^{-1} \cdot \frac{1}{4} \delta_0^2 \lambda_{\max}(\nabla^2 G(\lambda)) \right\} \geq 0 \right) = 0. \]

Note that the second inequality holds because the supremum over \( \lambda \notin B_{2 \epsilon_0}(\lambda^*) \) is unrelated to training data, therefore it’s independent of the process \( n \to \infty \) and we can swap the order of limit with supremum. Due to (34) and (35),

\[
P \left( \limsup_{n \to \infty} \|\hat{\lambda} - \lambda^*\|_2 > \delta_0 \right) \leq P \left( \limsup_{n \to \infty} \left[ \sup_{\lambda \in B_{2 \epsilon_0}(\lambda^*) \setminus B_{\epsilon_0}(\lambda^*)} |\hat{G}(\lambda) - \hat{G}(\lambda^*)| \right] \geq 0 \right)
+ P \left( \limsup_{n \to \infty} \left[ \sup_{\lambda \notin B_{2 \epsilon_0}(\lambda^*)} |\hat{G}(\lambda) - \hat{G}(\lambda^*)| \right] \geq 0 \right)
= 0.
\]

Because the conclusion holds for arbitrarily small \( \delta_0 \), by letting \( \delta_0 \to 0 \), we have \( \lim_{n \to \infty} \hat{\lambda} = \lambda^* \) a.s.. Recall that by strong law of large numbers, \( \lim_{n \to \infty} \pi = \pi^* \) a.s.. And by Assumption 2’, \( \lim_{n \to \infty} \tilde{P}_{Y|X=x}(Y = k) = \tilde{P}_{Y|X=x}(Y = k) \) and \( x \) a.s., w.r.t. the distribution of \( X \) (as well as the distribution of \( X|Y = k \) for any \( k \)), since \( \pi_k^* > 0 \) which implies \( \tilde{P}_{X|Y = k} \propto \tilde{P}_X \), for all \( k \)’s.

Denote \( \varphi_k(x; \lambda, \pi, \tilde{P}_{Y|X=x}) = c_k(\lambda, \pi)\tilde{P}_{Y|X=x}(Y = k) - \max_{j \neq k} c_j(\lambda, \pi)\tilde{P}_{Y|X=x}(Y = j) \), where \( \tilde{P}_{Y|X} \) can be any posterior distribution of \( Y|X \). Then by dominated convergence theorem and the continuity of \( \varphi_k(x; \lambda, \pi, \tilde{P}_{Y|X=x}) \) w.r.t. \( (\lambda, \pi, \tilde{P}_{Y|X=x})(Y = k) \),

\[
\lim_{n \to \infty} R_k(\phi) = \lim_{n \to \infty} \tilde{P}_{X|Y=k}(\varphi_k(X; \hat{\lambda}, \hat{\pi}, \hat{\tilde{P}}_{Y|X}) < 0)
= \tilde{P}_{X|Y=k} \left( \lim_{n \to \infty} \varphi_k(X; \hat{\lambda}, \hat{\pi}, \hat{\tilde{P}}_{Y|X}) < 0 \right)
= \tilde{P}_{X|Y=k} \left( \lim_{n \to \infty} \varphi_k(X; \lambda^*, \pi^*, \tilde{P}_{Y|X}) < 0 \right)
= R_k(\phi^*), \quad \text{a.s.,}
\]

for any \( k \). Followed by basic calculations, part (i) of Theorem 8 is proved.

Furthermore, if \( P(\hat{\lambda}_k > \delta_n) \to 1 \) for any vanishing sequence \( \{\delta_n\}_{n=1}^{\infty} \to 0 \), then by the consistency \( \lambda_k^* > 0 \), which implies \( R_k(\phi^*) = \alpha_k \) by complementary slackness (Boyd and Vandenberghe, 2004).

(ii) By strong duality, the infeasibility of NP problem leads to \( \sup_{\lambda \geq 0} G(\lambda) = +\infty \). There exists a sequence of compact sets \( \{\Lambda_j\}_{j=1}^{\infty} \) satisfying \( \sup_{\lambda \in \Lambda_j} G(\lambda) \to +\infty \) as \( j \to \infty \). Then for any \( M > 0 \), \( \exists \) a positive integer \( J = J(M) \), such that when \( j \geq J \), \( \sup_{\lambda \in \Lambda_j} G(\lambda) > 2M \).
It follows that
\[
\mathbb{P}
\left( \lim_{n \to \infty} \sup_{\lambda > 0} \hat{G}(\lambda) \geq M \right) \geq \mathbb{P}
\left( \lim_{n \to \infty} \sup_{\lambda \in \Lambda_j} |G(\lambda) - \hat{G}(\lambda)| \leq M, \sup_{\lambda \in \Lambda_j} G(\lambda) > 2M \right) = 1,
\]
due to (32). Specially, by letting \( M = 1 \), we have proved part (ii).

