Estimating the Arc Length of the Optimal ROC Curve and Lower Bounding the Maximal AUC

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Abstract

We show that when the data likelihood ratio is used as the score function, the arc length of the corresponding ROC curve gives rise to a novel f-divergence which measures differences between the positive and negative data distributions. This f-divergence can be expressed using a variational objective and estimated only using samples from the positive and negative *data* distributions. We show the empirical version of this variational objective is also a consistent estimator for the arctangent likelihood ratio with a non-parametric convergence rate $O_p(n^{-\beta/4})$ ($\beta \in (0, 1]$ depends on the smoothness). Moreover, we show the surface area below the optimal ROC curve can be expressed as a similar variational objective depending on the arctangent likelihood ratio. These new insights lead to a novel two-step procedure for finding a good score function by lower bounding the maximal AUC. Experiments on CIFAR-10 datasets show the proposed two-step procedure achieves good AUC performance in unbalanced binary classification tasks while being less computationally demanding.

1 Introduction

The study of Receiver operating characteristic (ROC) curves has a long history in medicine [24], psychology [13] and radiology [16, 11]. In machine learning, ROC curves have been primarily used to analyze the performance of different classification algorithms [6, 7]. Indeed, the Area Under the Curve (AUC) encodes the ranking accuracy of a classifier, which makes it a preferable performance metric for unbalanced class classification [6, 2]. In recent years, ROC curves have also been used in applications that compare two distributions and achieves promising results. Examples include analyzing the mode collapsing issue of Generative Adversarial nets (GAN) [23], and diagnosing the performance of an amortized Markov Chain Monte Carlo [18].

In applications that require computing statistical discrepancy between distributions (e.g. GAN [12] or Variational Inference (VI) [1]), f-divergences are a widely used discrepancy measure. The family of f-divergences includes Kullback-Leibler divergence [22] and Total Variational distance. It has been shown that f-divergences in general can be expressed via variational objectives and can be efficiently approximated from empirical samples [26, 27].

One might question that as the ROC curves are used as performance metrics in many two sample applications, are they in any way related to f-divergences? For example, can AUC be an f-divergence between positive and negative data densities given some score function? An earlier investigation proves that the answer is no when the score function is the likelihood ratio [28] . Nonetheless, this result inspired us to look for f-divergence from other geometries of the ROC curve.

In this paper we show that, when using the likelihood ratio score, a novel f-divergence arises from computing the *arc length* of the corresponding ROC curve. By leveraging this result, we can

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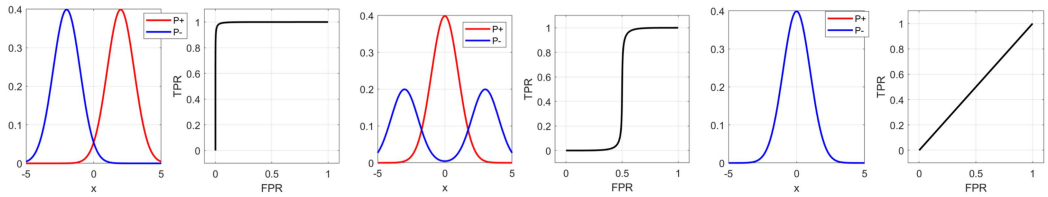

(a) different distributions, long ROC (b) different distributions, long ROC (c) same distribution, short ROC

Figure 1: ROC curves generated for one dimensional datasets using the identity score function $t(x) = x$. Notice that the arc length of ROC curves seem to be a good indication on how different the positive (red) and negative (blue) data distributions are.

express the arc length using a variational objective and approximate it using only samples from two distributions. We show this arc length estimator is also a consistent estimator to the arctangent of likelihood ratio and has a non-parametric convergence rate $O_p(n^{-\beta/4})$, where $\beta \in (0, 1]$ depends on the smoothness of the true arctangent likelihood ratio. Moreover, we show that by parameterizing the ROC curve of *mixtures* of positive and negative distributions, the surface area below the maximual ROC curve can be expressed via a similar variational objective. With the help of our arctangent ratio estimator, we can approximately maximize a lower bound to the maximal AUC. We point out the similarity between this lower bound maximization and the classic AUC maximization [2] and show our approximated optimal score achieves comparable performance to an AUC maximizer in an unbalanced classification problem while being less computationally demanding.

2 Background

2.1 An Illustrative Example

ROC curves are frequently used to visualize binary classification performance, and we often rely on the Area Under the Curve (AUC) as a numerical metric for selecting a good classifier. In this section, we highlight an often overlooked ROC geometry: arc length. We illustrate its potential as a good discrepancy measure between positive and negative data distributions.

Let us consider the one-dimensional distributions and the ROC curves in Figure 1. In this example, ROC curves are generated using the identity score function $t(x) = x$.

In both (a) and (b), p_+ and p_- are quite different, and thus the discrepancies between positive and negative distributions should be large in both cases. In (c), the densities p_+ and p_- are the same and consequently their discrepancy should be smaller than that of both (a) and (b). Further, notice that both (a) and (b) have long ROC curves (≈ 2) while (c) has a shorter one ($\approx \sqrt{2}$). This example therefore suggests that the more similar p_+ and p_- are, the shorter the ROC curve is.

However, we can see that $t(x) = x$ is a special choice: If $t(x) = 0$, the arc length will not reflect any discrepancy between data distributions at all. This simple observation promotes the following questions: Why is the arc length in this example good at telling the differences between two data distributions? Are there other score functions whose corresponding ROC arc length are good discrepancy measures between positive and negative data distributions? What are the practical applications of studying the arc length of ROC? In the following sections, we study the arc length of an ROC curve under a probabilistic framework and provide answers to these questions.

