Statistical Theory for Imbalanced Binary Classification

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Abstract

Within the vast body of statistical theory developed for binary classification, few meaningful results exist for imbalanced classification, in which data are dominated by samples from one of the two classes. Existing theory faces at least two main challenges. First, meaningful results must consider more complex performance measures than classification accuracy. To address this, we characterize a novel generalization of the Bayes-optimal classifier to any performance metric computed from the confusion matrix, and we use this to show how relative performance guarantees can be obtained in terms of the error of estimating the class probability function under uniform ($L_\infty$) loss. Second, as we show, optimal classification performance depends on certain properties of class imbalance that have not previously been formalized. Specifically, we propose a novel sub-type of class imbalance, which we call Uniform Class Imbalance. We analyze how Uniform Class Imbalance influences optimal classifier performance and show that it necessitates different classifier behavior than other types of class imbalance. We further illustrate these two contributions in the case of $k$-nearest neighbor classification, for which we develop novel guarantees. Together, these results provide some of the first meaningful finite-sample statistical theory for imbalanced binary classification.

1 Introduction

Many binary classification problems exhibit class imbalance, in which one of the two classes vastly outnumbers the other. Classifiers that perform well with balanced classes routinely fail for imbalanced classes, and developing reliable techniques for classification in the presence of severe class imbalance remains a challenging area of research [He and Ma, 2013, Krawczyk, 2016, Fernández et al., 2018]. Many practical approaches have been proposed to improve performance under class imbalance, including reweighting plug-in estimates of class probabilities [Lewis, 1995], resampling data to improve class imbalance [Chawla et al., 2002], or reformulating classification algorithms to optimize different performance metrics [Dembczynski et al., 2013, Fathony and Kolter, 2019, Joachims, 2005]. Extensive discussion of practical methods for handling class imbalance are surveyed in the books of He and Ma [2013] and Fernández et al. [2018].

Despite the pervasive challenge of class imbalance in practical problems, our theoretical understanding of class imbalance is quite limited. The vast majority of theoretical performance guarantees for classification characterize classification accuracy (or, equivalently, misclassification risk) [Mohri et al., 2018], which is typically an uninformative measure of performance for imbalanced classes. Under measures that are used with imbalanced classes in practice, such as precision,

∗The contributions in this paper were made prior to joining Amazon.
recall, $F_\beta$ scores, and class-weighted scores [Van Rijsbergen, 1974, 1979], existing theoretical guarantees are limited to statistical consistency, in that the algorithm under consideration asymptotically optimizes the metric of choice [Koyejo et al., 2014, Menon et al., 2013, Narasimhan et al., 2014]; specifically, there is no finite-sample theory that would allow comparison of an algorithm’s performance to that of other algorithms or to theoretically optimal performance levels. Additionally, existing theory for classification does not explicitly model the effects of class imbalance, especially severe imbalance (i.e., as the proportion of samples from the rare class vanishes), and hence sheds little light on how severe imbalance should influence the behavior of a classifier.

This paper provides two main contributions. First, in Section 4, we provide a novel characterization of classifiers optimizing general performance metrics that are functions of a classifier’s confusion matrix. This characterization generalizes a classical result – that the Bayes classifier optimizes classification accuracy – to a much larger class of performance measures, including those commonly used in imbalanced classification. While this generalization may be of independent interest, we use it here to show how to provide relative performance guarantees under these more general performance measures. We show, in particular, that performance guarantees can be derived in terms of the error of estimating the class probability function under uniform ($L_\infty$) loss.

This motivates our second main contribution, which is to provide an analysis of $k$-nearest neighbor ($k$NN) classification under uniform loss. In doing so, we also propose an explicit model of a sub-type of class imbalance, which we call Uniform Class Imbalance, and we show that the $k$NN classifier behaves quite differently under Uniform Class Imbalance than under other sub-types of class imbalance. To the best of our knowledge, such sub-types of class imbalance have not previously been distinguished in either the theoretical or practical literature, and we hope that identifying such relevant features of imbalanced datasets may facilitate the development of classifiers that perform well on specific imbalanced classification problems of practical importance.

Collectively, these contributions allow us to provide the first finite-sample performance guarantees for nonparametric binary classification in terms of performance metrics that are appropriate for imbalanced data and to show how these guarantees depend on the nature of imbalance in the data.

2 Related Work

Here, we discuss how our results relate to existing theoretical guarantees for imbalanced binary classification and prior analyses of $k$NN methods.

2.1 Theoretical Guarantees for Imbalanced Binary Classification

To the best of our knowledge, there are no existing statistical guarantees in terms of the functions of the confusion matrix in the generality that we propose. Extensive statistical learning theory for classification in terms of accuracy can be found in Mohri et al. [2018]. However, in the presence of severe class imbalance, accuracy ceases to be an informative measure of performance [Cortes and Mohri, 2004]. A straightforward alternative is cost-weighting. This is intuitive in applications where costs can be explicitly assigned, and statistically, weighting is equivalent to threshold selection in the case of binary classification. Interestingly, cost-weighting has been studied under the motivation of addressing class imbalance before [Scott, 2012], but in the context of calibrated losses, i.e., the guarantee that minimizing a surrogate loss for the zero-one classification loss leads to a Bayes-optimal estimator in the classical sense (see Eq. (1); Liu [2007], Tewari and Bartlett [2007]).

In addition to cost-weighting, other methods commonly used for imbalanced binary classification include resampling, margin adjustment, and Neyman-Pearson classification. Various forms of resampling appear most common in practice [He and Ma, 2013]. Undersampling the dominant class is straightforward and provides computational benefits, often with little loss in statistical performance [Fithian and Hastie, 2014], while interest in oversampling rare classes, sometimes referred to as data augmentation, has grown with the advent of sophisticated generative models (such as generative adversarial networks (GANs)) to produce additional data [Mariani et al., 2018]. However, the theoretical ramifications of oversampling techniques used for imbalanced classification, most commonly variants of SMOTE [Chawla et al., 2002], are poorly understood. Margin-adjustment involves adjusting the margins of support vector machines (SVMs) to appropriately handle class-
A family of techniques related to our work comes from the perspective of Neyman-Pearson classification, which attempts to minimize misclassification error on one class subject to a constraint on the maximum misclassification error on a second class, following the structure of statistical hypothesis testing. Our first main result (Theorem 3) implicitly involves re-framing optimization of general classification performance measures in the Neyman-Pearson framework, and some of our results for classification have analogues in the classical hypothesis testing literature [Lehmann and Romano, 2006]. Unlike many methods in imbalanced classification, substantial theoretical guarantees do exist for Neyman-Pearson classification [Rigollet and Tong, 2011, Tong, 2013, Tong et al., 2016], but these results focus on performance within the Neyman-Pearson framework, rather than in terms of general classification performance measures, which are the focus of our work.

Finally, the most similar existing results to our Theorem 3 are due to Yan et al. [2018] and Wang et al. [2019]; we discuss these results in detail after presenting Theorem 3 in Section 4.

2.2 kNN Classification and Regression

The kNN classifier, first published by Fix and Hodges [1951], is one of the oldest and most well-studied nonparametric classifiers. Early theoretical results include those of Cover and Hart [1967], who showed that the misclassification risk of the kNN classifier with \( k = 1 \) is at most twice that of the Bayes-optimal classifier, and Stone [1977], who showed that the kNN classifier is Bayes-consistent if \( k \to \infty \) and \( k/n \to 0 \). An extensive literature on the accuracy/misclassification risk of kNN classification has since developed [Devroye et al., 1996, Györfi et al., 2002, Samworth, 2012, Chaudhuri and Dasgupta, 2014, Biau and Devroye, 2015, Gadat et al., 2016, Döring et al., 2018, Cannings et al., 2019].

Rather than accuracy bounds for kNN classification, the bounds on uniform error we present in Section 5 are most closely related to risk bounds for kNN regression, of which the results of Biau et al. [2010] are representative. Biau et al. [2010] gives convergence rates for kNN regression in \( L_2 \) risk, weighted by the covariate distribution, in terms of noise variance and covering numbers of the covariate space. While closely related to our bounds on uniform (\( L_\infty \)) risk, their results differ in at least three main ways. First, minimax rates under \( L_\infty \) risk are necessarily worse than under \( L_2 \) risk by a logarithmic factor (as implied by our lower bounds). Second, that fact that Biau et al. [2010] use a risk that is weighted by the covariate distribution allows them to avoid our assumption that the covariate density is lower bounded away from 0, whereas, the lower boundedness assumption is unavoidable under \( L_\infty \) risk and is ultimately necessary for analyzing general classification performance measures. Finally, instead of Bernoulli noise, Biau et al. [2010] assume additive noise with finite variance; using Bernoulli noise is crucial for us to accurately model the effect of severe class imbalance.

Research on improving kNN for imbalanced classification has focused on algorithmic modifications, which are surveyed by Fernández et al. [2018]. Examples include prototype selection, in which representative points are selected from the training set to use with the kNN classifier [Liu and Chawla, 2011, López et al., 2014, Vluymans et al., 2016], and gravitational methods, in which the distance function is modified to resemble the gravitational force [Cano et al., 2013, Zhu et al., 2015]. However, to the best of our knowledge, no statistical guarantees exist for such methods.

3 Setup and Notation

Let \((\mathcal{X}, \rho)\) be a separable metric space, and let \(\mathcal{Y} = \{0, 1\}\) denote the set of classes. Consider a dataset of \(n\) independent samples \((X_1, Y_1), \ldots, (X_n, Y_n)\) drawn from a distribution \(P_{X,Y}\) on \(\mathcal{X} \times \mathcal{Y}\) with marginals \(P_X\) and \(P_Y\).

To construct classifiers that optimize general performance metrics, it will be necessary to consider stochastic classifiers, which may assign inputs to classes nondeterministically. Formally, letting \(B := \{Y \sim \text{Bernoulli}(p) : p \in [0, 1]\}\) denote the set of binary random variables, a stochastic classifier can be modeled as a mapping \(\hat{Y} : \mathcal{X} \to B\), where, for any \(x \in \mathcal{X}\), \(E[\hat{Y}(x)]\) is the probability that the classifier assigns \(x\) to class 1. We will use \(SC\) to denote the class of all stochastic classifiers.
The true regression function \( \eta : \mathcal{X} \to [0, 1] \) is defined by
\[
\eta^*(x) = \mathbb{P}[Y = 1 | X = x] = \mathbb{E}[Y | X = x];
\]
that is, given an instance \( X_i \), the label \( Y_i \) has a Bernoulli distribution with mean \( \eta(X_i) \). As we show in the next section, an optimal classifier can always be written in terms of the true regression function \( \eta \), motivating estimates \( \hat{\eta} : \mathcal{X} \to [0, 1] \) of \( \eta \). Such estimates \( \hat{\eta} \) are called “regressors”.

