Abstract

The accuracy of modern machine learning algorithms deteriorates severely on adversarially manipulated test data. Optimal adversarial risk quantifies the best error rate of any classifier in the presence of adversaries, and optimal adversarial classifiers are sought that minimize adversarial risk. In this paper, we investigate the optimal adversarial risk and optimal adversarial classifiers from an optimal transport perspective. We present a new and simple approach to show that the optimal adversarial risk for binary classification with $0 - 1$ loss function is completely characterized by an optimal transport cost between the probability distributions of the two classes, for a suitably defined cost function. We propose a novel coupling strategy that achieves the optimal transport cost for several univariate distributions like Gaussian, uniform and triangular. Using the optimal couplings, we obtain the optimal adversarial classifiers in these settings and show how they differ from optimal classifiers in the absence of adversaries. Based on our analysis, we evaluate algorithm-independent fundamental limits on adversarial risk for CIFAR-10, MNIST, Fashion-MNIST and SVHN datasets, and Gaussian mixtures based on them. In addition to the $0 - 1$ loss, we also derive bounds on the deviation of optimal risk and optimal classifier in the presence of adversaries for continuous loss functions, that are based on the convexity and smoothness of the loss functions.

1 Introduction

Modern machine learning algorithms based on deep learning have had tremendous success in recent times, producing state-of-the-art results in many domains such as image classification, game playing, speech and natural language processing. Along with the success, it was also discovered that these algorithms exhibit surprising vulnerability to adversarial perturbations that are imperceptible to humans. Since the discovery by Szegedy et al. [33], there has been a slew of adversarial attacks on neural network based classifiers [2, 6, 20] and defense methods against such attacks [25, 28, 8]. Often, the defense methods either fall short of new attacks or are computationally intractable for large neural networks. Recent work has focused on certifiable defenses that are provably robust against a pre-specified class of adversaries [9, 31, 30].

Theoretical investigation into the cause of adversarial examples has led to the hypothesis that adversarial examples may be inevitable in certain high-dimensional settings [1, 26]. Specifically, it has been shown that any classifier that works on data sampled from concentrated metric probability spaces is susceptible to a high adversarial risk. For instance, when the input distribution is uniform over a high dimensional sphere [17] or Boolean hypercube [11], or when the latent space of the data is a high dimensional Gaussian [14], the adversarial risk can be significantly higher than standard risk, even for small $\epsilon$. Moreover, it was recently proposed that adversarial risk may be
fundamentally at odds with standard risk—a claim that finds support both in theory [35] and in practice [32].

Our primary interest is in analyzing limits on the optimal adversarial risk without any dependence on the algorithm. The first question we investigate is the following:

**Question 1.** How much can the optimal adversarial risk differ from optimal standard risk?

It is easy to see that the optimal adversarial risk is at least as large as optimal standard risk (see Section 2.2). Is it possible to derive a tighter lower bound for the optimal adversarial risk? Recent works in this direction have addressed this question by deriving upper and lower bounds on the optimal adversarial risk with respect to a fixed set of classifiers, by extending the PAC learning theory to encompass adversaries. For instance, Khim and Loh [24] and Yin et al. [39] develop risk bounds based on a notion of adversarial Rademacher complexity, that is a function of both the data generating distribution and class of classifiers under consideration. In a similar vein, several works [3, 10] specifically focus on lower bounds for sample-complexity, in order to characterize the hardness of robust learning. However, deriving lower bounds on the optimal adversarial risk that are classifier agnostic has not received much attention. Another related question is the following: *How much adversarial perturbation is sufficient to make the optimal adversarial risk significantly greater than the optimal standard risk?* Relevant works in this direction have again focused on developing robustness metrics that are specific to the classifier [37, 40, 22].

In addition to Question 1, one might also consider the nature of the optimal classifier under the standard and adversarial settings. This motivates the following question:

**Question 2.** Does the optimal classifier in the adversarial setting differ from that in the standard setting? If so, by how much?

In a recent work, Moosavi-Dezfooli et al. [27] empirically observed that adversarial training significantly reduces the curvature of the loss function with respect to the input. Another line of work attempts to construct a provably robust classifier from a baseline classifier using randomized smoothing [9]. These works provide a clue that the optimal classifier may in fact be different in the presence of an adversary. Even so, many other interesting questions remain. For instance, is the optimal classifier without an adversary approximately the same as the optimal classifier with a small adversary (i.e., small $\epsilon$)? If decision boundaries change, do they change smoothly with increasing strength of an adversary, or do they change drastically?