2.2 ROC Curve in a Probabilistic Setting

Suppose we have positive and negative datasets $X_+ := \{\boldsymbol{x}_i^+\}_{i=1}^{n_+}$ and $X_- := \{\boldsymbol{x}_i^-\}_{i=1}^{n_-}$ drawn from two distributions $\mathbb{P}_+$ and $\mathbb{P}_-$ respectively. These distributions have respective probability density functions $p_+(\boldsymbol{x})$ and $p_-(\boldsymbol{x})$ that are both defined on the domain $\mathcal{X} \subseteq \mathbb{R}^d$. A score function takes a sample $\boldsymbol{x}$ as input and outputs a real-valued score. Suppose we have a score function $t(\boldsymbol{x}) \in \mathbb{R}$.

Let F_+ and F_- denote the Cumulative Distribution Functions (CDFs) of $t(\boldsymbol{x}^+)$ and $t(\boldsymbol{x}^-)$ respectively. Then we can define the following quantities:

- False Positive Rate (FPR), $\tilde{F}_- := 1 - F_-$
- True Positive Rate (TPR), $\tilde{F}_+ := 1 - F_+$
- The ROC curve of a score function t: the graph of function $\tilde{F}_+[\tilde{F}_-^{-1}(s)]$, where $s \in [0, 1]$.

The above definition of ROC curve requires F_- to be strictly increasing. In this paper, we assume F_+, F_- to be both strictly increasing. Both F_+ and F_- depend on the choice of score function t.

2.3 Arc Length of ROC Curve

Due to the strict monotonicity of CDFs, $\tilde{F}_+$ and $\tilde{F}_-$ form a bijective parameterization of the ROC curve in the sense that each point on this ROC curve can be written as $(\tilde{F}_-(\tau_0), \tilde{F}_+(\tau_0))$ for a unique $\tau_0 \in \mathbb{R}$. Using the line integral formula, the arc length of an ROC curve for a fixed score function t can be expressed using the derivatives of $\tilde{F}_-$ and $\tilde{F}_+$:

$$\widehat{\mathrm{ROC}}(t) := \int_{-\infty}^{\infty} \sqrt{\left[\partial_\tau \tilde{F}_+(\tau)\right]^2 + \partial_\tau \left[\tilde{F}_-(\tau)\right]^2} \mathrm{d}\tau = \int_{-\infty}^{\infty} \sqrt{f_+(\tau)^2 + f_-(\tau)^2} \mathrm{d}\tau, \qquad (1)$$

where $f_+(\tau)$ and $f_-(\tau)$ are the density functions of $t(\boldsymbol{x}^+)$ and $t(\boldsymbol{x}^-)$ respectively. Although (1) is an elementary result, it has been seldom discussed in the ROC literature. Authors in [3, 4] have proposed a performance metric computed over the "ROC hypersurface" and (1) is used to justify such a metric in a binary classification setting.

Using (1), we can confirm a simple geometric fact whose proof can be found in Appendix A:

Proposition 1. $\widehat{\mathrm{ROC}}(t) \in [\sqrt{2}, 2]$, *for all* t.

This result reflects the geometric observation that any monotone curve (such as ROC curve) starts and ends at two opposite corners of the ROC space $[0, 1]^2$ has an arc length between $\sqrt{2}$ and 2.

3 f-divergences Arising from ROC Arc Length

3.1 f-divergence of Score Distributions

Among many discrepancies measures, f-divergence has been widely used in many applications.

Definition 1. *Let p and q be densities of two continuous distributions. An f-divergence is defined as:* $\mathrm{D}_g(p|q) := \mathbb{E}_q \left[g\left(\frac{p(\boldsymbol{z})}{q(\boldsymbol{z})}\right)\right]$, *where g is convex and lower-semicontinuous satisfying $g(1) = 0$.*

Now let us slightly rewrite (1). Assuming f_- is strictly positive (in which case F_- is strictly increasing), we can write

$$\widehat{\mathrm{ROC}}(t) - \sqrt{2} = \mathbb{E}_{f_-} \sqrt{\left[\frac{f_+(\tau)}{f_-(\tau)}\right]^2 + 1} - \sqrt{2}. = \mathbb{E}_{f_-} \left[g\left(\frac{f_+(\tau)}{f_-(\tau)}\right)\right], \qquad (2)$$

where $g(s) = \sqrt{s^2 - 1} - \sqrt{2}$. Equation (2) yields the first important result of this paper: $\widehat{\mathrm{ROC}}(t) - \sqrt{2}$ is an f-divergence between score densities f_+ and f_- since $g(s)$ is a convex function and $g(1) = 0$. This result confirms, for any given t, $\widehat{\mathrm{ROC}}(t)$ is a good discrepancy for measuring positive and negative scores (i.e., score distributions). It also explains why the ROC arc length in Figure 1 is a good discrepancy measure: Given $t(x) = x$, the score distributions are same as the data distributions in each plot. The arc length of ROCs in Figure 1 plots are f-divergences of the score distributions hence are also f-divergences of data distributions.

Although $\widehat{\mathrm{ROC}}(t) - \sqrt{2}$ is an f-divergence of score distributions, it is not an f-divergence of the positive and negative *data* distributions for general t. The choice $t(x) = x$ in the toy example does not have simple analogues for higher dimensional datasets. Are there choices of t such that the arc lengths of their ROC curves are good discrepancy measures on data distribution? In what follows, we show when t is a bijective transform of the likelihood ratio $\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}$, $\widehat{\mathrm{ROC}}(t)$ encodes the differences between $p_+(\boldsymbol{x})$ and $p_-(\boldsymbol{x})$ in the form of an f-divergence between $p_+(\boldsymbol{x})$ and $p_-(\boldsymbol{x})$.

3.2 f-divergences of Data Distributions

Using the law of the unconscious statistician, we can express $\widehat{\mathrm{ROC}}(t)$ in terms of an expectation with respect to the negative data density $p_-(\boldsymbol{x})$: $\mathbb{E}_{p_-}\sqrt{\left[\frac{f_+(t(\boldsymbol{x}))}{f_-(t(\boldsymbol{x}))}\right]^2+1}$. Consider a special family of score functions: $t^*(\boldsymbol{x})=\gamma\left(\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}\right)$ where γ is any strictly increasing function. Due to the Neyman-Pearson lemma [25], $\mathrm{ROC}(t^*)$ has the highest TPR at any FPR level. Geometrically speaking, they dominate all other ROC cuves in an ROC plot. Hence, we refer to t^* as the optimal score and $\mathrm{ROC}(t^*)$ as the optimal ROC curve. For convenience, we denote the $\mathrm{ROC}(t^*)$ as ROC^* which reads "rock star".