## 4 Optimal Classification beyond Accuracy

A famous result states that classification accuracy is maximized by the “Bayes” classifier
\[
\hat{Y}(x) \sim \text{Bernoulli} \left( 1 \{ \eta^*(x) > 0.5 \} \right).
\] (1)

This result is of limited practical value when \( \eta^* \) is unknown, but it is a cornerstone of the statistical theory of binary classification because it provides an optimal performance benchmark against which a classifier of interest can be evaluated in terms of classification accuracy \[ \hat{\eta}(x) = \hat{Y}(x) \] wherein the true positive rate \( TP \) and the true and empirical false positive (FP) decrease. We therefore define the class of Confusion Matrix Measures (CMMs) as follows:

**Definition 1 (Confusion Matrix Measure (CMM)).** A function \( M : \mathcal{C} \to \mathbb{R} \) is called a confusion matrix measure (CMM) if, for any confusion matrix
\[
C = \begin{bmatrix}
TN & FP \\
FN & TP
\end{bmatrix} \in \mathcal{C}, \quad \epsilon_1 \in [0, FP], \text{ and } \epsilon_2 \in [0, FN], \text{ we have } M(C) \leq M \left( \begin{bmatrix}
TN + \epsilon_1 & FP - \epsilon_1 \\
FN - \epsilon_2 & TP + \epsilon_2
\end{bmatrix} \right).
\]

Under this definition, correcting any incorrect classification should not reduce a CMM. This mild condition is satisfied by all performance measures commonly used in practice, including weighted accuracies, precision, recall, \( F_\beta \) scores, and MCC. Our main result, presented below, will generalize the Bayes classifier (1) to arbitrary CMMs.
4.2 Generalizing the Bayes Classifier

The Bayes classifier given in Eq. (1) thresholds the regression function deterministically at the value 0.5. The following definition generalizes this to a stochastic threshold at an arbitrary value:

**Definition 2** (Regression-Thresholding Classifier). A classifier \( \hat{Y} : \mathcal{X} \to B \) is called a regression-thresholding classifier if, for some \( p, t \in [0, 1] \) and some \( \eta : \mathcal{X} \to [0, 1] \),

\[
\hat{Y}(x) \sim \text{Bernoulli}(p\{\eta(x) = t\} + 1\{\eta(x) > t\}), \quad \text{for all } x \in \mathcal{X}.
\]

In the sequel, we will denote such classifiers \( \hat{Y}_{p,t}\eta \) and refer to the pair \((p,t)\) as the threshold.

Given Definitions 1 and 2, we can state the main result of this section:

**Theorem 3.** If \( \arg\max_{\hat{Y} \in \mathcal{SC}} M(C_{\hat{Y}}) \neq \emptyset \), then there exists a regression-thresholding classifier

\[
\hat{Y}_{p,t,\eta} \in \arg\max_{\hat{Y} \in \mathcal{SC}} M(C_{\hat{Y}}).
\]

Theorem 3 states that, if a CMM \( M \) is maximized by any stochastic classifier, then \( M \) can be maximized by some regression-thresholding classifier. As a special case, the optimality of the classical Bayes classifier corresponds to \( M(C) = TN + TP, p = 0, \) and \( t = 0.5 \). Since classifiers of the form (4) generalize both the regression-thresholding structure and optimality properties of the Bayes classifier, we will refer to them, in the sequel, as generalized Bayes classifiers. Note that the existence of any maximizer \( \hat{Y} \) of \( M(C_{\hat{Y}}) \) depends on specific properties, such as (semi)continuity or convexity of \( M \); we do not investigate the question of existence here and focus only on characterizing a particular maximizer when it exists. Moreover, maximizers \( \hat{Y} \) of \( M(C_{\hat{Y}}) \) are typically not unique, since, for example, changing \( \hat{Y} \) on sets of \( P_X \)-measure 0 does not change \( C_{\hat{Y}} \); however, among maximizers, generalized Bayes classifiers are an important, mathematically well-behaved subclass.

To the best of our knowledge, no previous results provide such a precise and general characterization of an optimal classifier. The most similar results of which we are aware are those of Yan et al. [2018] and Wang et al. [2019]. Theorem 3.1 of Yan et al. [2018] shows that, under a “karmic” assumption slightly stronger than our monotonicity assumption in Definition 1, if the random variable \( \eta(X) \) is absolutely continuous (i.e., has a density with respect to Lebesgue measure on \([0, 1]\)), then an optimal classifier can be obtained by (deterministically) thresholding the regression function \( \eta \). Our Theorem 3 is strictly more general, since, if \( \eta(X) \) is absolutely continuous, then one can set \( p = 0 \) without changing \( C_{\hat{Y}_{p,t,\eta}} \). More recently, Wang et al. [2019] showed (in their Corollary 2), under absolute continuity of \( \eta(X) \) and a monotonicity assumption comparable to our Definition 1, that the optimal classifier can always be written as a mixture of two deterministic classifiers. Although Wang et al. [2019] consider more general multiclass and multilabel settings, in the binary setting, our result is more precise than theirs, since our regression-thresholding classifiers are deterministic except for a single value of \( \eta \). We leave it to future work to develop a similarly precise generalization of this result to multiclass and multilabel settings. Interestingly, Wang et al. [2019] claim that regularity assumptions on \( \eta(X) \) such as absolute continuity “seem to be unavoidable”, and our Theorem 3 appears to be the first result to omit such assumptions; specifically, we show that this comes at the cost of the optimal classifier possibly being non-deterministic for a single atom of \( \eta(X) \).

Finally, we note that there exist a number of relevant results that are specific to certain CMMs, such as Lemma 12 of Zhao et al. [2013], which provides a similar characterization of the (deterministic) classifier that maximizes the \( F_1 \) score.

We prove Theorem 3 in Appendix A using a series of variational arguments. Roughly speaking, given a classifier \( \hat{Y} \) not of the form (4), we construct a perturbation \( \hat{Y}' \) of \( \hat{Y} \) such that either \( M(C_{\hat{Y}}) < M(C_{\hat{Y}'}) \) or \( \hat{Y}' \) is of the form (4) and \( M(C_{\hat{Y}}) \leq M(C_{\hat{Y}'}) \). Since, in general, the classifier \( \hat{Y} \) might be quite poorly behaved (e.g., its behavior on sets of \( P_X \)-measure 0 could be arbitrary), the main technical complexity lies in constructing admissible perturbations (i.e., those that are well-defined classifiers). For this reason, the proof of Theorem 3 involves a series of constructions of increasingly well-behaved classifiers.

Theorem 3 shows that the generalized Bayes classifier can be written in terms of the regression function \( \eta \) and at most 2 scalar parameters \( p \) and \( t \) depending on the distribution of \( \eta(X) \) and the
CMM $M$. We now provide a simple example showing that the generalized Bayes classifier cannot be further simplified without additional assumptions:

**Example 4.** Suppose that $\mathcal{X} = \{0\}$ is a singleton, that $\eta(0) \in (0, 1)$, and, for some $\theta > 0$, $M(C) = (TP)^\theta TN$. One can easily check that $M$ is a valid CMM. Suppose $\hat{Y}$ is a classifier of the form (4), with generalized threshold $(p, t)$. It is straightforward to compute that $M(C_{\hat{Y}}) = (p\eta(0))^\theta(1-p)(1-\eta(0))\{t = \eta(0)\}$, and that $M(C_{\hat{Y}})$ is uniquely maximized by $p = \frac{\theta}{\theta+1} \in (0, 1)$ and $t = \eta(0) \in (0, 1)$. This shows that both generalized threshold parameters $p$ and $t$ in Eq. (4) are necessary in the absence of further assumptions on $M$ or $\eta$. This example also illustrates the need for stochasticity in classifiers optimizing general CMMs. Specifically, for any deterministic classifier $\hat{Y}$, either $\hat{Y}(0) = 0$ (so that $TP = 0$) or $\hat{Y}(0) = 1$ (so that $TN = 0$); in either case, $M(C_{\hat{Y}}) = 0$.

### 4.3 Relative Performance Guarantees in terms of the Generalized Bayes Classifier

Theorem 3 motivates a two-step approach to imbalanced classification in which one first estimates the regression function $\eta$ and then selects a generalized threshold $(p, t)$ that optimizes empirical performance $M(C_{\hat{Y}})$. Such an approach can have a number of practical advantages; for example, one can address covariate shift (specifically, a change in $P_Y | X$), or retrain a classifier trained under one CMM to perform well under another CMM, by simply re-selecting the two scalar parameters $p$ and $t$. This may be statistically and computationally much easier than retraining a classifier from scratch. In this section, we focus on an advantage for theoretical analysis, namely that the error of such a classifier can be decomposed into errors in selecting $(p, t)$ and errors in estimating $\eta$, facilitating the derivation of performance guarantees relative to the generalized Bayes classifier (4). All results in this section are proven in Appendix B.

Our first lemma bounds the performance difference of thresholds when two regressors in terms of their uniform distance. This will allow us to bound the error of using a regressor $\hat{\eta}$ instead of the true regression function $\eta$.

**Lemma 5.** Let $p, t \in [0, 1]$ and let $\eta, \eta' : \mathcal{X} \rightarrow [0, 1]$. Then,

$$\left\| C_{\hat{\eta}_{p,t,\eta}} - C_{\hat{\eta}_{p,t,\eta'}} \right\|_{\infty} \leq P \left[ |\eta(X) - t| \leq \|\eta - \eta'\|_{\infty} \right].$$

Intuitively, Lemma 5 bounds the largest difference in the confusion matrices of $\hat{\eta}_{p,t,\eta}$ and $\hat{\eta}_{p,t,\eta'}$ by the probability that the threshold $t$ lies between $\eta$ and $\eta'$. As we will show later, under standard margin assumptions, this can be bounded by the $L_{\infty}$ distance $\|\eta - \eta'\|_{\infty}$ between $\eta$ and $\eta'$.

Our second lemma bounds the worst-case error (over all thresholds $(p, t) \in [0, 1]$) of our estimated confusion matrix. This will allow us to bound the error due to using an empirically selected threshold $(\hat{p}, \hat{t})$ instead of the threshold $(p^*, t^*)$ that is optimal for the true regression function.

**Lemma 6.** Let $\eta : \mathcal{X} \rightarrow [0, 1]$ be any regression function. Then, with probability at least $1 - \delta$,

$$\sup_{p,t\in[0,1]} \|C_{\hat{\eta}_{p,t,\eta}} - C_{\hat{\eta}_{p,t,\eta'}}\|_{\infty} \leq \frac{8}{n} \log \left( \frac{32(2n+1)}{\delta} \right).$$

This result follows from a standard Vapnik-Chervonenkis-type bound on the complexity of the set $\{\hat{Y}_{p,t,\eta} : p, t \in [0, 1]\}$ of possible regression-thresholding classifiers with fixed regression function $\eta$. In fact, in the Appendix, we prove a generalization of Lemma 6 that bounds the error between the empirical and true confusion matrices uniformly over any family $\mathcal{F}$ of (potentially stochastic) classifiers in terms of the growth function of $\mathcal{F}$. As a consequence, for any class $\mathcal{F}$ with finite VC dimension, we obtain uniform convergence at the fairly fast rate $\sqrt{\frac{\log(n/\delta)}{n}}$. As we will formalize later in terms of Lipschitz constants, this suggests that the difficulty in tuning an imbalanced classifier to optimize a particular CMM $M$ comes not from difficulty in estimating the confusion matrix but rather from the instability of many commonly used CMMs. Because Theorem 3 shows that any CMM can be optimized by a regression-thresholding classifier, to reduce notational complexity, we state here only the specific result for regression-thresholding classifiers.

Before combining Lemmas 5 and 6 to give the main result of this section, we present a widely-used margin condition, which characterizes the separation between the two classes.
Definition 7 (Tsybakov Margin Condition). Let $C, \beta \geq 0$, $t \in (0, 1)$. A classification problem specified by covariate distribution $P_X$ and regression function $\eta$ is said so satisfy a $(C, \beta)$-margin condition around $t$ if, for any $\delta > 0$,

$$\mathbb{P} \left[ |\eta(X) - t| \leq \epsilon \right] \leq Ce^{\beta}.$$  

The Tsybakov margin condition, introduced by Mammen and Tsybakov [1999] in the special case $t = 0.5$, has been widely used to establish fast convergence rates for classification in terms of accuracy [Audibert and Tsybakov, 2007, Arlot et al., 2011, Chaudhuri and Dasgupta, 2014].