**B.3.4 Proof of Theorem 9**

Since all norms are equivalent in a finite-dimensional space, there exists \( R_1, R_2 > 0 \) such that
\[
\{ \lambda : \| \lambda \|_2 \leq R_1 \} \subseteq \{ \lambda : \| \lambda \|_\infty \leq R \} \subseteq \{ \lambda : \| \lambda \|_2 \leq R_2 \}.
\]

(i) Due to Assumption 3, for any sufficiently small \( \delta > 0 \), when \( \lambda \in \bar{B}_R(\lambda^*) \), \( \nabla^2 G(\lambda) \geq \frac{1}{2} \nabla^2 G(\lambda^*) \). Therefore, for any \( \lambda \notin \bar{B}_R(\lambda^*) \), \( \exists \lambda \in (0, 1) \) such that \( (1 - t_\lambda) \lambda^* + t_\lambda \lambda \in \bar{B}_R(\lambda^*) \), which combines with concavity leading to
\[
(1 - t_\lambda)G(\lambda^*) + t_\lambda G(\lambda) \leq G((1 - t_\lambda)\lambda^* + t_\lambda \lambda) \leq G(\lambda^*) + \frac{1}{4} \delta^2 \lambda_{\max}^* (\nabla^2 G(\lambda^*)).
\]

It follows that \( G(\lambda) \leq G(\lambda^*) + \frac{1}{4} \delta^2 \lambda_{\max}^* (\nabla^2 G(\lambda^*)) \) since \( t_\lambda^{-1} > 1 \). Therefore,
\[
\mathbb{P}(\| \lambda - \lambda^* \|_2 > \delta) = \mathbb{P}
\left( \sup_{\lambda \in \bar{B}_{R_2}(\lambda^*) \setminus \bar{B}_{R_1}(\lambda^*)} \hat{G}(\lambda) \geq \hat{G}(\lambda^*) \right)
\leq \mathbb{P}
\left( \sup_{\lambda \in \bar{B}_{R_2}(\lambda^*) \setminus \bar{B}_{R_1}(\lambda^*)} G(\lambda) + 2 \sup_{\lambda \in \bar{B}_{R_2}(\lambda^*)} |\hat{G}(\lambda) - G(\lambda)| \geq G(\lambda^*) \right)
\leq \mathbb{P}
\left( \sup_{\lambda \notin \bar{B}_{R_1}(\lambda^*)} G(\lambda) - \frac{1}{4} \delta^2 \lambda_{\max}^* (\nabla^2 G(\lambda^*)) \geq G(\lambda^*) \right)
+ \mathbb{P}
\left( \sup_{\lambda \in \bar{B}_{R_1}(\lambda^*)} |\hat{G}(\lambda) - G(\lambda)| \geq - \frac{1}{8} \delta^2 \lambda_{\max}^* (\nabla^2 G(\lambda^*)) \right)
\leq \exp\{-Cn\delta^4\} + \delta^{-2} \max_k \mathbb{E}[|\mathbb{P}_{Y|X}(Y = k) - \mathbb{P}_{Y|X}(Y = k)|],
\]
where the last inequality comes from Lemma 21. Denote \( \hat{g}_n^{(k)}(x) = c_k(\lambda, \pi)\hat{P}_{Y|X=x}(Y = k) - \max_{j \neq k}[c_j(\lambda, \pi)\hat{P}_{Y|X=x}(Y = j)] \) and \( \tilde{g}_n^{(k)}(x) = c_k(\lambda, \pi^*)\mathbb{P}_{Y|X=x}(Y = k) - \max_{j \neq k}[c_j(\lambda, \pi^*)\mathbb{P}_{Y|X=x}(Y = j)] \). Let \( t = (\delta/2)^{1/\gamma} \)
\[
\mathbb{P}(|R_k(\hat{\phi}) - R_k(\phi^*)| > \delta)
\]
step by step, and reaching the desired conclusion. We omit the details here.

\[
\exists \theta > \lambda
\]

The proof is almost the same as the proof of Theorem 3, which is done by starting from a

\[B.3.5 \text{ Proof of Theorem 12}\]

(ii) Recall part (ii) in the proof of Theorem 8. When

\[\delta > C\]

\[\sup \left\{ \pi_k - \pi_k^* \right\} > C \delta \]

\[\sup \left\{ \hat{\pi}_k - \pi_k^* \right\} > C \delta \]

\[\exp \left\{ -Cn\delta^{4/\gamma} \right\} + \delta^{-2\gamma(1-\delta)} \max_k \mathbb{E} \left| \hat{\pi}_k - \pi_k^* \right| \]

when \( \delta > C' n^{-\gamma/4} \) for some constant \( C' > 0 \), which completes our proof.