The closest work to ours is Bhagoji et al. [4], who develop the first classifier-agnostic lower bounds for learning in the presence of an adversary. Specifically, [4] contains a similar result to our Theorem 2 which gives the optimal adversarial risk for binary classification with $0 - 1$ loss in terms of an optimal transport cost between the probability distributions of the two classes. We provide a new, simpler proof of this characterization by applying the Kantorovich duality of optimal transport for $0 - 1$ cost functions. We shall discuss the results from Bhagoji et al. [4] and compare and contrast these with our results at appropriate points in the paper.

**Our contributions**

In this paper, we consider two types of adversaries: (i) data perturbing and (ii) distribution perturbing. We primarily focus on the binary classification setting under $0 - 1$ loss function. We answer Question 1 by providing universal bounds for adversarial risk under the two notions of adversaries that are agnostic to the classifier. We answer Question 2 by deriving the optimal adversarial classifier in some special settings, and by providing bounds on the deviation of the optimal adversarial
classifier from the standard optimal classifier in more general settings. Our contributions are listed below.

1. We provide a new and simple proof for the characterization of optimal adversarial risk for $0 - 1$ loss functions in terms of an optimal transport cost between the two data generating distributions, where the transport cost is given by $c_\epsilon(x, x') = 1\{d(x, x') > 2\epsilon\}$ and $\epsilon$ is the perturbation budget of the adversary. This is analogous to the optimal risk (i.e., Bayes risk) for binary classification in the standard setting, which is a function of the total variation distance between the two data generating distributions, which in turn is also an optimal transport cost with transport cost $c_0(x, x') = 1\{d(x, x') > 0\}$. This completely answers Question 1 for this setting. Our proof establishes connections between adversarial machine learning and well-known results in the theory of optimal transport.

2. We propose a novel coupling strategy that achieves the proposed optimal transport cost between the two class-conditional densities for several univariate distributions like Gaussian, triangular and uniform. Using the analysis of optimal couplings, we obtain the optimal adversarial classifiers for these settings. This answers Question 2 in these settings, and shows how the decision boundary of the optimal classifier changes in the presence of adversaries. In certain cases, we show that the decision boundary can change arbitrarily, even for small changes in the adversary budget $\epsilon$.

3. Using our analysis for $0 - 1$ loss, we obtain the exact optimal risk attainable for a range of adversarial budgets under $\ell_2$-norm and $\ell_\infty$-norm perturbation of data, for several real-world datasets, namely CIFAR10, MNIST, Fashion-MNIST, and SVHN. In addition, we analyze Gaussian mixture distributions based on these datasets and compute lower bounds on the optimal adversarial risk for them. These bounds indicate the optimal adversarial error achievable with data augmentation using Gaussian perturbations.

4. Addressing Questions 1 and 2 is more challenging for general continuous loss functions. We provide some preliminary results to address these that include upper and lower bounds on the optimal adversarial risk. These bounds depend on the convexity and smoothness of the loss function with respect to the data. For Question 2, we prove a result that quantifies the maximum amount by which the optimal classifier can deviate in the presence of an adversary, in terms of the curvature of the loss function at the optimal classifier for standard risk.

Structure: The rest of the paper is structured as follows: In Section 2, we introduce the two types of adversaries: (1) data perturbing and (2) distribution perturbing, and show that the optimal risk in the data perturbing case is lower. We also present a simple example to show that the optimal risk and optimal classifier can deviate significantly in the presence of adversaries. In Section 3, we discuss the optimal adversarial risk for binary classification with $0 - 1$ loss. We settle Question 1 in this setting by introducing the $D_\epsilon$ optimal transport cost that completely characterizes the optimal risk. In Section 4, we discuss the optimal adversarial classifier for binary classification with $0 - 1$ loss. We present a coupling strategy that achieves the optimal transport cost in special cases of interest. Using this coupling, we obtain the optimal adversarial classifier, thus settling Question 2 for these special cases. In Section 5.1, we discuss the optimal risk for general loss functions and present our bounds on the optimal adversarial risk. In Section 5.2, we discuss optimal classifiers for general loss functions and present our deviation bounds on the optimal adversarial classifier. Finally, in Section 6, we present adversarial risk lower bounds for real world datasets and evaluate our bounds for $0 - 1$ loss function.
Notation: The complement of a set $A$ is denoted by $A^c$. Define $1\{C\}$ to be the indicator function that maps all the inputs satisfying condition $C$ to 1 and the rest to 0. For a set $A$ in a Polish space $(\mathcal{X}, d)$, the set $A^\epsilon$ denotes the $\epsilon$-expansion of $A$ in $\mathcal{X}$. That is, $A^\epsilon = \{x \in \mathcal{X} : d(x, x') \leq \epsilon$ for some $x' \in A\}$. For any two probability measures $\mu$ and $\nu$ defined over the Polish space $(\mathcal{X}, d)$, we use $D_{TV}(\mu, \nu)$ to denote the set of all joint probability measures over $\mathcal{X} \times \mathcal{X}$ with marginals $\mu$ and $\nu$, respectively. We use $\|\cdot\|$ to denote a norm and $\|\cdot\|_*$ to denote its dual norm. The cumulative distribution function (cdf) of the standard normal distribution is denoted by $\Phi$. Denote $Q(x) := 1 - \Phi(x)$ to be the tail distribution function of a standard normal.