Together with the margin condition and a Lipschitz smoothness assumption on the CMM $M$, Lemmas 5 and 6 give the following bound on the sub-optimality of any regression-thresholding classifier, where the threshold is selected by maximizing the CMM $M$ on the empirical confusion matrix.

Corollary 8. Let $\eta : \mathcal{X} \to [0, 1]$ denote the true regression function, and let $\hat{\eta} : \mathcal{X} \to [0, 1]$ denote any regressor. Let

$$\left( \hat{p}, \hat{t} \right) := \arg\max_{(p, t) \in [0, 1]^2} M \left( \hat{C}_p, \hat{t}, \hat{\eta} \right) \quad \text{and} \quad \left( p^*, t^* \right) := \arg\max_{(p, t) \in [0, 1]^2} M \left( C, \beta \right),$$  

de note the empirically selected and true optimal thresholds, respectively. Suppose that $M$ is Lipschitz continuous with constant $L_M$ with respect to the uniform ($L_\infty$) metric on $C$. Finally, suppose that $P_X$ and $\eta$ satisfies a $(C, \beta)$-margin condition around $t^*$. Then, with probability at least $1 - \delta$,  

$$M \left( C, \beta \right) - M \left( \hat{C}_p, \hat{t}, \hat{\eta} \right) \leq L_M \left( C \|\eta - \hat{\eta}\|_\infty + 2 \frac{8}{n} \log \frac{32(2n + 1)}{\delta} \right).$$  

The computation of a Lipschitz constant $L_M$ is straightforward for some CMMs, such as weighted accuracy, but is more involved for many other CMMs such as precision, recall, and $F_\beta$ scores, which which the exact value of $L_M$ depends on the true distribution of class labels in the data. In Appendix B.1, we therefore demonstrate how to compute $L_M$ for a few of these standard CMMs.

5 Uniform Error of the $k$-Nearest Neighbor Regressor

In the previous section, for classifiers that threshold an estimate (a “regressor”) of the regression function, we bounded relative performance, as measured by arbitrary CMMs, in terms of the uniform ($L_\infty$) loss of the regression function estimate. In this section, we bound the uniform loss of one such regressor, the widely used $k$-nearest neighbor ($k$NN) regressor.

Our analyses include a parameter $r$, introduced in Section 5.2, that characterizes a novel sub-type of class imbalance, which we call Uniform Class Imbalance. As we discuss later, this leads to insights about how the behavior of the $k$NN classifier depends not only on the degree, but also on the structure, of class imbalance in a given dataset.

5.1 $k$-Nearest Neighbor Regressor

Given a point $x \in \mathcal{X}$, order the training data $X_{\sigma_1(x)}, \ldots, X_{\sigma_n(x)}$ such that

$$\rho \left( X_{\sigma_1(x)}, x \right) \leq \ldots \leq \rho \left( X_{\sigma_n(x)}, x \right);$$  

i.e., $X_{\sigma_i(x)}$ is the $i^{th}$-nearest neighbor of $x$ among $X_1, \ldots, X_n$.

For an integer $k > 0$, the $k$NN regressor $\hat{\eta}_k : \mathcal{X} \to [0, 1]$, is defined by the proportion

$$\hat{\eta}_k(x) = \frac{1}{k} \sum_{i=1}^{k} Y_{\sigma_i(x)}, \quad \text{for all } x \in \mathcal{X},$$  

(5)

of $x$’s $k$-nearest neighbors in class 1.
5.2 Uniform Class Imbalance

In this paper, we formalize a sub-type of class imbalance, which we refer to as Uniform Class Imbalance. We decompose the regression function as \( \eta = r\zeta \), where \( r \in (0, 1] \) and \( \zeta : \mathcal{X} \rightarrow [0, 1] \) is a regression function with \( \sup_{x \in \mathcal{X}} \zeta(x) = 1 \). Note that this decomposition loses no generality, as any regression function \( \eta \) can be written in this form. In Uniform Class Imbalance, \( r \approx 0 \), so that the class \( Y = 1 \) is rare regardless of the covariate \( X \) (hence the name “uniform”).

Uniform Class Imbalance tends to occur in “challenging” classification problems in which the covariate \( X \) provides only partial information about the class \( Y \). Practical examples include rare disease diagnosis [Schaefer et al., 2020], credit card fraud detection [Awonyi et al., 2017], or predicting whether an applicant will be offered a job when there are many more qualified applicants than openings. In practice, in such problems, the classifier’s role is often not so much to make a final class determination as to identify “high-risk” samples \( X \) such that \( \eta(X) \) is relatively elevated, for follow-up investigation. Uniform Class Imbalance can be distinguished from “easier” classification problems in which, for some values \( x \in \mathcal{X} \), \( \eta(X) \approx 1 \) and so a good classifier can confidently assign the label \( Y = 1 \). These include well-separated classes, or the extreme case where \( Y \) is a deterministic function of \( X \), such as in certain protein structure prediction problems [Noé et al., 2020].

5.3 Upper Bounds

In this section, we present bounds on the uniform error \( U(\hat{\eta}) := \|\eta - \hat{\eta}\|_\infty \) of the kNN regressor \( \hat{\eta}_k \), where, for a function \( f : \mathcal{X} \rightarrow \mathbb{R} \), \( \|f\|_{\infty} := \sup_{x \in \mathcal{X}} |f(x)| \) denotes the \( \sup \)-norm of \( f \).

Before presenting our bounds, we define two standard quantities, covering numbers and shattering coefficients, by which we measure the complexity of the feature space.

**Definition 9 (Covering Number).** Suppose \((\mathcal{X}, \rho)\) is a totally bounded metric space. Then, for any \( \epsilon > 0 \), the \( \epsilon \)-covering number \( N(\epsilon) \) of \((\mathcal{X}, \rho)\) is the smallest integer such that there exist \( N(\epsilon) \) points \( x_1, \ldots, x_{N(\epsilon)} \in X \) satisfying \( \mathcal{X} \subseteq \bigcup_{i=1}^{N(\epsilon)} B(x_i, \epsilon) \).

**Definition 10 (Shattering Coefficient of Balls).** For positive integers \( n \),

\[
S(n) := \sup_{x_1, \ldots, x_n \in \mathcal{X}} \left| \{ x_1, \ldots, x_n \} \cap B(x, \epsilon) : x \in \mathcal{X}, \epsilon \geq 0 \right|
\]

denotes the shattering coefficient of open balls in \((\mathcal{X}, \rho)\).

We now state two assumptions we make on the joint distribution \( P_{X,Y} \) of the data

**Assumption 11 (Dense Covariates Assumption).** The marginal distribution \( P_X \) of the covariates is lower bounded in the sense that, for some constants \( p, \alpha, d > 0 \), for any point \( x \in \mathcal{X} \) and radius \( \epsilon \in (0, \epsilon^*) \), we have the inequality \( P_X(B_{\epsilon}(x)) \geq p\epsilon^d \).

Assumption 11 ensures that each query point’s nearest neighbor is sufficiently near. We will also need to assume that the regression function \( \zeta \) is sufficiently smooth:

**Assumption 12 (Hölder Continuity).** \( \zeta \) is \((\alpha, L)\)-Hölder continuous; that is, for all \( x, x' \in \mathcal{X} \), \( |\zeta(x) - \zeta(x')| \leq L\rho^\alpha(x, x') \).

We now provide our upper bound on the uniform error, proven in Appendix C.1.

**Theorem 13.** Under Assumptions 11 and 12, whenever \( k/n \leq p_\epsilon(\epsilon^*)^d/2 \), for any \( \delta > 0 \), with probability at least \( 1 - N \left( (2k/(p_\epsilon n)^{1/d}) \epsilon^{-k/4} - \delta \right) \), we have the uniform error bound

\[
\|\eta - \hat{\eta}\|_\infty \leq 2^\alpha Lr \left( \frac{2k}{p_\epsilon n} \right)^{\alpha/d} + \frac{2}{3k} \log \frac{2S(n)}{\delta} + \sqrt{\frac{2r \log 2S(n)}{k}}. \tag{6}
\]

If \( r \in O \left( \frac{\log S(n)}{n} \right) \), this bound is minimized by \( k \approx n \), giving \( \|\eta - \hat{\eta}\|_\infty \in O_P \left( \frac{\log S(n)}{n} \right) \). Otherwise, under a mild simplifying assumption that \( N(\epsilon) \) increases at most polynomially with \( 1/\epsilon \), this bound is minimized by \( k \approx n^\frac{2\alpha}{1+\alpha} (\log S(n))^{\frac{1}{1+\alpha}} r^{-\frac{\alpha+2}{1+\alpha}} \), giving

\[
\|\eta - \hat{\eta}\|_\infty \in O_P \left( \left( \frac{\log S(n)}{n} \right)^{\frac{\alpha}{1+\alpha}} r^{\frac{\alpha+2}{1+\alpha}} \right). \tag{7}
\]
of the three terms in (6), the first term, of order $r(k/n)^{α/d}$, comes from smoothing bias of the kNN classifier. The second and third terms are due to label noise, with the second term dominating under extreme class imbalance ($r \in O \left( \frac{\log S(n)}{n} \right)$) and the third term dominating otherwise. Theorem 6 shows that the optimal choice of the tuning parameter $k$ is much larger under Uniform Class Imbalance than in the case of balanced classes; indeed, one can check that setting $k \asymp n^{2α/(2α+d)} (\log S(n))^{-d/(2α+d)}$, which is optimal in the balanced case, gives a rate that slower by a factor of $r^{-d/(2α+d)}$. One interpretation is that a larger number of neighbors is needed to obtain enough samples from the rare class to make a reliable prediction at any given point.

The following two examples demonstrate how to apply Theorem 13 in specific settings of interest:

**Corollary 14 (Euclidean, Absolutely Continuous Case).** Suppose $(X, ρ) = ([0, 1]^d, \| \cdot \|_2)$ is the unit cube in $\mathbb{R}^d$, equipped with the Euclidean metric, and $P_X$ has a density that is lower bounded away from 0 on $X$. Then, $N(ε) \leq (2/ε)^d$ and $S(n) \leq 2n^{d+1} + 2$, and so, for $k \asymp n^{2α/(2α+d)} (\log n)^{d/(2α+d)} r^{-d/(2α+d)}$, by Theorem 13,

$$||\hat{η} - η||_∞ \in O_P \left( \left( \frac{\log n}{n} \right)^{\frac{α}{2α+d}} r^\frac{\alpha+d}{2α+d} \right).$$

The most problematic term in this bound is the exponential dependence on the dimension $d$ of the covariates. Fortunately, since Theorem 13 utilizes covering numbers, it improves if the covariates exhibit structure, such as that of a low-dimensional manifold. The next example formalizes this.