It can be shown that

$$\frac{f_+(t^*(\boldsymbol{x}_0))}{f_-(t^*(\boldsymbol{x}_0))}=\frac{\int_{\boldsymbol{x}:\gamma\left(\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}\right)=t^*(\boldsymbol{x}_0)}p_+(\boldsymbol{x})\mathrm{d}\boldsymbol{x}}{\int_{\boldsymbol{x}:\gamma\left(\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}\right)=t^*(\boldsymbol{x}_0)}p_-(\boldsymbol{x})\mathrm{d}\boldsymbol{x}}=\frac{p_+(\boldsymbol{x}_0)}{p_-(\boldsymbol{x}_0)},\quad\forall\gamma \tag{3}$$

where the second equality holds due to $\frac{\int_D a(\boldsymbol{x})\mathrm{d}\boldsymbol{x}}{\int_D b(\boldsymbol{x})\mathrm{d}\boldsymbol{x}}=\gamma^{-1}(C)$, when $\gamma\left(\frac{a(\boldsymbol{x})}{b(\boldsymbol{x})}\right)\equiv C,\ \forall\boldsymbol{x}\in D$. When $\gamma(\boldsymbol{x})=\boldsymbol{x}$, (3) expresses a known result [5], and is often given in plain English as "the density ratio of the likelihood ratio score is the likelihood ratio itself".

Finally, $\widehat{\mathrm{ROC}^*}$ takes an elegant form free from t^* or γ: $\mathbb{E}_{p_-(\boldsymbol{x})}\sqrt{\left[\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}\right]^2+1}$. Equivalently, we can write

$$\widehat{\mathrm{ROC}^*}-\sqrt{2}=\mathbb{E}_{p_-(\boldsymbol{x})}\left[g\left(\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}\right)\right] \tag{4}$$

We can see that the same f-divergence arises from computing the arc length of ROC^*. However, unlike the f-divergence given in (2), (4) is an f-divergence between *data* distributions, not score distributions. It shows that as long as we use the the optimal scores, the arc length of the optimal ROC can indeed reflect the differences between *data* distributions. From now on, we will refer to $\widehat{\mathrm{ROC}^*}-\sqrt{2}$ as the ROC divergence. To the best of our knowledge, (4) has not been presented in literature before.

By definition, the ROC divergence is symmetric. Moreover, as a result of Proposition 1, the ROC divergence is upper bounded by $2-\sqrt{2}$ and lower bounded by 0.

As we mentioned earlier, ROC^* has the maximal AUC. Here we prove a result regarding some other geometric properties of ROC^*.

Proposition 2. ROC^* *is a convex curve and* $\widehat{\mathrm{ROC}^*}$ *is the longest among all convex ROC curves.*

The proof of this proposition can be found in Appendix B in the supplementary material.

4 Estimating the Arc Length of ROC^*

4.1 A Variational Objective

To numerically approximate the arc length using samples alone, we leverage that $\widehat{\mathrm{ROC}^*}-\sqrt{2}$ is an f-divergence. Utilizing Fenchel's duality [20], Authors in [26] show that an f-divergence $\mathrm{D}_g(p_+|p_-)$ has a variational representation:

$$\begin{aligned}\mathrm{D}_g(p_+|p_-)=\int_{\mathcal{X}}p_-(\boldsymbol{x})g\left[\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}\right]\mathrm{d}\boldsymbol{x}&=\int_{\mathcal{X}}p_-(\boldsymbol{x})\sup_u\left\{u(\boldsymbol{x})\cdot\left[\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}\right]-g'[u(\boldsymbol{x})]\right\}\mathrm{d}\boldsymbol{x}\\&=\sup_u\int_{\mathcal{X}}p_+(\boldsymbol{x})u(\boldsymbol{x})-\int_{\mathcal{X}}p_-(\boldsymbol{x})g'[u(\boldsymbol{x})]\mathrm{d}\boldsymbol{x},\end{aligned}$$

where g' is the convex conjugate of g and the supremum is taken over all measurable functions. In the case of the ROC divergence, $g(z)=\sqrt{z^2+1}-\sqrt{2}$ with $z\in[0,\infty]$ thus g has a convex

conjugate $g'(z') = -\sqrt{1-z'^2} - \sqrt{2}$, $z' \in [0,1]$. Rewriting $\widehat{\mathrm{ROC}}^* - \sqrt{2}$ using the above variational representation and dropping the $-\sqrt{2}$, we obtain:

$$\widehat{\mathrm{ROC}}^* = \sup_{u \in [0,1]} \mathbb{E}_{p_+}[u(\boldsymbol{x})] + \mathbb{E}_{p_-}[\sqrt{1-u^2(\boldsymbol{x})}].$$

We reparameterize $u(\boldsymbol{x}) = \sin[v(\boldsymbol{x})]$, where $v \in [0, \pi/2]$:

$$\widehat{\mathrm{ROC}}^* = \sup_{v \in [0,\pi/2]} \mathbb{E}_{p_+} \sin[v(\boldsymbol{x})] + \mathbb{E}_{p_-} \cos[v(\boldsymbol{x})]. \tag{5}$$

Differentiating the objective in (5) for v, we can see the supremum is attained at $v^* = \operatorname{atan} \frac{p_+}{p_-}$. In other words, the optimal v^* is the arctangent likelihood ratio function. Thus, our assumptions on the likelihood ratio $\frac{p_+}{p_-}$ can provide valuable guidance when designing a suitable function class for v when solving (5) in practice.