2 Preliminaries

In the framework of statistical learning, let $z = (x, y)$ denote labeled data points drawn i.i.d. from an unknown distribution $\rho$ over $Z = \mathcal{X} \times \mathcal{Y}$, where $\mathcal{X}$ is the input space and $\mathcal{Y}$ is the label space. Consider a hypothesis class parametrized by $w \in W$, where $W$ is a compact subset of $\mathbb{R}^p$. Let $\ell : Z \times W \rightarrow \mathbb{R}^+$ denote the loss function. Let $d : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}^+$ be a distance metric on the space $\mathcal{X}$.

2.1 Types of adversaries

To quantify the impact of an adversary, notions of adversarial risk have been proposed in the literature. We discuss two such notions here: (i) adversary perturbs data points, and (ii) adversary perturbs data distributions.

Data perturbing adversary: Let the data distribution be $\rho$. The adversarial loss (or robust loss) incurred by a hypothesis $w \in W$ in the presence of a data perturbing adversary with a budget $\epsilon$ is defined as follows:

$$R_\epsilon(\ell, w) = \mathbb{E}_{(x,y) \sim \rho} \left[ \sup_{d(x, x') \leq \epsilon} \ell((x', y), w) \right].$$

Define the optimal adversarial loss attainable over the parameters $w \in \mathbb{R}^p$ as the optimal adversarial risk or optimal robust risk,

$$R^*_\epsilon = \inf_{w \in W} R_\epsilon(\ell, w).$$

The classifier attaining the optimal adversarial risk is called the optimal adversarial classifier or optimal robust classifier. The parameter vector of such a classifier is denoted by $w^*_\epsilon$. Note that for $\epsilon = 0$, the adversarial loss reduces to the standard loss, and the adversarial risk reduces to the standard risk (or Bayes risk), $R^*_0 = \inf_w \mathbb{E}_{z \sim \rho} [\ell(z, w)]$.

Distribution perturbing adversary: The adversarial loss incurred by a hypothesis $w \in W$ in the presence of a distribution perturbing adversary with a budget $\epsilon$ is defined as follows:

$$\hat{R}_\epsilon(\ell, w) = \sup_{\rho' \in B_\epsilon(\rho)} \mathbb{E}_{z \sim \rho'} \ell(z, w),$$

where $B_\epsilon(\rho)$ may be thought of as a ball of radius $\epsilon$ around $\rho$, the true data generating distribution. The Wasserstein distance has been one of the more popular metrics used to define $B_\epsilon(\cdot)$ in the
space of distributions [38, 5, 16, 15, 13, 41]. In this paper, we shall assume the distance being used is the 1-Wasserstein distance, unless otherwise stated. The optimal adversarial risk is defined as

\[ \hat{R}_\epsilon^* = \inf_{w \in \mathcal{W}} \hat{R}_\epsilon^*(\ell, w). \]  

(3)

The optimizing \( w \) for the adversarial risk is denoted by \( \hat{w}_\epsilon^* \). Note that \( \hat{w}_0^* = w_0^* \). A distribution perturbing adversary is considerably more powerful than a data perturbing adversary. For any fixed \( w \in \mathcal{W} \), and for each \( z = (x, y) \), we may define \( z' = (x', y) \), where \( x' \) achieves the supremum in equation (1). It is easily checked that the 1-Wasserstein distance between the distributions of \( Z \) and \( Z' \) is upper-bounded by \( \epsilon \). Thus, we have

\[ R_\epsilon(\ell, w) \leq \hat{R}_\epsilon(\ell, w), \]

and taking the infimum with respect to \( w \in \mathcal{W} \) yields

\[ R_\epsilon^* \leq \hat{R}_\epsilon^*. \]

**A remark on the risk bounds for adversaries:** All risk bounds proved in this paper are valid for both adversaries. Since the distribution perturbing adversary is stronger than the data perturbing adversary, any lower bound that holds for the latter holds for the former. Analogously, any upper bound for the distribution perturbing adversary holds for the data perturbing adversary.

### 2.2 A trivial lower bound

We start by presenting a trivial lower bound on the optimal adversarial risk. To derive the bound, we use the fact that the adversarial loss \( R_\epsilon(\ell, w) \) for any classifier (i.e., for any \( w \)) is lower-bounded by the standard loss \( R_0(\ell, w) \) for that classifier.