**Corollary 15 (Implicit Manifold Case).** Suppose $Z$ is a $[0, 1]^d$-valued random variable with a density lower bounded away from 0, and suppose that, for some Lipschitz map $T : [0, 1]^d \to \mathbb{R}^D$, $X = T(Z)$. Then, $N(ε) \leq (2/ε)^d$, and $S(n) \leq 2n^{D+1} + 2$, and so, by Theorem 13, $k \asymp n^{2α/(2α+D)} (\log n)^{D/(2α+D)} r^{-D/(2α+D)}$,

$$||\hat{η} - η||_∞ \in O_P \left( \left( \frac{\log n}{n} \right)^{\frac{α}{2α+D}} r^\frac{\alpha+D}{2α+D} \right).$$

This shows that, if the $D$ covariates lie implicitly on a $d$-dimensional manifold (e.g., if the covariates are strongly correlated), convergence rates depend on $d$, which may be much smaller than $D$.

We close this section with a lower bound, proven in Appendix C.2, on the minimax uniform error, showing that the rate provided in Theorem 13 is minimax optimal over $(α, L)$-Hölder regression functions, up to a polylogarithmic factor in $r$:

**Theorem 16.** Suppose $X = [0, 1]^d$ is the $d$-dimensional unit cube and the marginal distribution of $X$ is uniform on $X$. Let $Σ^α(L)$ denote the family of $(α, L)$-Hölder continuous regression function. Then, for any $α, L > 0$, there exist constants $n_0$ and $c > 0$ (depending only on $α$, $L$, and $d$) such that, for all $n \geq n_0$, and any estimator $\hat{η}$,

$$\sup_{ζ \in Σ^α(L)} \mathbb{P} \left[ \|\hat{η} - η\|_∞ \geq c \left( \frac{\log(nr)}{n} \right)^{\frac{α}{α+d}} r^{\frac{α+d}{2α+d}} \right] \geq \frac{1}{8}.$$

### 5.4 Discussion

The upper bounds on $||\hat{η} - η||_∞$ given in this section can be plugged directly into Corollary 8 to provide error bound under arbitrary CMMs, in terms of the sample size $n$, hyperparameter $k$, degree $d$ of Uniform Class Imbalance, and complexity parameters (margin $β$, smoothness $α$, intrinsic dimension $d$, etc.) of $X$ and $P_{X,Y}$. Thus, these results collectively give some of the first finite-sample guarantees under general performance metrics used for imbalanced classification.

As noted previously, our analysis shows that, under severe Uniform Class Imbalance, the optimal choice of the hyperparameter $k$ is much larger than in balanced classification. Importantly, this larger choice of $k$, leads to sub-optimal, or even inconsistent, estimates of the regression function under other (nonuniform) forms of class imbalance. The following example illustrates this:
**Example 17.** Suppose $\mathcal{X} = [0, 1]$, $X \sim \text{Uniform}([0, 1])$, and $r \in (0, 1)$. Consider two regression functions $\eta_1(x) = r(1 - x)$ and $\eta_2(x) = \max\{0, 1 - x/r\}$. Both $\eta_1$ and $\eta_2$ exhibit the same degree of overall class imbalance, with the proportion of samples from class 1 being $r/2$. The regression function $\eta_1$ satisfies Uniform Class Imbalance of degree $r$, whereas $\eta_2$ does not satisfy a nontrivial degree of Uniform Class Imbalance, since $\eta_2(0) = 1$. For sufficiently small $r \in (0, 1)$, specifically $r \in o\left(n^{-\frac{\alpha}{d+2}}\right)$, Theorem 13 gives that the optimal choice of $k$ under $\eta_1$ satisfies $k \in \omega(rn)$. On the other hand, if $k \in \omega(rn)$, then, under $\eta_2$, $\mathbb{E}\left[\hat{\eta}_k(0)\right] \to 0$, so that $\hat{\eta}_k(0)$ is an inconsistent estimate of $\eta_2(0) = 1$.

This example demonstrates that constructing classifiers that perform well under severe class imbalance may require distinguishing different sub-types of class imbalance, such as Uniform Class Imbalance.

6 Conclusions

The main conclusions of this paper are as follows. First, the Bayes classifier, which optimizes classification performance in terms of accuracy, can be generalized to many other measures of classification performance using a simple thresholding procedure with only two additional scalar parameters. This Generalized Bayes Classifier provides an optimal performance benchmark, relative to which one can evaluate many classifiers of interest in terms of their ability to estimate the regression function in uniform loss. This includes the widely-used $k$NN classifier, for which we provided a number of guarantees, showing that it performs minimax optimally under uniform loss in a number of settings, including that of severe Uniform Class Imbalance. On the other hand, we showed that the optimal tuning of $k$ can differ significantly between different sub-types of imbalanced classification, suggesting that developing reliable classifiers for severely imbalanced classification may require a more nuanced understanding of the nature of class imbalance intrinsic to the problem at hand.

We hope that some of these ideas, especially the generalized Bayes classifier and the distinction of sub-types of class imbalance, will play a role in developing a coherent and insightful statistical theory of imbalanced classification, and that this theory will inform the construction of more reliable classifiers for challenging real-world imbalanced classification problems. Additionally, these ideas should be generalized to the multi-class case, in which severe class imbalance emerges naturally when the number of classes is large and existing statistical theory is quite limited.

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A Derivation of the Generalized Bayes Classifier (Theorem 3)

In this Appendix, we prove Theorem 3, in which we characterize a generalization of the Bayes classifier to arbitrary CMMs. We reiterate the theorem for the reader here:

**Theorem 3.** If \( \arg\max_{\hat{Y} \in \mathcal{SC}} M(C_{\hat{Y}}) \neq \emptyset \), then there exists a regression-thresholding classifier

\[
\hat{Y}_{p,t,\eta} \in \arg\max_{\hat{Y} \in \mathcal{SC}} M(C_{\hat{Y}}).
\]

As described in the main paper, the proof of Theorem 3 is given in a sequence of steps constructing optimal classifiers in forms progressively closer to that of the generalized Bayes classifier described in Theorem 3. Specifically, we first show, in Lemma 18, that there exists an optimal classifier that is a (stochastic) function of the regression function \( \eta \). We then construct an optimal classifier in which this function of \( \eta \) is non-decreasing. Finally, we construct an optimal classifier in which this function of \( \eta \) is a threshold function, as in Theorem 3.

**Lemma 18.** For any stochastic classifier \( \hat{Y} : \mathcal{X} \to \mathcal{P}(\{0, 1\}) \), there is a stochastic classifier \( \hat{Y}' : \mathcal{X} \to \mathcal{P}(\{0, 1\}) \) of the form

\[
\hat{Y}'(x) \sim \text{Bernoulli}(f(\eta(x))),
\]

for some \( f : [0, 1] \to [0, 1] \), such that \( C_{\hat{Y}'} = C_{\hat{Y}} \).

**Proof.** Define \( \hat{Y}' : \mathcal{X} \to \mathcal{P}(\{0, 1\}) \) by

\[
\hat{Y}'(x) \sim \text{Bernoulli} \left( \mathbb{E}_{Z \sim P_X} \left[ \hat{Y}(Z) | \eta(Z) = \eta(x) \right] \right),
\]

and note that \( \hat{Y}' \) has the desired form. Note that both \( \hat{Y}(X) \) and \( \hat{Y}'(X) \) are conditionally independent of the true label \( Y \) given \( \eta(X) \). Thus,

\[
\mathbb{E} \left[ Y \hat{Y}'(X) \right] = \mathbb{E} \left[ \mathbb{E} \left[ Y \hat{Y}'(X) | \eta(X) \right] \right] = \mathbb{E} \left[ \mathbb{E} \left[ Y | \eta(X) \right] \mathbb{E} \left[ \hat{Y}'(X) | \eta(X) \right] \right] = \mathbb{E} \left[ \eta(X) \mathbb{E} \left[ \hat{Y}'(X) | \eta(X) \right] \right]
\]

and, similarly,

\[
\mathbb{E} \left[ Y \hat{Y}(X) \right] = \mathbb{E} \left[ \eta(X) \mathbb{E} \left[ \hat{Y}(X) | \eta(X) \right] \right].
\]

Additionally, by construction of \( \hat{Y}' \),

\[
\mathbb{E} \left[ \hat{Y}'(X) | \eta(X) \right] = \mathbb{E} \left[ \mathbb{E}_{Z \sim P_X} \left[ \hat{Y}(Z) | \eta(Z) = \eta(X) \right] | \eta(X) \right] = \mathbb{E} \left[ \hat{Y}(X) | \eta(X) \right].
\]

Putting these together, we have

\[
\text{TP}_{\hat{Y}'} = \mathbb{E} \left[ Y \hat{Y}'(X) \right] = \mathbb{E} \left[ \eta(X) \mathbb{E} \left[ \hat{Y}'(X) | \eta(X) \right] \right] = \mathbb{E} \left[ \eta(X) \mathbb{E} \left[ \hat{Y}(X) | \eta(X) \right] \right] = \mathbb{E} \left[ Y \hat{Y}(X) \right] = \text{TP}_{\hat{Y}}.
\]

Similarly, one can check that \( C_{\hat{Y}'} = C_{\hat{Y}} \). \( \Box \)

It follows from Lemma 18 that, if \( M(C_{\hat{Y}}) \) is maximized by any classifier, then it is maximized by a classifier \( \hat{Y} \) of the form in Eq. (8). It remains to show that \( f \) in Eq. (8) can be of the form \( z \mapsto p1 \{ z = t \} + 1 \{ z > t \} \) for some threshold \( (p, t) \in [0, 1]^2 \). Before proving this, we give a simplifying lemma showing that the problem of maximizing a CMM can be equivalently framed as a particular functional optimization problem. This will allow us to to significantly simplify the notation in the subsequent proofs.
Lemma 19. Let $M$ be a CMM, and suppose that $M(C_Y)$ is maximized (over SC) by a classifier $\hat{Y}$ of the form
\[ \hat{Y}(x) \sim \text{Bernoulli}(f^*(\eta(x))), \]
for some $f^* : [0, 1] \to [0, 1]$. Let $f$ be a solution to the optimization problem
\[ \max_{f: [0, 1] \to [0, 1]} \mathbb{E}[\eta(X)f(\eta(X))] \quad \text{subject to} \quad \mathbb{E}[(1 - \eta(X))f(\eta(X))] \leq \mathbb{E}[(1 - \eta(X))f^*(\eta(X))]. \]
Then, the classifier
\[ \hat{Y}'(x) \sim \text{Bernoulli}(f(\eta(x))), \]
also maximizes $M(C_{\hat{Y}'})$ (over SC).

Proof. This result follows from the definition (Definition 1) of a CMM. Specifically, by construction of $\hat{Y}'$,
\[ \text{TP}_{\hat{Y}'} = \mathbb{E}[\eta(X)f(\eta(X))] \geq \mathbb{E}[\eta(X)f^*(\eta(X))] = \text{TP}_{\hat{Y}} \]
and
\[ \text{FP}_{\hat{Y}'} = \mathbb{E}[(1 - \eta(X))f(\eta(X))] \leq \mathbb{E}[(1 - \eta(X))f^*(\eta(X))] = \text{FP}_{\hat{Y}}. \]
Moreover, since the actual proportions of positives and negatives are fixed (i.e., $\text{TP}_{\hat{Y}'} + \text{FN}_{\hat{Y}'} = \text{TP}_{\hat{Y}} + \text{FN}_{\hat{Y}}$ and $\text{FP}_{\hat{Y}'} + \text{TN}_{\hat{Y}'} = \text{FP}_{\hat{Y}} + \text{TN}_{\hat{Y}}$), we have
\[ C_{\hat{Y}'} = \begin{bmatrix} \text{TN}_{\hat{Y}} + \epsilon_1 & \text{FP}_{\hat{Y}} - \epsilon_1 \\ \text{FN}_{\hat{Y}} - \epsilon_2 & \text{TP}_{\hat{Y}} + \epsilon_2 \end{bmatrix}, \]
where $\epsilon_1 := \text{FP}_{\hat{Y}} - \text{FP}_{\hat{Y}} \in [0, \text{FP}_{\hat{Y}}]$ and $\epsilon_2 := \text{TP}_{\hat{Y}} - \text{TP}_{\hat{Y}} \in [0, \text{FN}]$. Thus, by the definition (Definition 1) of a CMM, $M(C_{\hat{Y}'}) \geq M(C_{\hat{Y}}).$ \hfill $\square$

Lemma 19 essentially shows that maximizing any CMM $M$ is equivalent to performing Neyman-Pearson classification, at a some particular false positive level $\alpha$ depending on $M$ (through $f^*$) and on the distribution of $\eta(X)$. For our purposes, this simplifies the remaining steps in proving Theorem 3 by allowing us to ignore the details of the particular CMM $M$ and regression function $\eta$ and focus on characterizing solutions to an optimization problem of the form (9) (see, specifically, (10) below).