(ii) Recall part (ii) in the proof of Theorem 8. When \( R \) is sufficiently large such that

\[\exists R_1 > 0 \text{ satisfying } \{ \lambda : \|\lambda\|_2 \leq R_1 \} \subset \{ \lambda : \|\lambda\|_\infty \leq R \} \text{ and } \sup_{\lambda \in \mathbb{R}^{|A|}, \|\lambda\|_2 \leq R_1} G(\lambda) > 1 + \theta \]

for some \( \theta > 0 \). Therefore,

\[
\mathbb{P} \left( \sup_{\lambda \in \mathbb{R}^{|A|}, \|\lambda\|_\infty \leq R} \hat{G}(\lambda) > 1 \right) \geq \mathbb{P} \left( \sup_{\lambda \in \mathbb{R}^{|A|}, \|\lambda\|_2 \leq R_1} |G(\lambda) - \hat{G}(\lambda)| \leq \theta, \sup_{\lambda \in \mathbb{R}^{|A|}, \|\lambda\|_2 \leq R_1} G(\lambda) > 1 + \theta \right)
\]

\[
= \mathbb{P} \left( \sup_{\lambda \in \mathbb{R}^{|A|}, \|\lambda\|_2 \leq R_1} |G(\lambda) - \hat{G}(\lambda)| \leq \theta \right)
\]

\[
\geq 1 - C \left( \max_k \mathbb{E} |\hat{\pi}_k - \pi_k| + \exp\{-Cn\} \right),
\]

which completes the proof.

B.3.5 Proof of Theorem 12

The proof is almost the same as the proof of Theorem 3, which is done by starting from an NP feasible classifier obtained by the cost-sensitive learning problem, manipulating the \( \lambda \) step by step, and reaching the desired conclusion. We omit the details here.
B.3.6 Proof of Theorem 13

The proof is almost identical to the proof of Theorem 6. We can first prove a similar uniform concentration result as in Lemma 17, then apply a similar analysis used in the proof of Theorem 6.

B.3.7 Proof of Theorem 16

The proof is almost identical to the proof of Theorem 9. We can first prove a similar uniform concentration result as in Lemma 21, then apply a similar analysis used in the proof of Theorem 6. The only difference is in the proof of Lemma 21, we shall replace the inequality (27) with the following one: For any $X = \mathbf{x}$ and $\lambda$, suppose $k = \hat{\phi}_\lambda(\mathbf{x})$ and $k^* = \phi^*_\lambda(\mathbf{x})$,

$$0 \leq \sum_{k \neq k^*} c_{kk}(\lambda, \hat{\pi}) \mathbb{P}_{Y|X=\mathbf{x}}(Y = k) - \sum_{k \neq k^*} c_{kk^*}(\lambda, \pi^*) \mathbb{P}_{Y|X=\mathbf{x}}(Y = k)$$

$$= \sum_{k \neq k^*} c_{kk}(\lambda, \hat{\pi}) \mathbb{P}_{Y|X=\mathbf{x}}(Y = k) - \sum_{k \neq k^*} c_{kk^*}(\lambda, \hat{\pi}) \mathbb{P}_{Y|X=\mathbf{x}}(Y = k)$$

$$+ \sum_{k \neq k^*} c_{kk}(\lambda, \hat{\pi}) \mathbb{P}_{Y|X=\mathbf{x}}(Y = k) - \sum_{k \neq k^*} c_{kk^*}(\lambda, \hat{\pi}) \mathbb{P}_{Y|X=\mathbf{x}}(Y = k)$$

$$+ \sum_{k \neq k^*} c_{kk^*}(\lambda, \hat{\pi}) \mathbb{P}_{Y|X=\mathbf{x}}(Y = k) - \sum_{k \neq k^*} c_{kk^*}(\lambda, \pi^*) \mathbb{P}_{Y|X=\mathbf{x}}(Y = k)$$

$$\leq \max_{r=1:K} \left| \sum_{k \neq r} c_{kr}(\lambda, \hat{\pi}) \mathbb{P}_{Y|X=\mathbf{x}}(Y = k) - c_{kr}(\lambda, \pi^*) \mathbb{P}_{Y|X=\mathbf{x}}(Y = k) \right|$$

$$+ \max_{r=1:K} \left| \sum_{k \neq r} \mathbb{P}_{Y|X=\mathbf{x}}(Y = k) - \mathbb{P}_{Y|X=\mathbf{x}}(Y = k) \right| \cdot \max_{k \neq r} c_{kr}(\lambda, \pi^*)$$

$$\leq 2 \max_{r=1:K} \left| \sum_{k \neq r} c_{kr}(\lambda, \hat{\pi}) - c_{kr}(\lambda, \pi^*) \right|$$

$$+ 2 \max_{r=1:K} \left| \sum_{k \neq r} \mathbb{P}_{Y|X=\mathbf{x}}(Y = k) - \mathbb{P}_{Y|X=\mathbf{x}}(Y = k) \right| \cdot \max_{k \neq r} c_{kr}(\lambda, \pi^*)$$

$$\leq \max_{k=1:K} \left| \hat{\pi}_k - \pi_k \right| + \max_{k=1:K} \left| \mathbb{P}_{Y|X=\mathbf{x}}(Y = k) - \mathbb{P}_{Y|X=\mathbf{x}}(Y = k) \right|,$$

where we used the fact that $\sum_{k \neq \hat{k}} c_{kk}(\lambda, \hat{\pi}) \mathbb{P}_{Y|X=\mathbf{x}}(Y = k) - \sum_{k \neq k^*} c_{kk^*}(\lambda, \hat{\pi}) \mathbb{P}_{Y|X=\mathbf{x}}(Y = k) \leq 0.$