**Theorem 1.** The optimal adversarial risk is at least as large as the optimal standard risk, that is, \( R_\epsilon^* \geq R_0^* \).

**Proof.** We have the sequence of inequalities:

\[ R_\epsilon^* = R_\epsilon(\ell, w_\epsilon^*) \geq R_0(\ell, w_\epsilon^*) \geq R_0(\ell, w_0^*) = R_0^*. \]

The first inequality holds because \( R_\epsilon(\ell, w) \) is a non-decreasing function of \( \epsilon \) for any fixed \( \ell \) and \( w \). The second inequality follows from the fact that the adversarially optimal classifier \( w_\epsilon^* \) is sub-optimal for minimizing the standard risk.

Note that the bound in Theorem 1 does not depend on the strength of the adversary \( \epsilon \), and hence it may not be very tight for large \( \epsilon \). In what follows, we show tighter lower bounds for \( R_\epsilon^* \) that depend on \( \epsilon \).

### 2.3 A motivating example

Here, we present a simple binary classification problem with Gaussian class conditional densities which shows that the optimal classifier indeed differs from the Bayes optimal classifier, in the presence of an adversary. For this example, we are able to explicitly compute the optimal adversarial risk and the optimal adversarial classifier as a function of the adversarial budget \( \epsilon \). The detailed proof of this fact is found in Theorem 7.
Let \( x|y = i \sim \mathcal{N}(0, \sigma_i^2) \) for \( i = 0, 1 \) (\( \sigma_1 < \sigma_0 \)). Let \( \Phi_i \) denote the cumulative distribution function for \( \mathcal{N}(0, \sigma_i) \). Let the class labels 0 and 1 be equally likely. Consider classifiers parametrized by \( \mathcal{W} = \{ w \in \mathbb{R} : w > 0 \} \) as follows: \( f(x) = 1\{x \in [-w, w]\} \). Let \( k = \left( \frac{\sigma_0^2 + \sigma_1^2}{\sigma_0^2 - \sigma_1^2} \right) \). Then the optimal adversarial risk and classifier are given by

\[
w^*_\epsilon = w^*_0 \sqrt{1 + \frac{\epsilon^2(k^2 - 1)}{(w^*_0)^2}} + \epsilon k, \tag{4}
\]

\[
R^*_\epsilon = \frac{1}{2} \left[ 1 - 2 (\Phi_1(w^*_\epsilon - \epsilon) - \Phi_0(w^*_\epsilon + \epsilon)) \right]. \tag{5}
\]

Equation (5) shows that the optimal adversarial risk increases with increasing power of the adversary (i.e., increasing \( \epsilon \)). Moreover, we see from (4) the optimal adversarial classifier can differ significantly from the Bayes optimal classifier when \( \sigma_0 \) is close to \( \sigma_1 \) (i.e., when \( k \) is large). Figure 1 shows a specific instance of this example.

Figure 1: Optimal classifier in the standard setting and adversarial setting for two centered Gaussian distributions. Here, \( \sigma_0 = 1, \sigma_1 = 0.5, \) and \( \epsilon = 0.3 \). The optimal adversarial boundary bisects the line segment of length \( 2\epsilon \) that matches \( \phi_0 \) and \( \phi_1 \).

### 3 Optimal adversarial risk via optimal transport

In this section, we present our results on adversarial risk under \( 0-1 \) loss in the binary classification setting. We first define the optimal transport cost \( D_\epsilon(\mu, \nu) \) between two probability measures \( \mu \) and \( \nu \) over a metric space \( (X, d) \), as follows.

**Definition 1 (Optimal transport cost).** For \( \epsilon \geq 0 \), define the cost function \( c_\epsilon : X \times X \rightarrow \mathbb{R} \) as \( c_\epsilon(x, y) = 1\{d(x, y) > 2\epsilon\} \). The optimal transport cost \( D_\epsilon \) is defined as

\[
D_\epsilon(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \mathbb{E}_{(x, x') \sim \pi} c_\epsilon(x, x'). \tag{6}
\]

**Remark 1.** For \( \epsilon = 0 \), the optimal cost is equivalent to the total variation distance, i.e., \( D_0(\mu, \nu) = D_{TV}(\mu, \nu) \). For \( \epsilon > 0 \), this cost does not define a metric over the space of distributions. This is because \( D_\epsilon(\mu, \nu) = 0 \) does not imply \( \mu \) and \( \nu \) are identical. Moreover, it also does not define a pseudometric since the triangle inequality is not satisfied. To see this, observe that if \( \mu_1, \mu_2, \) and \( \mu_3 \) are unit point masses at 0, \( 2\epsilon \), and \( 4\epsilon \), then \( D_\epsilon(\mu_1, \mu_3) = 1 > 0 = D_\epsilon(\mu_1, \mu_2) + D_\epsilon(\mu_2, \mu_3) \).
Next, we present the main theorem of this section that gives the optimal risk under the binary classification setup for a data perturbing adversary.