It is also interesting to see how v^* is visualized in the ROC plot. We can see the tangent of ROC^* at an FPR level $s_0 \in [0,1]$ is $\partial_s \tilde{F}_+(\tilde{F}_-^{-1}(s_0)) = \frac{f_+(\tilde{F}_-^{-1}(s_0))}{f_-(\tilde{F}_-^{-1}(s_0))} = \frac{p_+(\boldsymbol{x}_0)}{p_-(\boldsymbol{x}_0)}$, where $\boldsymbol{x}_0$ is any point in $\mathcal{X}$ that satisfies the equality $\gamma\left(\frac{p_+(\boldsymbol{x}_0)}{p_-(\boldsymbol{x}_0)}\right) = \tilde{F}_-^{-1}(s_0)$. It can be seen that the likelihood ratio characterizes the slope of ROC^* and thus $v^* = \operatorname{atan} \frac{p_+}{p_-}$ is the *slope angle* of ROC^*. Hence, the boundary constraint for $v(\boldsymbol{x})$ in (5) coincides with the geometric fact that the slope angle of any ROC curve is in between 0 and $\pi/2$.

Moreover, using (5), we can obtain a relationship between $\widehat{\mathrm{ROC}}^*$ and the total variation distance between $\mathbb{P}_+$ and $\mathbb{P}_-$ (denoted as $\mathrm{TV}(\mathbb{P}_+, \mathbb{P}_-)$).

Proposition 3. $\widehat{\mathrm{ROC}}^*$ *has a lower and upper bound expressed via* $\mathrm{TV}(\mathbb{P}_+, \mathbb{P}_-)$*:*

$$\frac{1}{2}\mathrm{TV}(\mathbb{P}_+, \mathbb{P}_-) + 1 \leq \widehat{\mathrm{ROC}}^* \leq \frac{\pi}{4}\mathrm{TV}(\mathbb{P}_+, \mathbb{P}_-) + \frac{\pi}{2}.$$

Proof of this proposition can be found at Section C. This proposition further justifies that $\widehat{\mathrm{ROC}}^*$ is a valid measure of the discrepancy between $\mathbb{P}_+$ and $\mathbb{P}_-$.

4.2 Designing of $\mathcal{F}$ and Two Estimators

To use (5) in practice, we need to find appropriate function class $\mathcal{F}$ as well as using empirical average over X_+ and X_- to replace the expectations. Consider two different modelling choices of v:

Estimating $\operatorname{atan}\left[\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}\right]$ **directly:** We can simply restrict v to a bounded (parametric/non-parametric) function class $\mathcal{F}$ and solve the sample version of (5). Then (5) becomes

$$\max_{v \in [0,\pi/2], v \in \mathcal{F}} \frac{1}{n_+} \sum_{i=1}^{n_+} \sin(v(\boldsymbol{x}_i)) + \frac{1}{n_-} \sum_{i=1}^{n_-} \cos(v(\boldsymbol{x}_i)). \tag{6}$$

where, for ease, we write $\sum_{i=1}^{n_+} f(\boldsymbol{x}_i^+)$ as $\sum_{i=1}^{n_+} f(\boldsymbol{x}_i)$, a convention which will adopted henceforth.

In practice, enforcing the boundedness $v \in [0, \pi/2]$ over $\mathcal{X}$ is difficult. We can relax (6) by only enforcing the boundedness constraint of v on our finite sample dataset $X_+ \cup X_-$.

For example, by letting $\mathcal{F}$ be a Reproducing Kernel Hilbert Space (RKHS) [30], we can translate (6) into the following optimization problem:

$$\begin{aligned} \hat{v} &:= \operatorname*{argmin}_{v \in \mathcal{H}} \ell(v) + \frac{\lambda}{2}\|v\|_{\mathcal{H}}^2, \quad \ell(v) := -\frac{1}{n_+}\sum_{i=1}^{n_+} \sin\langle v, \varphi(\boldsymbol{x}_i)\rangle - \frac{1}{n_-}\sum_{i=1}^{n_-} \cos\langle v, \varphi(\boldsymbol{x}_i)\rangle \\ &\text{s.t: } \langle v, \varphi(\boldsymbol{x})\rangle \in \left[0, \frac{\pi}{2}\right], \quad \forall \boldsymbol{x} \in X_+ \cup X_-, \end{aligned} \tag{7}$$

where $\mathcal{H}$ is a RKHS with a positive definite kernel $k(\boldsymbol{x}, \boldsymbol{x}') = \langle \varphi(\boldsymbol{x}), \varphi(\boldsymbol{x}')\rangle$, $\|\cdot\|_{\mathcal{H}}$ is the RKHS norm and $\frac{\lambda}{2}\|v\|_{\mathcal{H}}^2$ is the regularization term. $\langle \hat{v}, \varphi(\boldsymbol{x})\rangle$ is an estimation of $v^*(\boldsymbol{x})$, the arctangent of the likelihood ratio. (7) is a strictly convex optimization and thus, if a solution $\hat{v}$ exists, it must be unique.

Estimating $\log\left[\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}\right]$**:** We can also leverage that v^* is the arctangent of the likelihood ratio and introduce mild assumptions on p_+ and p_-. When $p_+(\boldsymbol{x})$ and $p_-(\boldsymbol{x})$ are both members of the exponential family and share the same sufficient statistic $\boldsymbol{h}(\boldsymbol{x}) \in \mathbb{R}^m$, then $\exists \boldsymbol{v}^* \in \mathbb{R}^m$ such that $\log\left[\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}\right] = \langle \boldsymbol{v}^*, \boldsymbol{h}(\boldsymbol{x})\rangle + C$, where C is a constant. If we choose to parameterize the log likelihood ratio using a linear model, $\langle \boldsymbol{v}, \boldsymbol{h}(\boldsymbol{x})\rangle + v_0$, then (6) becomes

$$(\hat{\boldsymbol{v}}, \hat{v}_0) := \operatorname*{argmax}_{\substack{\boldsymbol{v}\in\mathbb{R}^m,\\ v_0\in\mathbb{R}}} \frac{1}{n_+}\sum_{i=1}^{n_+} \sin[\operatorname{atan}\exp(\langle \boldsymbol{v}, \boldsymbol{h}(\boldsymbol{x}_i)\rangle + v_0)] + \frac{1}{n_-}\sum_{i=1}^{n_-} \cos[\operatorname{atan}\exp(\langle \boldsymbol{v}, \boldsymbol{h}(\boldsymbol{x}_i)\rangle + v_0)]. \tag{8}$$

Note we do not have to restrict the optimization to a bounded function family as $\log\left[\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}\right] \in \mathbb{R}$, and $\langle \hat{\boldsymbol{v}}, \boldsymbol{h}(\boldsymbol{x})\rangle + \hat{v_0}$ is an estimate of the likelihood ratio.