To characterize solutions to this optimization problem, we will repeatedly utilize the following measure-theoretic technical lemma:

Lemma 20. Let $\mu$ be a measure on $[0, 1]$ with $\mu([0, 1]) > 0$. Then, there exists $z \in \mathbb{R}$ such that, for all $\epsilon > 0$, $\mu([0, 1] \cap (z - \epsilon, z)) > 0$.

Proof. We prove the contrapositive. Suppose that, for every $z \in [0, 1]$, there exists $\epsilon_z > 0$ such that $\mu([0, 1] \cap (z - \epsilon_z, z)) = 0$. The family $S := \{[0, 1] \cap (z - \epsilon_z, z) : z \in \mathbb{R}\}$ is an open cover of $[0, 1]$. Since $[0, 1]$ is compact, there exists a finite sub-cover $S' \subseteq S$ of $[0, 1]$. Thus, by countable subadditivity of measures,
\[ \mu([0, 1]) \leq \sum_{S \in S'} \mu(S) = 0. \]
\hfill $\square$

We are now ready for the main remaining step in the proof of Theorem 3, namely characterizing solutions of (a generalization of) the optimization problem (9):

Lemma 21. Let $Z$ be a $[0, 1]$-valued random variable, and let $c \in [0, 1]$. Suppose that the optimization problem
\[ \max_{f: [0, 1] \to [0, 1]} \mathbb{E}[Zf(Z)] \quad \text{subject to} \quad \mathbb{E}[(1 - Z)f(Z)] \leq c \]
has a solution. Then, there is a solution to (10) that is a generalized threshold function.
We now show that $g$ while where the essential supremum and infimum are taken with respect to the measure $Z$ and $P$. Suppose, for sake of contradiction, that, for some $g(z) = 0$, whenever $P_Z([0, z]) = 0$ and $h(z) = 1$ whenever $P_Z((z, 1]) = 0$. We first show that, for all $z \in [0, 1]$, $g(z) \leq h(z)$. We will then use this to show that $g = f$ except on a set of measure $0$ (i.e., $P_Z(\{ z \in [0, 1] : g(z) \neq f(z) \}) = 0$). Therefore, both $E[Z_g(Z)] = E[Z_f(Z)]$ and $E[(1-Z)g(Z)] = E[(1-Z)f(Z)]$. Since $g : [0, 1] \rightarrow [0, 1]$ is clearly monotone non-decreasing, the result follows.

Suppose, for sake of contradiction, that, for some $z \in [0, 1]$, $g(z) > h(z)$. Then there exist $A \subseteq [0, z]$ and $B \subseteq (z, 1]$ such that $\inf_{z \in A} f(z) \geq \sup_{z \in B} f(z)$ and $P_Z(A), P_Z(B) > 0$. Define $z_A := E[Z|Z \in A]$ and $z_B := E[Z|Z \in B]$, and note that, since $A \subseteq [0, z]$ and $B \subseteq (z, 1]$, $z_A < z_B$. Define,

$$
\epsilon := \min \left\{ \frac{P_Z(A)(1-z_A)}{P_Z(B)(1-z_B)} \inf_{z \in A} f(z), \sup_{z \in B} f(z) \right\} > 0
$$

and define $\phi : [0, 1] \rightarrow [0, 1]$ by

$$
\phi(z) := \begin{cases} 
  f(z) - \epsilon \frac{P_Z(B)(1-z_B)}{P_Z(A)(1-z_A)} & \text{if } z \in A \\
  f(z) + \epsilon & \text{if } z \in B \\
  f(z) & \text{otherwise,}
\end{cases}
$$

noting that, by construction of $\epsilon$, $\phi(z) \in [0, 1]$ for all $z \in [0, 1]$. Then, by construction of $\phi$,

$$
E[(1-Z)\phi(Z)] - E[(1-Z)f(Z)] = -(1-z_A)\epsilon \frac{P_Z(B)(1-z_B)}{P_Z(A)(1-z_A)} P_Z(A) + (1-z_B)\epsilon P_Z(B)
$$

while

$$
E[Z\phi(Z)] - E[Zf(Z)] = -z_A\epsilon \frac{P_Z(B)(1-z_B)}{P_Z(A)(1-z_A)} P_Z(A) + z_B\epsilon P_Z(B)
$$

$$
= \left( -\frac{z_A}{1-z_A} (1-z_B) + z_B \right) \epsilon P_Z(B) > 0,
$$

since the function $z \mapsto \frac{z}{1-z}$ is strictly increasing. This contradicts the assumption that $f$ optimizes (10), implying $g \leq h$.

We now show that $g = f$ except on a set of $P_Z$ measure 0. First, note that, if $g(z) \neq f(z)$, then $g(z) = \esssup_{z \in [0, z]} f(z) = \esssup_{z \in [0, z]},$ and so $g$ is left-continuous at $z$.

For any $\delta > 0$, define

$$
A_\delta := \{ z \in [0, 1] : g(z) < f(z) - \delta \} \quad \text{and} \quad B_\delta := \{ z \in [0, 1] : g(z) > f(z) + \delta \}.
$$

Since

$$
\{ z \in [0, 1] : g(z) < f(z) \} = \bigcup_{j=1}^\infty \left\{ z \in [0, 1] : g(z) < f(z) - \frac{1}{j} \right\}
$$

and

$$
\{ z \in [0, 1] : g(z) > f(z) \} = \bigcup_{j=1}^\infty \left\{ z \in [0, 1] : g(z) > f(z) + \frac{1}{j} \right\},
$$

by countable subadditivity, it suffices to show that $P_Z(A_\delta) = P_Z(B_\delta) = 0$ for all $\delta > 0$. 

Proof. Suppose that there exists a solution $f$ to (10). We will construct a generalized threshold function that solves (10) in two main steps. First, we will construct a monotone solution to (10). Second, we will show that this monotone solution is equal to a generalized threshold function except perhaps on a set of probability 0 with respect to $Z$. This generalized threshold function is therefore a solution to (10).

Construction of Monotone Solution to (10): Define

$$
g(z) := \esssup_{z \in A} f([0, z]) \quad \text{and} \quad h(z) := \essinf_{z \in B} f((z, 1]),
$$

where the essential supremum and infimum are taken with respect to the measure $Z$. Since the function $\phi$ is strictly increasing. This contradicts the assumption that $f$ optimizes (10), implying $g \leq h$. 

We now show that $g = f$ except on a set of $P_Z$ measure 0. First, note that, if $g(z) \neq f(z)$, then $g(z) = \esssup_{z \in [0, z]} f(z)$, and so $g$ is left-continuous at $z$.
Suppose, for sake of contradiction, that \( P_Z(A_\delta) > 0 \). Applying Lemma 20 to the measure \( E \mapsto P_Z(A_\delta \cap E) \), there exists \( z \in \mathbb{R} \) such that, for any \( \epsilon > 0 \), \( P_Z(A_\delta \cap (z - \epsilon, z)) > 0 \). Since \( g \) is continuous at \( z \), there exists \( \epsilon > 0 \) such that \( g(z - \epsilon) \geq g(z) - \delta \), so that, for all \( z \in A_\delta \cap (z - \epsilon, z) \), \( f(z) > g(z) + \delta \). Then, since \( P_Z(A_\delta \cap (z - \epsilon, z)) > 0 \), we have the contradiction
\[
g(z) \geq \text{ess sup} f(A_\delta \cap (z - \epsilon, z)) > g(z).
\]

On the other hand, suppose, for sake of contradiction, that \( P_Z(B_\delta) > 0 \). Applying Lemma 20 to the measure \( E \mapsto P_Z(B_\delta \cap E) \), there exists \( z \in \mathbb{R} \) such that, for any \( \epsilon > 0 \), \( P_Z(B_\delta \cap (z - \epsilon, z)) > 0 \). Since \( g \) is continuous at \( z \), there exists \( \epsilon > 0 \) such that \( g(z - \epsilon) \geq g(z) - \delta \). At the same time, since \( g \) is non-decreasing, for \( t \in B_\delta \cap (z - \epsilon, z) \), \( f(t) < g(t) - \delta \leq g(z) - \delta \). Thus, since \( P_Z(B_\delta \cap (z - \epsilon, z)) > 0 \), we have \( h(z - \epsilon) < g(z) - \delta < g(z - \epsilon) \), contradicting the previously shown fact that \( g \leq h \).

To conclude, we have shown that \( P_Z(\{z \in [0,1] : g(z) \neq f(z)\}) = 0 \).

**Construction of a Generalized Threshold Solution:** We now construct a solution to (10) that is equal to a generalized threshold function (i.e., a function that has the form \( 0 \leq f(z) \leq 1 \)) except on a set of \( P_Z \)-measure 0. To show this, it suffices to construct a function \( f : [0,1] \to [0,1] \) such that (a) \( f \) is monotone non-decreasing and (b) the set \( f^{-1}((0,1)) \) is the union of the singleton \( \{t\} \) and a set of \( P_Z \)-measure 0.

From the previous step of this proof, we may assume that we have a solution \( f \) to (10) that is monotone non-decreasing. It suffices therefore to show that \( A := f^{-1}((0,1)) \) is the union of a singleton and a set of \( P_Z \)-measure 0. Define
\[
t_0 := \inf \{z \in [0,1] : P_Z(A \cap [0,z]) > 0\} \quad \text{and} \quad t_1 := \sup \{z \in [0,1] : P_Z(A \cap [z,1]) > 0\}.
\]

Then, for all \( \epsilon > 0 \), \( P_Z(A \cap [0, t_0 - \epsilon]) = P_Z(A \cap [t_1 + \epsilon, 1]) = 0 \). If \( t_0 = t_1 \), then, since
\[
A \setminus \{t_0\} = \bigcup_{j=1}^{\infty} A \cap ([0, t_0 - 1/j] \cup [t_0 + 1/j, 1])
\]
by countable subadditivity, \( P_Z(A \setminus \{t_0\}) = 0 \), which implies that \( A = \{t_0\} \cup (A \setminus \{t_0\}) \) is the union of a singleton and a set of \( P_Z \)-measure 0.