**Theorem 2.** Consider the binary classification setup with \( \mathcal{Y} = \{0, 1\} \), where the input \( x \in \mathcal{X} \) is drawn with equal probability from two distributions \( p_0 \) (for label 0) and \( p_1 \) (for label 0). We consider a set of binary classifiers of the form \( 1 \{x \in A\} \), where \( A \subseteq \mathcal{X} \) is a topologically closed set. That is, the classifier corresponding to \( A \) assigns the label 1 for all \( x \in A \) and the label 0 for all \( x \notin A \). Consider the 0−1 loss function \( \ell((x, y), A) = 1\{x \in A, y = 0\} + 1\{x \notin A, y = 1\} \). The adversarial risk with the data perturbing adversary is given by

\[
R^*_\epsilon = \frac{1}{2} \left[ 1 - D_\epsilon(p_0, p_1) \right].
\]  

(7)

Instantiating Theorem 2 for \( \epsilon = 0 \), we get

\[
R^*_0 = \frac{1}{2} \left[ 1 - D_0(p_0, p_1) \right] = \frac{1}{2} \left[ 1 - D_{TV}(p_0, p_1) \right],
\]

which is the Bayes risk. It is also possible to derive weaker bounds in terms of the \( p \)-Wasserstein distance between the distributions of the two data classes, as shown in the following corollary:

**Corollary 3.1.** Under the setup considered in Theorem 2, we have the following bound for \( p \geq 1 \):

\[
R^*_\epsilon \geq \frac{1}{2} \left[ 1 - \left( \frac{W_p(p_0, p_1)}{2\epsilon} \right)^p \right].
\]  

(8)

**Proof of Theorem 2.** Let \( A \subseteq \mathcal{X} \) be a closed set such that the classifier declares 1 on \( A \) and 0 on \( A^c \). The robust risk over the hypothesis class of closed sets is given by

\[
R^*_\epsilon = \min_{A \subseteq \mathcal{X}} \frac{1}{2} \left( p_0(A^c) + p_1((A^c)^c) \right)
\]

\[
= \frac{1}{2} \left( 1 - \sup_{A \text{ closed}} \left\{ p_1(A^c) - p_0(A^c) \right\} \right),
\]

where we define \( A^{-\epsilon} := ((A^c)^c)^c \). For any two distributions, Strassen’s theorem (stated in Appendix A.1) states that

\[
D_\epsilon(p_0, p_1) = \sup_{A \text{ closed}} \left\{ p_0(A) - p_1(A^{2\epsilon}) \right\}.
\]

To prove the equality \( R^*_\epsilon = \frac{1}{2}[1 - D_\epsilon(p_0, p_1)] \), notice that it is enough to prove that for measures \( \mu \) and \( \nu \),

\[
\sup_{A \text{ closed}} \mu(A^{-\epsilon}) - \nu(A^c) = \sup_{A \text{ closed}} \mu(A) - \nu(A^{2\epsilon}).
\]  

(9)

To do so, we first we show that \( A^\epsilon \) and \( A^{-\epsilon} \) are also closed sets if \( A \) is a closed set:

**Lemma 3.1** (Proof in Appendix A.2). If \( A \) is closed, then \( A^\epsilon \) is also closed. Similarly, if \( A \) is closed, then \( A^{-\epsilon} \) is also closed.

Next, we show the order in which a set is thickened by \( \epsilon \) and thinned by \( \epsilon \) affects the size of the original set in opposing ways:

**Lemma 3.2** (Proof in Appendix A.3). Let \( A \) be a closed set. Then \( (A^{-\epsilon})^\epsilon \subseteq A \) and \( A \subseteq (A^\epsilon)^{-\epsilon} \).
Figure 2: Illustration of $A^\epsilon, A^-\epsilon, (A^\epsilon)^{-\epsilon}$, and $(A^-\epsilon)^\epsilon$ for a square in $(\mathbb{R}^2, \| \cdot \|_2)$. Observe that $(A^-\epsilon)^\epsilon \subseteq A$ and $A \subseteq (A^\epsilon)^{-\epsilon}$.