In this paper, we focus on (7) since the objective in (8) is non-convex with respect to $\boldsymbol{v}$ thus presents extra challenges in the theoretical analysis, although (8) is easier to implement in practice due to its unconstrained nature.

4.3 Finite Sample Guarantee

In this section, we show that $\langle \hat{v}, \varphi(\boldsymbol{x})\rangle$ converges to the true arctangent likelihood ratio (or its projection onto $\mathcal{H}$) as the number of samples goes to infinity. Below are a few regularity conditions.

Assumption 1. *There exists a unique $v^* \in \mathcal{H}$, such that $\mathbb{E}[\nabla_v \ell(v^*)] = 0$ and $\langle v^*, \varphi(\boldsymbol{x})\rangle \in [0, \pi/2]$ holds for all $\boldsymbol{x} \in \mathcal{X}$.*

A sufficient condition of the above condition is specified in the following proposition.

Proposition 4. *If there exists a unique $v^* \in \mathcal{H}$, such that $\langle v^*, \varphi(\boldsymbol{x})\rangle = \operatorname{atan}\left[\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}\right]$ then Assumption 1 holds.*

Proof of this Proposition can be found in Appendix F. Proposition 4 states if model is correctly specified and identifiable then Assumption 1 holds. It is possible that there exists a $v^* \in \mathcal{H}$ satisfying $\mathbb{E}[\nabla_v \ell(v^*)] = 0$ which does not meet the boundedness constraint $[0, \pi/2]$. In this paper we only consider situations where Assumption 1 holds, which includes all situations where the model is correctly specified and some situations where the model is misspecified.

Assumption 2. *Let $n_{\min} = \min(n_+, n_-)$. There exists a subspace $\mathcal{H}^* := \{v \in \mathcal{H} | \|v - v^*\|_{\mathcal{H}}^2 \leq \delta_{n_{\min}}^2\}$, such that $\forall v \in \mathcal{H}^*, \forall \boldsymbol{x} \in X_+ \cup X_-, \langle v, \varphi(\boldsymbol{x})\rangle \in (0, \frac{\pi}{2})$ holds with high probability. The sequence $\delta_{n_{\min}}$ is monotonically decreasing as $n_{\min}$ grows to infinity.*

Assumption 2 states all v within a vicinity of v^* are in the interior of (7)'s feasible region with high probability. The following proposition gives a sufficient condition under which Assumption 2 holds.

Proposition 5. *Suppose $\|\varphi(\boldsymbol{x})\|_{\mathcal{H}} \leq 1$. If our model is correctly specified as described in Proposition 4 and $\forall \boldsymbol{x} \in \mathcal{X}$, $\operatorname{atan}\left[\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}\right] \in [R_1, R_2]$, for some R_1 and R_2 such that $\frac{\pi}{2} > R_2 > R_1 > 0$, then there exists $N > 0$ such that Assumption 2 holds when $n_{\min} > N$.*

The proof can be found in Appendix D. Since we use RKHS as the estimator function class, our final assumption is that v^* should be reasonably smooth. In previous works such an assumption depends on the decay of the integral operator's eigenvalues [33, 8]. In this paper, we measure the smoothness using the *range space* technique which has recently been adopted in [9, 32]. We define

$$\boldsymbol{\Sigma}_v := \mathbb{E}[\nabla_f^2 \ell(v)] = \mathbb{E}_{p_+}[\sin\langle v, \varphi(\boldsymbol{x})\rangle \cdot \varphi(\boldsymbol{x}, \cdot) \otimes \varphi(\boldsymbol{x}, \cdot)] + \mathbb{E}_{p_-}[\cos\langle v, \varphi(\boldsymbol{x})\rangle \cdot \varphi(\boldsymbol{x}, \cdot) \otimes \varphi(\boldsymbol{x}, \cdot)],$$

where $\otimes$ denotes the outer product. Given $v_0 \in \mathcal{H}$, $\boldsymbol{\Sigma}_{v_0}$ is an integral operator on $u \in \mathcal{H}$ and

$$\boldsymbol{\Sigma}_{v_0} u = \mathbb{E}_{p_+}[\sin\langle v_0, \varphi(\boldsymbol{x})\rangle \cdot \varphi(\boldsymbol{x}, \cdot) \cdot u(\boldsymbol{x})] + \mathbb{E}_{p_-}[\cos\langle v_0, \varphi(\boldsymbol{x})\rangle \cdot \varphi(\boldsymbol{x}, \cdot) \cdot u(\boldsymbol{x})].$$

By definition $\boldsymbol{\Sigma}_{v_0}$ is a positive, self-adjoint operator, in the sense that $\langle u, \boldsymbol{\Sigma}_{v_0} u\rangle \geq 0$, $\langle u, \boldsymbol{\Sigma}_{v_0} v\rangle = \langle \boldsymbol{\Sigma}_{v_0} u, v\rangle, \forall v, u \in \mathcal{H}$. Moreover, some algebra shows that $\boldsymbol{\Sigma}_{v_0}$ is also a bounded and compact operator. See Section G for more details.

Next, we assume the true arctangent ratio function (or its projection on $\mathcal{H}$) is in the range space of $\boldsymbol{\Sigma}_{v^*}$.