It suffices therefore to prove that \( t_0 = t_1 \). Suppose, for sake of contradiction, that \( t_0 < t_1 \). Then, there exists \( t \in (t_0, t_1) \), and, by definition of \( t_0 \) and \( t_1 \), both \( P_Z(A \cap [0,t]) > 0 \) and \( P_Z(A \cap (t, 1]) > 0 \). For any \( \delta \geq 0 \), define
\[
B_\delta := \{z \in [0,t] : \delta < f(z) < 1 - \delta\} \quad \text{and} \quad C_\delta := \{z \in (t, 1] : \delta < f(z) < 1 - \delta\},
\]
so that \( P_Z(B_\delta) > 0 \) and \( P_Z(C_\delta) > 0 \). By countable subadditivity, there exists \( \delta > 0 \) such that \( P_Z(B_\delta) > 0 \) and \( P_Z(C_\delta) > 0 \).

Define \( \epsilon := \delta \cdot \min\{P_Z(B_\delta), P_Z(C_\delta)\} > 0 \). Define \( g : [0,1] \to \mathbb{R} \) for all \( z \in [0,1] \) by
\[
g(z) = \begin{cases} 
  f(z) - P_Z(B_\delta) & \text{if } z \in B_\delta \\
  f(z) + P_Z(C_\delta) & \text{if } z \in C_\delta \\
  f(z) & \text{otherwise}
\end{cases}
\]
and note that, by definition of \( \epsilon, B_\delta, \) and \( C_\delta, g : [0,1] \to [0,1] \). Then,
\[
\mathbb{E}[g(Z)] - \mathbb{E}[f(Z)] = -\frac{\epsilon}{P_Z(B_\delta)} P_Z(B_\delta) + \frac{\epsilon}{P_Z(C_\delta)} P_Z(C_\delta) = 0,
\]
while
\[
\mathbb{E}[Z g(Z)] - \mathbb{E}[Z f(Z)] = -\mathbb{E}[Z | Z \in B_\delta] \frac{\epsilon}{P_Z(B_\delta)} P_Z(B_\delta) + \mathbb{E}[Z | Z \in C_\delta] \frac{\epsilon}{P_Z(C_\delta)} P_Z(C_\delta) = \epsilon (\mathbb{E}[Z | Z \in C_\delta] - \mathbb{E}[Z | Z \in B_\delta]).
\]

Since \( B_\delta \subseteq [0,t) \) and \( C_\delta \subseteq (t,1] \), this difference is strictly positive, contradicting the assumption that \( f \) optimizes (10).

Combining Lemma 21 with Lemma 19 completes the proof of our main result, Theorem 3.
B Relative Performance Guarantees in terms of the Generalized Bayes Classifier

In this Appendix, we prove Lemmas 5 and 6, as well as their consequence, Corollary 8. Also, in Section B.1, we demonstrate, in a few key examples, how to compute the Lipschitz constant used in Corollary 8.

We begin with the proof of Lemma 5, which, at a given threshold \((p, t)\), bounds the difference between the confusion matrices of the true regression function \(\eta\) and an estimate \(\eta'\) of \(\eta\). We restate the result for the reader’s convenience:

**Lemma 5.** Let \(p, t \in [0, 1]\) and let \(\eta, \eta' : \mathcal{X} \to [0, 1]\). Then,

\[
\left\| C_{\hat{Y}_{p,t,\eta}} - C_{\hat{Y}_{p,t,\eta'}} \right\|_{\infty} \leq \mathbb{P} [\|\eta(X) - t\| \leq \|\eta - \eta'\|_{\infty}].
\]

**Proof.** For the true negative rate, we have

\[
\left|\text{TN}_{\hat{Y}_{p,t,\eta}} - \text{TN}_{\hat{Y}_{p,t,\eta'}}\right| = |\mathbb{P}[Y = 0, \eta'(X) \leq t < \eta(X)] - \mathbb{P}[Y = 0, \eta(X) \leq t < \eta'(X)]|
\leq \mathbb{P} [\|\eta(X) - t\| \leq \|\eta - \eta'\|_{\infty}].
\]

This type of inequality is standard and follows from the fact that, if \(t\) lies between \(\eta\) and \(\eta'\), then the difference of \(\eta\) and \(t\) is necessarily less than \(\eta\) and \(\eta'\). Repeating this calculation for the true positive, false positive, and false negative rates gives (11).

Note that, in the presence of degree \(r\) Uniform Class Imbalance (see Section 5.2), one can obtain a tighter error bound \(\mathbb{P} [\|\eta'(X) - t\| \leq \|\eta - \eta'\|_{\infty}]\) for the true positive and false negative rates because, for all \(x \in \mathcal{X}\), \(\mathbb{P}[Y = 1 | X = x] \leq r\). However, the weaker bound (11) simplifies the exposition.

We now turn to proving Lemma 6, which we use to bound the maximum difference between the empirical and true confusion matrices of a regression-thresholding classifier over thresholds \((p, t)\).

Specifically, we will use this result to bound the difference in confusion matrices between the optimal threshold \((p^*, t^*)\) and the threshold \((\hat{p}, \hat{t})\) selected by maximizing the empirical CMM. We actually prove a more general version of Lemma 6, for arbitrary classifiers, based on the following definition:

**Definition 22 (Stochastic Growth Function).** Let \(\mathcal{F}\) be a family of \([0, 1]\)-valued functions on \(\mathcal{X}\). The stochastic growth function \(\Pi_{\mathcal{F}} : \mathbb{N} \to \mathbb{N}\), defined by

\[
\Pi_{\mathcal{F}}(n) := \max_{\{f \in \mathcal{F}\}} \left| \left\{ \{f(x_i) > z_i\} \right\}_{i=1}^{n} : f \in \mathcal{F} \right| \text{ for all } n \in \mathbb{N},
\]

is the maximum number of distinct classifications of \(n\) points \(x_1, \ldots, x_n\) by a stochastic classifier \(\hat{Y}\) with \((x \mapsto \mathbb{E}[\hat{Y}(x)]) \in \mathcal{F}\) and randomness given by \(z_1, \ldots, z_n\).

Definition 22 generalizes the growth function [Mohri et al., 2018], a classical measure of the complexity of a hypothesis class originally due to Vapnik and Chervonenkis [1971], to non-deterministic classifiers. Importantly for our purposes, one can easily bound the stochastic growth function of regression-thresholding classifiers:

**Example 23 (Stochastic Growth Function of Regression-Thresholding Classifiers).** Suppose \(\mathcal{F} = \{f : \mathcal{X} \to [0, 1]\} \) for some \(p, t \in [0, 1]\), \(f(x) = p \cdot 1\{\eta(x) = t\} + 1\{\eta(x) > t\}\) for all \(x \in \mathcal{X}\), so that \(\{\hat{Y}_{f,\eta} : f \in \mathcal{F}\}\) is the class of regression-thresholding classifiers. Any set of points \((x_1, z_1), \ldots, (x_n, z_n)\), can be sorted in increasing order by \(\eta(x)\)’s, breaking ties in decreasing order by \(x\)’s. Having sorted the points in this way, \(\{f(x) > z\} = 0\) for the first \(j\) points and \(\{f(x) > z\} = 1\) for the remaining \(n - j\) points, for some \(j \in [n] \cup \{0\}\). Thus, \(\Pi_{\mathcal{F}}(n) = n + 1\).

We will now prove the following result, from which, together with Example 23, Lemma 6 follows immediately:
Lemma 6 (Generalized Version). Let $\mathcal{F}$ be a family of $[0, 1]$-valued functions on $X$. Then, with probability at least $1 - \delta$,
\[
\sup_{f \in \mathcal{F}} \left\| \hat{C}_{\hat{Y}_f} - C_{\hat{Y}_f} \right\|_\infty \leq \sqrt{\frac{8}{n} \log \frac{32\Pi \mathcal{F}(2n)}{\delta}}.
\]

Before proving Lemma 6, we note a standard symmetrization lemma, which allows us to replace the expectation of $\hat{T}_{\mathcal{F}, f, i, n}$ with its value on an independent, identically distributed “ghost sample".

Lemma 24 (Symmetrization; Lemma 2 of Bousquet et al. [2003]). Let $X$ and $X'$ be independent realizations of a random variable with respect to which $\mathcal{F}$ is a family of integrable functions. Then, for any $\epsilon > 0$,
\[
P \left[ \sup_{f \in \mathcal{F}} f(X) - \mathbb{E} f(X) > \epsilon \right] \leq 2 \mathbb{P} \left[ \sup_{f \in \mathcal{F}} \left| f(X) - f(X') \right| > \epsilon/2 \right].
\]

We now use this lemma to prove Lemma 6.

Proof. To facilitate analyzing the stochastic aspect of the classifier $\hat{Y}_{f, n}$, let $Z_1, \ldots, Z_n \sim \text{Uniform}([0, 1])$, such that $\hat{Y}_{f, n}(X_i) = 1\{Z_i < f(\eta((X_i)))\}$.

Now suppose that we have a ghost sample $(X'_1, Y'_1, Z'_1), \ldots, (X'_n, Y'_n, Z'_n)$. Let $\hat{T}_{\mathcal{F}, f, n}$ denote the empirical true negative rate computed on this ghost sample, and let $\hat{T}_{\mathcal{F}, f, n}^{(i)}$ denote the empirical true negative rate computed on $(X_1, Y_1, Z_1), \ldots, (X_{i-1}, Y_{i-1}, Z_{i-1}), (X'_i, Y'_i, Z'_i), (X_{i+1}, Y_{i+1}, Z_{i+1}), \ldots, (X_n, Y_n, Z_n)$ (i.e., replacing only the $i^{th}$ sample with its ghost). By the Symmetrization Lemma,
\[
P \left[ \sup_{f \in \mathcal{F}} \hat{T}_{\mathcal{F}, f, n} - \mathbb{E} \hat{T}_{\mathcal{F}, f, n} > \epsilon \right] \leq 2 \mathbb{P} \left[ \sup_{f \in \mathcal{F}} \hat{T}_{\mathcal{F}, f, n} - \hat{T}_{\mathcal{F}, f, n}^{(i)} > \epsilon/2 \right]
\leq 2 \Pi \mathcal{F}(2n) \sup_{f \in \mathcal{F}} \mathbb{P} \left[ \hat{T}_{\mathcal{F}, f, n} - \hat{T}_{\mathcal{F}, f, n}^{(i)} > \epsilon/2 \right]
\leq 4 \Pi \mathcal{F}(2n) \sup_{f \in \mathcal{F}} \left[ \hat{T}_{\mathcal{F}, f, n} - \mathbb{E} \hat{T}_{\mathcal{F}, f, n}^{(i)} > \epsilon/4 \right],
\]
where the second inequality is a union bound over the $\Pi \mathcal{F}(2n)$ distinct classifications of $2n$ points that can be assigned by $\hat{Y}_{f, n}$ with $f \in \mathcal{F}$, and the last inequality is from the fact that $\hat{T}_{\mathcal{F}, f, n}$ and $\hat{T}_{\mathcal{F}, f, n}^{(i)}$ are identically distributed and the algebraic fact that, if $a - b > \epsilon$, then either $a - c > \epsilon/2$ or $b - c > \epsilon/2$.