Figure 2 illustrates the above lemma when $A$ is a square in $\mathbb{R}^2$ with the Euclidean distance metric. Using the above lemmas, we now establish the desired equality from (9): We have the sequence of inequalities
\[
\sup_{A \text{ closed}} \mu(A) - \nu(A^{2\epsilon}) \geq \sup_{A \text{ closed}} \mu(A^{-\epsilon}) - \nu((A^{-\epsilon})^{2\epsilon}) \\
\geq \sup_{A \text{ closed}} \mu(A^{-\epsilon}) - \nu(A^\epsilon).
\]
Here, (a) follows because $A^{-\epsilon}$ is contained in the set of all closed sets by Lemma 3.1. Inequality (b) follows using Lemma 3.2, since
\[(A^{-\epsilon})^{2\epsilon} = [(A^{-\epsilon})^\epsilon]^{\epsilon} \subseteq A^\epsilon,
\]and so $\nu((A^{-\epsilon})^{2\epsilon}) \leq \nu(A^\epsilon)$.

For the other direction, notice that
\[
\sup_{A \text{ closed}} \mu(A^{-\epsilon}) - \nu(A^\epsilon) \geq \sup_{A \text{ closed}} \mu((A^\epsilon)^{-\epsilon}) - \nu((A^\epsilon)^\epsilon) \\
\geq \sup_{A \text{ closed}} \mu((A^\epsilon)^{-\epsilon}) - \nu(A^{2\epsilon}).
\]
Here, (a) follows because $A^\epsilon$ is a closed set according to Lemma 3.1. To see (b), first note that $(A^\epsilon)^{-\epsilon} = A^{2\epsilon}$, and so $\nu((A^\epsilon)^{-\epsilon}) = \nu(A^{2\epsilon})$. Moreover, Lemma 3.2 states that
\[A \subseteq (A^\epsilon)^{-\epsilon},\]
and so $\mu(A) \leq \mu((A^\epsilon)^{-\epsilon})$. This completes the proof. \qed

Comparison with Bhagoji et al. [4]: We point out that a similar result was obtained recently in [4]. A key difference is that the proof in [4] was established for a larger hypothesis class of measurable sets $A$; i.e., the following equality was established:
\[
\sup_{A \text{ measurable}} \mu(A^{-\epsilon}) - \nu(A^\epsilon) = \sup_{A \text{ measurable}} \mu(A) - \nu(A^{2\epsilon}).
\]
As pointed out in [4], we may restrict to the smaller hypothesis class of closed sets $A$ to obtain an inequality
\[
\sup_{A \text{ closed}} \mu(A^{-\epsilon}) - \nu(A^\epsilon) \leq \sup_{A \text{ measurable}} \mu(A) - \nu(A^{2\epsilon}).
\]
Our result shows that we can obtain an equality if the supremum over the right hand side is also taken over closed sets. Using closed sets and directly using Strassen’s theorem allows us to considerably simplify the technical details as compared to the proof from [4].

**Proof of Corollary 3.1.** From Theorem 2, we have
\[
R^*_\epsilon = \frac{1}{2} \left[ 1 - \inf_{\pi \in \Pi(\mu, \nu)} \mathbb{E}_{(x, x') \sim \pi} [\mathbbm{1}\{d(x, x') > 2\epsilon\}] \right].
\]
For $p \geq 1$ and any $\pi \in \Pi(\mu, \nu)$, we have the following:
\[
\mathbb{E}_{(x, x') \sim \pi} [\mathbbm{1}\{d(x, x') > 2\epsilon\}] = \mathbb{E}_{(x, x') \sim \pi} [\mathbbm{1}\{d(x, x')^p > (2\epsilon)^p\}] \leq \mathbb{E}_{(x, x') \sim \pi} \left[ \left( \frac{d(x, x')}{2\epsilon} \right)^p \right],
\]
where the last inequality follows from Markov’s inequality. Therefore,
\[
R^*_\epsilon = \frac{1}{2} \left[ 1 - \inf_{\pi \in \Pi(\mu, \nu)} \mathbb{E}_{(x, x') \sim \pi} \left[ \left( \frac{d(x, x')}{2\epsilon} \right)^p \right] \right] = \frac{1}{2} \left[ 1 - \left( \frac{W_p(p_0, p_1)}{2\epsilon} \right)^p \right].
\]

4 **Optimal adversarial classifiers via optimal couplings**

In this section, we explicitly compute the optimal risk and optimal classifier for a data perturbing adversary in some special cases. Instead of using $D_\epsilon$, we have shown in Corollary 2 that the optimal adversarial risk can be lower-bounded using other well-understood metrics such as the $W_p$ distances. However, these bounds are often too loose to use in practice, and this motivates us to study the optimal cost $D_\epsilon$ directly. In this section, we show that in certain special cases, the optimal coupling corresponding to calculating $D_\epsilon$ may be explicitly evaluated. Furthermore, in these cases, we can exactly characterize the optimal classifier and the optimal risk in the presence of an adversary.