Assumption 3. *Let $\mathcal{R}(\mathbf{\Sigma}_{v^*})$ denote the range space of $\mathbf{\Sigma}_{v^*}$. There exists $0 < \beta \leq 1$, $v^* \in \mathcal{R}(\mathbf{\Sigma}_{v^*}^{\beta})$, where C^{β} is the fraction power of a compact, positive and self-adjoint operator C.*

Note that the larger β is, the smoother the functions in the range space are. More discussions on the range space assumption can be found in Section 4.2, [32]. Now we are ready to state our theorem:

Theorem 1 (Convergence Rate of $\hat{v}$)**.** *Suppose Assumptions 1, 2 and 3 hold and $\hat{v}$ exists. If $\|\varphi(\boldsymbol{x})\|_{\mathcal{H}} \leq 1$ and*

$$\lambda = \frac{T}{n_{\min}^{1/4}}, \quad \frac{K}{n_{\min}^{\beta/4}} \leq \delta_{n_{\min}} \leq \frac{4}{\max\left(B_+, B_-\right)},$$

where $B_+ = \|\left(\mathbf{\Sigma}_{v^*} + \lambda \boldsymbol{I}\right)^{-1} \mathbb{E}_{p_+}[\varphi(\boldsymbol{x})]\|_{\mathcal{H}}$, $B_- = \|\left(\mathbf{\Sigma}_{v^*} + \lambda \boldsymbol{I}\right)^{-1} \mathbb{E}_{p_-}[\varphi(\boldsymbol{x})]\|_{\mathcal{H}}$, and $T \geq 1, K > 0$ are constants that do not depend on $n_{\min}$, then there exists a constant $N > 0$ such that when $n_{\min} > N$, $\|\hat{v} - v^*\|_{\mathcal{H}} = O_p(n_{\min}^{-\beta/4})$.

The proof can be found at Appendix E. Theorem 1 shows that, under mild assumptions, $\hat{v}$ is indeed a good estimator for $\operatorname{atan}\left[\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}\right]$. Since $\operatorname{atan}\left[\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}\right]$ is an optimal score, our estimator may have some interesting applications such as outlier detection [19] or Neyman-Pearson classification [35]. We will defer discussions on those applications in future works. In the next section, we employ our arctangent likelihood ratio estimator in an application of lower bounding the maximal AUC.

5 Lower Bounding the Maximum AUC

Finding a score function t that approximately maximizes AUC is an important task in binary classification. Due to the Neyman-Pearson lemma, ROC^* has the maximum AUC among all ROC curves. Let us denote the AUC of ROC^* as AUC^*. Consider the following inequalities:

$$\mathrm{AUC}^* = \underbrace{\sup_t \mathbb{E}_{p_-}\mathbb{E}_{p_+}\left[\mathbb{1}\left(t(\boldsymbol{x}_+) \geq t(\boldsymbol{x}_-)\right)\right]}_{(i)} \geq \sup_{t \in \mathcal{F}'} \underbrace{\mathbb{E}_{p_-}\mathbb{E}_{p_+}\left[L\left(t(\boldsymbol{x}_+), t(\boldsymbol{x}_-)\right)\right]}_{(ii)}, \tag{9}$$

where $L(a, b)$ is a continuous and concave lower bound of the indicator function $\mathbb{1}(a > b)$. It can be seen that $\mathbb{E}_{p_-}\mathbb{E}_{p_+}\left[\mathbb{1}\left(t(\boldsymbol{x}_+) \geq t(\boldsymbol{x}_-)\right)\right] = \int_{[0,1]} \tilde{F}_+(\tilde{F}_-^{-1}(s))\mathrm{d}s$ is the AUC of $\mathrm{ROC}(t)$. Due to the Neyman-Pearson lemma, the supremum of (i) is only attained when $t(\boldsymbol{x}) = \gamma\left(\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}\right)$ where γ is a strictly increasing function. Replacing the expectations in (ii) with sample averages, we obtain the optimization problem of AUC maximization [2, 10]. Therefore, we can see that AUC maximization is a procedure that approximates an optimal score function by maximizing a lower bound of AUC^*.

Now, we show a different way of lower bounding AUC^* with the help of $\operatorname{atan}\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}$. We have seen that how $(\tilde{F}_-(\tau), \tilde{F}_+(\tau))$ parameterizes an ROC curve given a score function t in Section 2.3. In fact, the surface between ROC^* and the diagonal line between $(0, 0)$ and $(1, 1)$ can be similarly parameterized by considering ROC curves of *mixtures* between positive and negative score distributions. Let F_+^* and F_-^* denote CDFs of any optimal score. For $\alpha \in [0, .5]$, we define FPR and TPR for α-mixtures of F_+^* and F_-^*:

$$\tilde{F}_-^*(\tau, \alpha) := 1 - [(1-\alpha)F_-^*(\tau) + \alpha F_+^*(\tau)], \quad \tilde{F}_+^*(\tau, \alpha) := 1 - [\alpha F_-^*(\tau) + (1-\alpha)F_+^*(\tau)].$$

We can see the 2-dimensional coordinate $\boldsymbol{r}(\tau, \alpha) := (\tilde{F}_+^*(\tau, \alpha), \tilde{F}_-^*(\tau, \alpha))$ parameterizes the area between ROC^* and the diagonal line in $[0, 1]^2$: When fixing α and varying τ, the coordinates give rise to a smooth curve in ROC space from $[0, 0]$ to $[1, 1]$. When $\alpha = 0$, such a curve is ROC^*. When $\alpha = .5$, such a curve is the diagonal line. When fixing $\tau = \tau_0$ and varying α, the coordinates produce a straight line segment connecting $(\tilde{F}_-^*(\tau_0, 0), \tilde{F}_+^*(\tau_0, 0))$ and $(\tilde{F}_-^*(\tau_0, .5), \tilde{F}_+^*(\tau_0, .5))$. The left plot in Figure 2 visualizes this parameterization. Now the surface area sandwiched between ROC^* and the diagonal line can be computed using a surface integration:

$$\mathrm{AUC}^* - .5 = \int_{\mathrm{dom}(\tau)} \int_{[0,.5]} \|\partial_\tau \boldsymbol{r}(\tau, \alpha) \times \partial_\alpha \boldsymbol{r}(\tau, \alpha)\| \, \mathrm{d}\alpha \mathrm{d}\tau, \tag{10}$$

where $\times$ denotes the cross product. After some algebra and applying the Fenchel duality technique in Section 4.1, we prove that AUC^* can also be expressed as the supremum of a variational objective similar to (5):