For any particular $f \in \mathcal{F}$, by McDiarmid’s inequality [McDiarmid, 1998],
\[
P \left[ \hat{T}_{\mathcal{F}, f, n} - \mathbb{E} \hat{T}_{\mathcal{F}, f, n}^{(i)} > \epsilon/4 \right] \leq e^{-nc^2/8},
\]
we have
\[
P \left[ \sup_{f \in \mathcal{F}} \hat{T}_{\mathcal{F}, f, n} - \mathbb{E} \hat{T}_{\mathcal{F}, f, n}^{(i)} > \epsilon \right] \leq 4 \Pi \mathcal{F}(2n) e^{-nc^2/8}.
\]
Repeating this argument with $\hat{T}_{\mathcal{F}, f, n}$ instead of $\hat{T}_{\mathcal{F}, f, n}^{(i)}$, as well as with $\hat{Y}_{f, n}, \hat{T}_{\mathcal{F}, f, n}$ and their negatives, and taking a union bound over these $8 \delta$ cases, gives the desired result.
Finally, we will use these two lemmas, together with the margin and Lipschitz assumptions, to prove Corollary 8, which bounds the sub-optimality of the trained classifier, relative to the generalized Bayes classifier, in terms of the desired CMM.

**Corollary 8.** Let \( \eta : \mathcal{X} \to [0, 1] \) denote the true regression function, and let \( \hat{\eta} : \mathcal{X} \to [0, 1] \) denote any empirical regressor. Let

\[
(p, \hat{t}) := \arg\max_{(p, t) \in [0, 1]^2} M \left( \hat{C}_{p,t,\hat{\eta}} \right) \quad \text{and} \quad (p^*, t^*) := \arg\max_{(p, t) \in [0, 1]^2} M \left( C_{p,t,\eta} \right)
\]

denote the empirically selected and true optimal thresholds, respectively. Suppose that \( M \) is Lipschitz continuous with constant \( L_M \) with respect to the uniform (\( L_\infty \)) metric on \( C \). Finally, suppose that \( P_X \) and \( \eta \) satisfies a \((C, \beta)\)-margin condition around \( t^* \). Then, with probability at least \( 1 - \delta \),

\[
M \left( C_{p,t,\eta} (p^*, t^*) \right) - M \left( \hat{C}_{p,t,\hat{\eta}} (p^*, \hat{\eta}) \right) \leq L_M \left( C \|\eta - \hat{\eta}\|_\infty + 2 \sqrt{\frac{8}{n} \log \frac{32(2n + 1)}{\delta}} \right).
\]

**Proof.** First, note that

\[
M \left( C_{p,t,\eta} (p^*, t^*) \right) - M \left( \hat{C}_{p,t,\hat{\eta}} (p^*, \hat{\eta}) \right) \leq M \left( C_{p,t,\eta} (p^*, t^*) \right) - M \left( \hat{C}_{p,t,\hat{\eta}} (p^*, \hat{\eta}) \right) \\
+ M \left( C_{p,t,\eta} (p^*, \hat{\eta}) \right) - M \left( \hat{C}_{p,t,\hat{\eta}} (p^*, \hat{\eta}) \right) \\
+ M \left( \hat{C}_{p,t,\hat{\eta}} (p^*, \hat{\eta}) \right) - M \left( C_{p,t,\hat{\eta}} (p^*, \hat{\eta}) \right),
\]

since, by definition of \((p, \hat{t})\),

\[
M \left( \hat{C}_{p,t,\hat{\eta}} (p^*, \hat{\eta}) \right) - M \left( C_{p,t,\hat{\eta}} (p^*, \hat{\eta}) \right) \leq 0;
\]

this term sits between the second and third lines above. By the Lipschitz assumption,

\[
M \left( C_{p,t,\eta} (p^*, t^*) \right) - M \left( \hat{C}_{p,t,\hat{\eta}} (p^*, \hat{\eta}) \right) \leq L_M \left( \left\| C_{p,t,\eta} (p^*, t^*) - C_{p,t,\hat{\eta}} (p^*, \hat{\eta}) \right\|_\infty \right) \tag{14}
\]

\[
+ \left\| C_{p,t,\eta} (p^*, \hat{\eta}) - \hat{C}_{p,t,\hat{\eta}} (p^*, \hat{\eta}) \right\|_\infty \tag{15}
\]

\[
+ \left\| \hat{C}_{p,t,\hat{\eta}} (p^*, \hat{\eta}) - C_{p,t,\hat{\eta}} (p^*, \hat{\eta}) \right\|_\infty \tag{16}
\]

Corollary 8 follows by applying Lemma 5 and the \((C, \beta)\)-margin condition to (14) and applying Lemma 6 to both terms (15) and (16).

### B.1 Lipschitz constants for some common CMMs

Corollary 8 assumed that the CMM \( M \) was Lipschitz continuous with respect to the sup-norm on confusion matrices. In this section, we show how to compute appropriate Lipschitz constants for several simple example CMMs. We begin with a simple example:

**Example 25 (Weighted Accuracy).** For a fixed \( w \in (0, 1) \), the \( w \)-weighted accuracy is given by \( M(C) = (1 - w)TP + wTN \). In this case, \( M \) clearly has Lipschitz constant \( L_M = \max\{w, 1 - w\} \).

For the remainder of this section (only), we will use \( P := E[Y] \) to denote the positive rate of the true labels and \( \hat{P} := \frac{1}{n} \sum_{i=1}^{n} Y_i \) to denote the empirical positive rate of the true labels. Many CMMs of interest, such as Recall and \( F_\beta \) scores, are not Lipschitz continuous over all of \( C \). Fortunately, inspecting the proof of Corollary 8, it suffices for the CMM \( M \) to be Lipschitz continuous on the line segments between three specific pairs of confusion matrices, given in Eqs. (14), (15), and (16). Deriving the appropriate Lipschitz constants is a bit more complex, and we demonstrate here how to derive them for the specific CMMs of Recall and \( F_\beta \) scores.
Of the six confusion matrices in Eqs. (14), (15), and (16), four are true confusion matrices. These four matrices have the same positive rate $TP + FN = P$, which is a function of the true distribution of labels. The remaining two matrices are empirical confusion matrices, and hence have the positive rate $\hat{TP} + \hat{FN} = \hat{P}$, which is a function of the data. By a multiplicative Chernoff bound, with probability at least $1 - e^{-nP/\delta}$, $\hat{P} \geq P/2$. Thus, with high probability, it suffices for the CMM $M$ to be Lipschitz continuous over confusion matrices with positive rate at least $P/2$. For Recall and $F_\beta$ scores, this gives the following Lipschitz constants:

**Example 26 (Recall).** Recall is given by $M(C) = \frac{TP}{TP + FN} = \frac{TP}{P}$. Thus, $M$ is Lipschitz continuous with constant $L_M = \frac{1}{P}$ over the confusion matrices in Eqs. (14), (15), and (16).

**Example 27 ($F_\beta$ Score).** For $\beta \in (0, \infty)$, the $F_\beta$ score is given by

$$M(C) = \frac{(1 + \beta^2)TP}{(1 + \beta^2)TP + FP + \beta^2 FN} = \frac{(1 + \beta^2)TP}{TP + FP + \beta^2 P}.$$ 

Hence,

$$\frac{\partial}{\partial TP} M(C) = (1 + \beta^2) \frac{FP + \beta^2 P}{(TP + FP + \beta^2 P)^2} \leq \frac{1 + \beta^2}{\beta^3 P},$$

while, since $TP \leq P$,

$$\frac{\partial}{\partial FP} M(C) = (1 + \beta^2) \frac{TP}{(TP + FP + \beta^2 P)^2} \leq \frac{1 + \beta^2}{\beta^4 P}.$$ 

Hence, $M$ is Lipschitz continuous with constant $\frac{2(1 + \beta^2)}{P} \max \{\beta^{-2}, \beta^{-4}\}$ over the confusion matrices in Eqs. (14), (15), and (16).

As Examples 26 and 27 demonstrate, the Lipschitz constants of many CMMs can become large when the proportion $P$ is positive samples is small. In particular, when $P \in O\left(\sqrt{\log \frac{n}{\delta}}\right)$, the $\asymp L_M \sqrt{\log \frac{n}{\delta}}$ term of Corollary 8 fails to vanish as $n \to \infty$. We believe that some loss of convergence rate is inevitable if $P \to 0$ as $n \to \infty$, due to the inherent instability of such metrics, but further work is needed to understand if the rates given by Corollary 8 are optimal under these metrics. See also Dembczyński et al. [2017] for detailed discussion of Lipschitz constants of many common CMMs.

### C Bounds on Uniform Error of the Nearest Neighbor Regressor

In this appendix, we prove our upper bound on the uniform risk of the $k$NN regressor (Theorem 13), as well as the corresponding minimax lower bound (Theorem 16).

#### C.1 Upper Bounds

In this section, we prove Theorem 13, our upper bound on the uniform error of the $k$-NN regressor. The main result is restated below:

**Theorem 13.** Under Assumptions 11 and 12, whenever $k/n \leq p_*(\epsilon^*)^d/2$, for any $\delta > 0$, with probability at least $1 - N\left((2k/(p_*)n)^{1/d}\right) e^{-k/4} - \delta$, we have the uniform error bound

$$\|\eta - \tilde{\eta}\|_\infty \leq 2^a L_r \left(\frac{2k}{p_* n}\right)^{\alpha/d} + \frac{2}{3k} \log \frac{2S(n)}{\delta} + \sqrt{\frac{2r}{k} \log \frac{2S(n)}{\delta}}. \quad (17)$$

For any $x \in \mathcal{X}$, let

$$\tilde{\eta}_k(x) := \frac{1}{k} \sum_{j=1}^{k} \eta(X_{\sigma_j(x)})$$

denote the mean of the true regression function over the $k$ nearest neighbors of $x$. By the triangle inequality,

$$\|\eta - \bar{\eta}\|_\infty \leq \|\eta - \tilde{\eta}\|_\infty + \|\tilde{\eta}_k - \bar{\eta}\|_\infty,$$
wherein \( \|\eta - \hat{\eta}_k\|_\infty \) captures bias due to smoothing and \( \|\hat{\eta}_k - \hat{\eta}\|_\infty \) captures variance due to label noise. We separately show that, with probability at least \( 1 - N \left( \frac{2k}{p \cdot n} \right)^{1/d} \),

\[
\|\eta - \hat{\eta}_k\|_\infty \leq 2^\alpha L r \left( \frac{2k}{p \cdot n} \right)^{\alpha/d},
\]

and that, with probability at least \( 1 - \delta \),

\[
\|\hat{\eta}_k - \hat{\eta}\|_\infty \leq \frac{2}{3k} \log \frac{2S(n)}{\delta} + \sqrt{\frac{2r}{k} \log \frac{2S(n)}{\delta}}.
\]

**Bounding the smoothing bias** Fix some \( r > 0 \) to be determined, and let \( \{B_r(z_1), \ldots, B_r(z_{N(r)})\} \) be a covering of \( (\mathcal{X}, \rho) \) by \( N(r) \) balls of radius \( r \), with centers \( z_1, \ldots, z_{N(r)} \in \mathcal{X} \).

By the lower bound assumption on \( P_X \), each \( P_X(B_r(z_j)) \geq p_r r^d \). Therefore, by a multiplicative Chernoff bound, with probability at least \( 1 - N(r) e^{-p_r n r^d/8} \), each \( B_r(z_j) \) contains at least \( p_r n r^d/2 \) samples. In particular, if \( r \geq \left( \frac{2k}{p \cdot n} \right)^{1/d} \), then each \( B_k \) contains at least \( k \) samples, and it follows that, for every \( x \in \mathcal{X} \), \( \rho(x, X_{\sigma_0(x)}) \leq 2r \). Thus, by Hölder continuity of \( \eta \),

\[
|\eta(x) - \hat{\eta}_k(x)| = |\eta(x) - \frac{1}{k} \sum_{j=1}^k \eta(X_{\sigma_j(x)})| \leq \frac{1}{k} \sum_{j=1}^k |\eta(x) - \eta(X_{\sigma_j(x)})| \leq L(2r)^\alpha.
\]

Finally, if \( \frac{k}{n} \leq \frac{2^\alpha}{2^\alpha} (r^*)^d \), then we can let \( r = \left( \frac{2k}{p \cdot n} \right)^{1/d} \).