Given measures $\mu$ and $\nu$ corresponding to the two (equally likely) data classes, the general strategy we employ consists of the following steps:

1. Propose a coupling $\pi$ between $\mu$ and $\nu$.

2. Using this coupling, obtain the upper bound
\[
D_\epsilon(\mu, \nu) \leq \mathbb{E}_{(x, x') \sim \pi} c_\epsilon(x, x').
\]

3. Identify a closed set $A$ and compute a lower bound using
\[
D_\epsilon(\mu, \nu) \geq \mu(A^{-\epsilon}) - \nu(A^\epsilon).
\]

4. Show that the lower and upper bounds match. This shows that the proposed coupling is optimal, and the sets $A$ and $A^c$ define the two regions of the optimal robust classifier.

In the examples we consider, guessing the set $A$ corresponding to the optimal robust classifier is easy. The challenging part is proposing a coupling and establishing its optimality. Although we shall focus on real-valued random variables, some of our results will also naturally extend to higher dimensional distributions.
4.1 Gaussian distributions with identical variances

**Theorem 3.** Let \( p_0 = N(\mu_0, \sigma^2) \) and \( p_1 = N(\mu_1, \sigma^2) \) in the metric space \((\mathbb{R}, |\cdot|)\). Assume \( \mu_0 < \mu_1 \) without loss of generality. Then the following hold:

1. If \( \epsilon \geq \frac{|\mu_0 - \mu_1|}{2} \), the optimal robust risk is \( \frac{1}{2} \). A constant classifier achieves this risk.
2. If \( \epsilon < \frac{|\mu_0 - \mu_1|}{2} \), the optimal classifier satisfies \( A = [\frac{\mu_1 + \mu_0}{2}, +\infty] \), where \( A \) is the region where the classifier decides 1. The optimal risk in this case is \( \int_{\frac{\mu_1 + \mu_0}{2} - \epsilon}^{\infty} p_0(x)dx = Q\left(\frac{\frac{\mu_1}{\sigma} - \frac{\mu_0}{\sigma} - \epsilon}{2}\right) \).

The lower bound of \( \frac{1}{2} \) on the adversarial risk is trivially achieved by the constant classifier. Part (1) of the theorem states that for large enough \( \epsilon \), this is the best one can do. For smaller values of \( \epsilon \), the above theorem shows that the most robust classifier is the same as the MLE classifier. Surprisingly, for larger values of \( \epsilon \) the MLE classifier has a risk larger than \( \frac{1}{2} \); i.e., it is worse than the constant classifier.

**Proof.** We shall prove (1) first. Note that if \( \epsilon \geq \frac{|\mu_1 - \mu_0|}{2} \), the transport map \( T \) defined by \( T(x) = x + (\mu_1 - \mu_0) \) transports \( p_0 \) to \( p_1 \). Moreover, this coupling satisfies \( |T(x) - x| = \mu_1 - \mu_0 \leq 2\epsilon \). Thus, the optimal transport cost for this coupling is 0, and therefore so is \( D_\epsilon(p_0, p_1) \). This gives the lower bound

\[
R^*_\epsilon \geq \frac{1}{2}.
\]

However, since the constant classifier achieves the lower bound, we conclude \( R^*_\epsilon = 1/2 \).

Figure 3: Optimal coupling for two Gaussians with identical variances. The shaded region within \( p_0 \) is translated by \( 2\epsilon \) to \( p_1 \), whereas the remaining is mass in \( p_0 \) is moved at a cost of 1 per unit mass.

For part (2), we consider the following strategy. As shown in Figure 3, consider the distribution \( \tilde{p}_1 \) obtained by shifting \( p_1 \) to the left by \( 2\epsilon \). It is evident that the overlapping area between \( \tilde{p}_1 \) and \( p_0 \) maybe be translated by \( 2\epsilon \) so that it lies entirely with \( p_1 \). This means that the overlapping area may be transported at 0 cost. It is easily verified that the overlapping area contains \( 2Q\left(\frac{\frac{\mu_1 - \mu_0}{2} - \epsilon}{\sigma}\right) \) mass, and so the total cost of transportation is at most \( 1 - 2Q\left(\frac{\frac{\mu_1 - \mu_0}{2} - \epsilon}{\sigma}\right) \). Plugging this into the lower bound, we see that

\[
R^*_\epsilon \geq Q\left(\frac{\frac{\mu_1 - \mu_0}{2} - \epsilon}{\sigma}\right) \cdot \frac{1}{2}.
\]

Since this risk is achieved by the MLE classifier, we conclude that this is the optimal robust risk and the MLE classifier is the optimal robust classifier.
Theorem 3 can be easily extended to $d$-dimensional Gaussians with the same identity covariances. Our results may be summarized in the following theorem:

**Theorem 4.** Let $p_0 = \mathcal{N}(\mu_0, \sigma^2 I_d)$ and $p_1 = \mathcal{N}(\mu_1, \sigma^2 I_d)$ in the metric space $(\mathbb{R}, || \cdot ||_2)$. Then the following hold:

1. If $\epsilon \geq \frac{||\mu_0 - \mu_1||_2^2}{2}$, the optimal robust risk is $1/2$. A constant classifier achieves this risk.