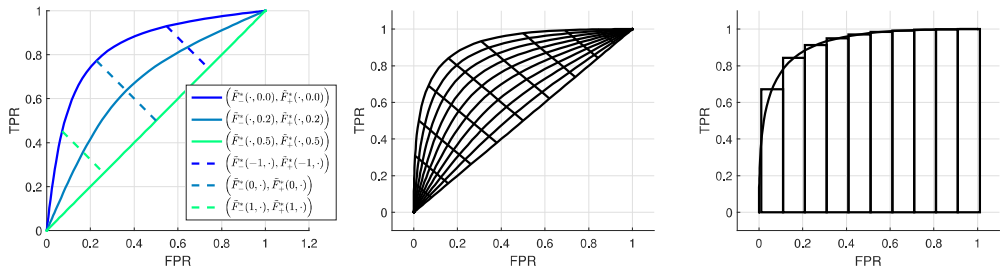

Figure 2: Left: $(\tilde{F}_+^*(\tau,\alpha), \tilde{F}_-^*(\tau,\alpha))$ parameterizes the surface between ROC^* and the diagonal line in $[0,1]^2$. This plot is created by setting $p_+ = \mathcal{N}(1,1)$, $p_- = \mathcal{N}(-1,1)$ and $t^*(x) = \frac{1}{2}\log\frac{p_+(x)}{p_-(x)} = x$. Middle: Our parameterization "mesh" divides AUC into surface elements (small patches on the plot). Right: Wilcoxon-Mann-Whitney statistic divides AUC into histograms bars.

Proposition 6. $\mathrm{AUC}^* = \frac{\sqrt{2}A}{2} + \frac{1}{2}$,

$$A := \sup_{v\in[0,\pi/2]} \mathbb{E}_{p_+}\left[w\left(\operatorname{atan}\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}\right)\sin[v(\boldsymbol{x})]\right] + \mathbb{E}_{p_-}\left[w\left(\operatorname{atan}\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}\right)\cos[v(\boldsymbol{x})]\right], \quad (11)$$

where $w(\tau) := \sin(\tau + \frac{\pi}{4}) \cdot |F_+^*(\tau) - F_-^*(\tau)|$. *The supremum of* (11) *is attained at* $v^* = \operatorname{atan}\frac{p_+}{p_-}$.

The proof can be found in Appendix H in the supplementary material. A lower bound of A can be obtained by restricting v to a function class. Evaluating w requires us to evaluate $\operatorname{atan}\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}$, F_+^* and F_-^* which are not readily available. However, Section 4.3 shows that the empirical estimator (7) is a consistent estimator of $\operatorname{atan}\frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}$ under mild conditions. Therefore, we propose the following two-step procedure to approximately lowerbound A:

1. Obtain $\hat{t}(\boldsymbol{x}) := \langle \hat{v}, \phi(\boldsymbol{x})\rangle$ using (7). Approximate F_+^* and F_-^* using $\hat{F}_+$ and $\hat{F}_-$ which are empirical CDFs of $\hat{t}(\boldsymbol{x}^+)$ and $\hat{t}(\boldsymbol{x}^-)$.
2. Optimize the empirical version of (11) by restricting v to a feasible function class and plugging in estimates obtained in the earlier step, i.e.,

$$\hat{\hat{v}} := \operatorname*{argmax}_{v\in[0,\pi/2], v\in\mathcal{F}} \frac{1}{n_+}\sum_{i=1}^{n_+} \hat{w}\left[\hat{t}(\boldsymbol{x}_i)\right]\cdot\sin[v(\boldsymbol{x}_i)] + \frac{1}{n_-}\sum_{i=1}^{n_-} \hat{w}\left[\hat{t}(\boldsymbol{x}_i)\right]\cdot\cos[v(\boldsymbol{x}_i)], \quad (12)$$

   where $\hat{w}(\tau) := \sin(\tau + \frac{\pi}{4})\left|\hat{F}_+(\tau) - \hat{F}_-(\tau)\right|$.

Note that (12) is nothing but a weighted sample objective (6). Thus, it can be easily optimized by the same algorithm that solves a weighted version of (6) given the approximated weights in the first step. In practice, we simply run (7) twice: The first time we run it without weights then run it again with weights $\hat{w}\left[\hat{t}(\boldsymbol{x}_i)\right]$ calculated from the first run.

Since the above algorithm also approximates an optimal score ($\operatorname{atan}\frac{p_+}{p_-}$) by maximizing a lower bound of AUC^*, it is natural to wonder how the maximizer $\hat{\hat{v}}$ of (12) would perform in AUC maximization tasks. In the next section, we show our two-step algorithm achieves a promising AUC performance when compared with an AUC maximizer.

Comparing to the traditional AUC maximizer, the proposed algorithm has a lower computational cost. Without loss of generality, assuming $n_+ = n_- = n$, the AUC maximization problem derived from the Wilcoxon-Mann-Whitney statistic [16] has a computational complexity $O(n^2)$. In comparison, (12) has a computational complexity $O(n)$. Computing $\hat{F}_+$ and $\hat{F}_-$ requires sorting our datasets which has an average computational complexity $O(n\log n)$. However, once our datasets are sorted, $\hat{F}_+\left(\hat{t}(\boldsymbol{x}_0)\right) = \frac{i}{n_+}$, where i is the index of $\hat{t}(x_0)$ in the sorted set $\{\hat{t}(x_i)\}_{i=1}^{n_+}$.