**Bounding variance due to label noise** Let \( \Sigma := \{\sigma(x) \in [\eta]^k : x \in \mathcal{X}\} \) denote the set of possible \( k \)-nearest neighbor index sets. One can check from the definition of the shattering coefficient that \( |\Sigma| \leq S(n) \).

For any \( \sigma \in [\eta]^k \), let \( Z_\sigma := \sum_{j=1}^k Y_{\sigma_j} \) and let \( \mu_\sigma := \mathbb{E}[Z_\sigma] \). Note that the conditional random variables \( Y_{\sigma_j} | X_1, \ldots, X_n \) have conditionally independent Bernoulli distributions with means \( \mathbb{E}[Y_{\sigma_j} | X_1, \ldots, X_n] = \eta(X_{\sigma_j}) \) and variances \( \mathbb{E}\left[ (Y_{\sigma_j} - \eta(X_{\sigma_j}))^2 | X_1, \ldots, X_n \right] = \eta(X_{\sigma_j})(1 - \eta(X_{\sigma_j})) \leq r \). Therefore, by Bernstein’s inequality (Eq. (2.10) of Boucheron et al. [2013]), for any \( \epsilon > 0 \),

\[
\mathbb{P}\left[ |Z_\sigma/k - \mu_\sigma| \geq \epsilon \right] \leq 2 \exp\left( -\frac{k \epsilon^2}{2(k+\epsilon/3)} \right).
\]

Moreover, for any \( x \in \mathcal{X} \), \( \mu_{\sigma(x)} = \bar{\eta}_k(x) \) and \( Z_{\sigma(x)}/k = \bar{\eta}(x) \). Hence, by a union bound over \( \sigma \) in \( \Sigma \),

\[
\mathbb{P}\left( \sup_{x \in \mathcal{X}} |\bar{\eta}_k(x) - \bar{\eta}(x)| > \epsilon \left| X_1, \ldots, X_n \right. \right) \leq \mathbb{P}\left( \sup_{x \in \mathcal{X}} |\mu_{\sigma(x)} - Z_{\sigma(x)}/k| > \epsilon \left| X_1, \ldots, X_n \right. \right) \leq \mathbb{P}\left( \sup_{\sigma \in \Sigma} |\mu_\sigma - Z_\sigma/k| > \epsilon \left| X_1, \ldots, X_n \right. \right) \leq \frac{2S(n)}{\epsilon} \exp\left( -\frac{k \epsilon^2}{2(k+\epsilon/3)} \right).
\]

Since the right-hand side is independent of \( X_1, \ldots, X_n \), the unconditional bound

\[
\mathbb{P}\left( \sup_{x \in \mathcal{X}} \|\bar{\eta}_k(x) - \bar{\eta}(x)\|_\infty > \epsilon \right) \leq 2S(n) \exp\left( -\frac{k \epsilon^2}{2(k+\epsilon/3)} \right)
\]

follows. Plugging in

\[
\epsilon = \frac{1}{3k} \log \frac{2S(n)}{\delta} + \sqrt{\left( \frac{1}{3k} \log \frac{2S(n)}{\delta} \right)^2 + \frac{2r}{k} \log \frac{2S(n)}{\delta} \leq \frac{2}{3k} \log \frac{2S(n)}{\delta} + \sqrt{\frac{2r}{k} \log \frac{2S(n)}{\delta}}}
\]

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and simplifying gives the final result.

Recall that there is a small (polylogarithmic in $r$) gap between our upper and lower bounds. We believe that the upper bound may be slightly loose, and that this might be tightened by using a stronger concentration inequality, such as Bennett’s inequality [Bennett, 1962], instead of Bernstein’s inequality in Inequality (18).

**C.2 Lower Bounds**

In this section, we prove Theorem 16, our lower bound on the minimax uniform error of estimating a Hölder continuous regression function. We use a standard approach based on the following version of Fano’s lemma:

**Lemma 28.** (Fano’s Lemma; Simplified Form of Theorem 2.5 of Tsybakov 2009) Fix a family $\mathcal{P}$ of distributions over a sample space $\mathcal{X}$ and fix a pseudo-metric $\rho : \mathcal{P} \times \mathcal{P} \to [0, \infty]$ over $\mathcal{P}$. Suppose there exist $P_0 \in \mathcal{P}$ and a set $T \subseteq \mathcal{P}$ such that

$$\sup_{P \in T} D_{KL}(P, P_0) \leq \frac{\log |T|}{16},$$

where $D_{KL} : \mathcal{P} \times \mathcal{P} \to [0, \infty]$ denotes Kullback-Leibler divergence. Then,

$$\inf_{\hat{P}} \sup_{P \in \mathcal{P}} \mathbb{P} \left( \rho(P, \hat{P}) \geq \frac{1}{2} \inf_{P \in T} \rho(P, P_0) \right) \geq 1/8,$$

where the first inf is taken over all estimators $\hat{P}$.

Now, we proceed with the proof. We now proceed to construct an appropriate $P_0 \in \mathcal{P}$ and $T \subseteq \mathcal{P}$. Let $g : [-1, 1]^d \to [0, 1]$ defined by

$$g(x) = \begin{cases} \exp \left( 1 - \frac{1}{1 - \|x\|_2^2} \right) & \text{if } \|x\|_2 < 1 \\ 0 & \text{else} \end{cases}$$

denote the standard bump function supported on $[-1, 1]^d$, scaled to have $\|g\|_{\mathcal{X}, \infty} = 1$. Since $g$ is infinitely differentiable and compactly supported, it has a finite $\alpha$-Hölder semi-norm:

$$\|g\|_{\Sigma^\alpha} := \sup_{\ell \in \mathbb{N}^d : \ell \leq \alpha} \sup_{x \neq y \in \mathcal{X}} \frac{|g^\ell(x) - g^\ell(y)|}{\|x - y\|^\alpha \|\ell\|_1} < \infty,$$

where $\ell$ is any $[\beta]$-order multi-index and $g^\ell$ is the corresponding mixed derivative of $g$. Define $M := \left( \frac{64(2^{2d}+d)nr}{d \log(nr)} \right)^{-\frac{1}{\beta + 1}} \geq 1$, since $r \geq 1/n$. For each $m \in [M]^d$, define $g_m : \mathcal{X} \to [0, 1]$ by

$$g_m(x) := g \left( Mx - \frac{2m - 1}{2} \right),$$

so that $\{g_m : m \in [M]^d\}$ is a grid of $M^d$ bump functions with disjoint supports. Let $\zeta_0 \equiv \frac{1}{4}$ denote the constant-$\frac{1}{4}$ function on $\mathcal{X}$. Finally, for each $m \in [M]^d$, define $\zeta_m : \mathcal{X} \to [0, 1]$ by

$$\zeta_m := \zeta_0 + \min \left\{ \frac{1}{2}, \frac{L \|g\|_{\Sigma^\alpha}}{\|g\|_{\Sigma^\alpha}} \right\} M^{-\alpha} g_m.$$

(20)

Note that, for any $m \in [M]^d$,

$$\|\zeta_m\|_{\Sigma^\alpha} \leq LM^{-\alpha} \frac{\|g_m\|_{\Sigma^\alpha}}{\|g\|_{\Sigma^\alpha}} = L,$$

so that $\zeta_m$ satisfies the Hölder smoothness condition. For any particular $\eta$, let $P_{\eta}$ denote the joint distribution of $(X, Y)$. Note that $P_{\eta}(x, 1) = \zeta(x) \geq 1/4$. Moreover, one can check that, for all
\(x \geq -2/3, \ -\log(1 + x) \leq x^2 - x.\) Hence, for any \(x \in \mathcal{X},\)

\[
P_{\eta_n}(x, 1) \log \frac{P_{\eta_n}(x, 1)}{P_{\eta}(x, 1)} = r \zeta_m(x, 1) \log \frac{P_{\zeta_m}(x, 1)}{P_{\zeta}(x, 1)}
\]

\[
= r \zeta_m(x) \log \frac{\zeta_m(x)}{\zeta(x)}
\]

\[
= -r \zeta_m(x) \log \left(1 + \frac{\zeta(x) - \zeta_m(x)}{\zeta_m(x)}\right)
\]

\[
\leq r \zeta_m(x) \left(\frac{(\zeta(x) - \zeta_m(x))^2}{\zeta_m(x)} - \frac{\zeta(x) - \zeta_m(x)}{\zeta_m(x)}\right)
\]

\[
= r \left(4(\zeta(x) - \zeta_m(x))^2 + \zeta(x) - \zeta_m(x)\right)
\]

and, similarly, since \(P_\zeta(x, 0) = 1 - \zeta(x) \geq 1/4,

\[
P_{\eta_n}(x, 0) \log \frac{P_{\eta_n}(x, 0)}{P_{\eta}(x, 0)} \leq r \left(4(\zeta(x) - \zeta_m(x))^2 + \zeta(x) - \zeta_m(x)\right).
\]

Adding these two terms gives

\[
D_{KL}(P_{\eta_n}, \eta) = n \left(\int_{\mathcal{X}} P_{\eta_n}(x, 0) \log \frac{P_{\eta_n}(x, 0)}{P_{\eta_n}(x, 0)} \ dx + \int_{\mathcal{X}} P_{\eta_n}(x, 1) \log \frac{P_{\eta}(x, 1)}{P_{\eta_n}(x, 1)} \ dx\right)
\]

\[
\leq 8nr \int_{\mathcal{X}} (\zeta(x) - \zeta_m(x))^2 \ dx
\]

\[
= 8nr \|\zeta - \zeta_m\|_2^2
\]

\[
\leq 2nr M^{-2\alpha} \|g_m\|_2^2
\]

\[
= 2nr M^{-2\alpha + d} \|g\|_2^2
\]

\[
= 2nr \left(\frac{64(2\alpha + d)nr}{d \log(nr)}\right)^{-(2\alpha + d)} \|g\|_2^2
\]

\[
= \frac{1}{32} \left(\frac{d}{2\alpha + d}\right) \|g\|_2^2 \log(nr)
\]

\[
\leq \frac{1}{16} \left(\frac{d}{2\alpha + d}\right) \left(\log(nr) - \log(\log(nr) + \log \frac{64(2\alpha + d)}{d}\right)
\]

\[
= \frac{\log(|M|)}{16}
\]

where the second inequality comes from the definition of \(\zeta_m\) (Eq. 20) and the third inequality comes from the facts that \(\|g\|_2^2 \leq 1\) and \(\log \log x \leq \frac{1}{2} \log x\) for all \(x > 1\). Fano’s lemma therefore implies the lower bound

\[
\inf_{\mathcal{H}_n} \sup_{r \in (0, 1), \zeta \in \Sigma^\alpha(L)} \mathbb{P}_{\mathcal{H}_n} \left(\left\|r\zeta - \hat{r}\zeta\right\|_\infty \geq \frac{1}{2} \min \left\{\frac{1}{2}, \left\|\frac{L}{\|\zeta\|_2}\right\|\right\} \left(\frac{d \log(nr)}{64(2\alpha + d)n}\right)^{\frac{n}{d + \alpha}}\right) \geq \frac{1}{8},
\]

which completes the proof. \(\square\)