(10) computes AUC^* differently from the conventional Wilcoxon-Mann-Whitney statistic: Our approach divides the space sandwiched between ROC^* and the diagonal into small surface elements

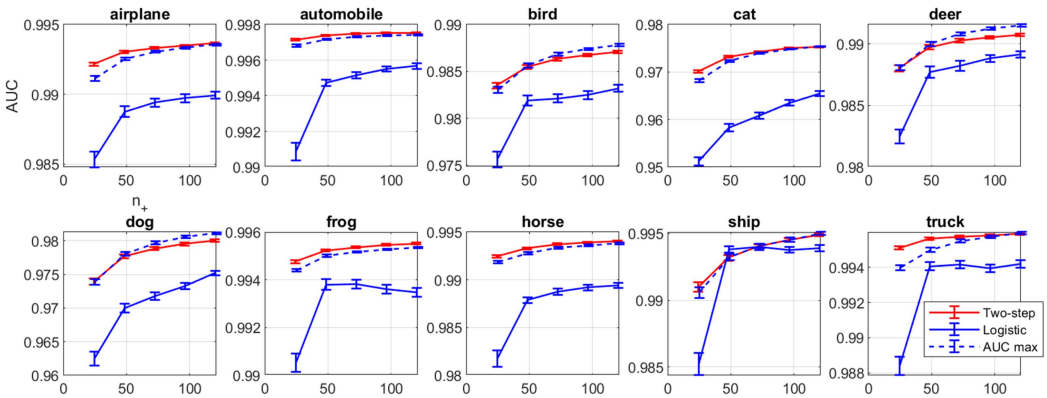

Figure 3: Testing AUC of one-versus-the-rest classification on CIFAR-10 dataset.

then adds them up while Wilcoxon-Mann-Whitney statistic adds up all histogram bars which are TPRs at different FPR levels. Our approach require $\tilde{F}_+$ and $\tilde{F}_-$ to be differentiable with respect to τ, which means the score distributions cannot be discrete. However, Wilcoxon-Mann-Whitney can compute the AUC of discrete score distributions without any problem. This difference is visualized in the middle and right plot of Figure 2.

6 AUC for Unbalanced Classification on CIFAR-10

In this section, we test if the $\hat{v}$ obtained in our two-step procedure (12) is indeed a good score function in terms of AUC in unbalanced classification tasks. We use a widely known image classification dataset CIFAR-10 [21]. The performance is compared with an AUC maximizer which maximizes the empirical lower bound in (9) and is compared with a logistic regression classifier. We set $L(a,b) := -(1-(a-b))^2$ in the AUC maximizer, as suggested in [10]. All methods use linear models with no regularization terms since our models are simple and samples are sufficient. Particularly, the $\hat{t}$ and $\hat{v}$ in our two-step algorithm is obtained using (7) by setting $\phi(\boldsymbol{x}) = \boldsymbol{x}$ and $\lambda = 0$.

Instead of using the raw features, we extract 50 dimensional bounded features by training a residual network [17] on the training dataset using the 10-class cross entropy loss. The structure of the network is included in the supplementary material. After obtaining features, we construct datasets for 10 different one-versus-the-rest classification tasks. For a single task, we pick a class and attain X_+ by randomly sampling from this class n_+ times in the training set. Similarly, X_- is attained by randomly sampling from the rest of the classes n_- times. In our experiments, we set $n_+ = 24, 48, 72, 96, 120$ and fix $n_- = 1000$ to create unbalanced positive and negative datasets. We run all three methods and obtain the corresponding score functions. For each class, we repeat the experiment 96 times using different random samples. We use the testing and training split provided by the dataset itself.

Our experiments can be seen as a transfer learning task which reuses predictive features trained for a multi-class classifier for one-versus-the-rest binary classification tasks.

The average AUCs computed on the testing dataset and their standard errors over 96 runs over different n_+ sample sizes are shown in Figure 3. It can be seen that our method has approximately equal performance with the AUC maximizer despite not directly maximizing the AUC and having a lower computational complexity. This observation indicates that $\hat{v}$ can be a good score function in AUC maximization tasks. Both of the methods significantly outperform vanilla logistic regression.

7 Conclusions

In this paper, we showed that the arc length of the optimal ROC curve could be expressed as an f-divergence between the positive and negative data distribution. This f-divergence and an optimal score $\operatorname{atan} \frac{p_+(\boldsymbol{x})}{p_-(\boldsymbol{x})}$ could be consistently estimated using samples. We then showed this estimator could be employed to lower bound the maximal AUC. Experiments on unbalanced classification tasks showed the score function obtained from our two-step procedure produced promising results.

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope?
   [Yes] In introduction, we discussed the background/usages ROC curves, f-divergence estimation and provided a full paragraph summary of the contribution of this paper. We give the same contribution rundown in the abstract as well.

(b) Did you describe the limitations of your work?
[Yes] In Section 5, we included a brief discussion comparing the proposed maximal AUC lower bounding approach vs. the classic Wilcoxon-Mann-Whitney statistic.

(c) Did you discuss any potential negative societal impacts of your work? [N/A]

(d) Have you read the ethics review guidelines and ensured that your paper conforms to them?
[Yes]

2. If you are including theoretical results...

(a) Did you state the full set of assumptions of all theoretical results?
[Yes] See Section 4.3

(b) Did you include complete proofs of all theoretical results?
[Yes] See Appendix

3. If you ran experiments...

(a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)?
[Yes] Full instructions on how to reproduce our experiments is provided in the supplementary material.

(b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)?
[Yes] See Section 6

(c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)?
[Yes] See Section 6

(d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)?
[N/A] The Computation time is not compared in this paper.

4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...

(a) If your work uses existing assets, did you cite the creators?
[Yes] See Section 6

(b) Did you mention the license of the assets?
[No] The authors of CIFAR-10 do not specify a license for the dataset.

(c) Did you include any new assets either in the supplemental material or as a URL?
[No] We did not create any new asset in this research.

(d) Did you discuss whether and how consent was obtained from people whose data you're using/curating?
[No] We did not collect any data ourselves.

(e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content?
[N/A] CIFAR-10 dataset we use in our experiment does not contain any identifiable human information.

5. If you used crowdsourcing or conducted research with human subjects...

(a) Did you include the full text of instructions given to participants and screenshots, if applicable?
[N/A]

(b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable?
[N/A]

(c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation?
[N/A]