2. If $\epsilon < \frac{||\mu_0 - \mu_1||_2^2}{2}$, the optimal classifier is given by the following halfspace:

$$A = \left\{ x : (\mu_1 - \mu_0) \left( x - \frac{\mu_0 + \mu_1}{2} \right) \geq 0 \right\}. \quad (10)$$

**Comparison to Bhagoji et al. [4]:** Bhagoji et al. also explore optimal classifiers for multivariate normal distributions. In fact, they show a more general version of our Theorems 3 and 4 by considering data distributions $\mathcal{N}(\mu, \Sigma)$ and $\mathcal{N}(\mu_2, \Sigma)$, and an adversary that perturbs within $L_p$ balls.

In the following subsections, we shall generalize Theorem 3 in a different way by considering various interesting examples of univariate distributions and identifying optimal couplings for these.

### 4.2 Gaussians with arbitrary means and variances

We shall introduce a general coupling strategy and apply it to the special case of Gaussian random variables. Given two probability measures $\mu$ and $\nu$ on $\mathbb{R}$, our strategy consists of the following steps:

1. Partition the real line into $K \geq 1$ intervals $S_i, 1 \leq i \leq K$, and let the restriction of $\mu$ to $S_i$ be $\mu_i$.

2. Partition the real line into $K \geq 1$ intervals $T_i, 1 \leq i \leq K$, and let the restriction of $\nu$ to $T_i$ be $\nu_i$.

3. Transport mass from $\mu_i$ to $\nu_i$ such that $D_\epsilon(\mu_i, \nu_i) = 0$. (We shall define an appropriate notion of mass transport between measures with unequal masses shortly.) The transport maps used in these $K$ problems may be arbitrary; however, we shall often use versions of the monotone optimal transport map [36].

Our first result identifies a necessary and sufficient condition for $D_\epsilon(\mu, \nu) = 0$ for arbitrary measures on $\mathbb{R}^d$.

**Theorem 5.** Let $\mu$ and $\nu$ be finite positive measures on $\mathbb{R}^d$ that are absolutely continuous with respect to the Lebesgue measure and have bounded supports. Then $D_\epsilon(\mu, \nu) = 0$ if and only if $W_\infty(\mu, \nu) \leq 2\epsilon$. Here, $W_\infty(\mu, \nu) = \lim_{p \to \infty} W_p(\mu, \nu)$.

**Proof.** An alternate description of $W_\infty(\mu, \nu)$ as per Givens and Shortt [18] is

$$W_\infty(\mu, \nu) = \inf\{\delta > 0 : \mu(A) \leq \nu(A^\delta) \text{ for all measurable } A\}.$$

Naturally, if $W_\infty(\mu, \nu) \leq 2\epsilon$, then $\mu(A) \leq \nu(A^{2\epsilon})$ for all closed sets $A$. Hence,

$$D_\epsilon(\mu, \nu) = \sup_{A \text{ closed}} \mu(A) - \nu(A^{2\epsilon}) \leq 0.$$
Since $D_*(\mu, \nu) \geq 0$, we conclude that $D_*(\mu, \nu) = 0$.

For the reverse direction, suppose that $D_*(\mu, \nu) = 0$. This means there exists a sequence of couplings $\{\pi_i\}_{i \geq 1}$ such that $\mathbb{E}_{\pi_i} c_*(x, x') \to 0$ where $\pi_i \in \Pi(\mu, \nu)$. Equivalently, the probability $\alpha_i := \mathbb{P}_{\pi_i}(\|x - x'\| > 2\epsilon) \to 0$ as $i \to \infty$. For any fixed $p \geq 1$, we have the inequality
\[
W_p(\mu, \nu) \leq (\mathbb{E}_{\pi_i} \|x - x'\|^p)^{1/p} 
\leq ((2\epsilon)^p (1 - \alpha_i) + C^p \alpha_i)^{1/p},
\]
where $C = \sup \|x - x'\|$ which is a constant since $\mu$ and $\nu$ are assumed to have bounded supports. Pick $i_0$ large enough so that $(2\epsilon)^p (1 - \alpha_{i_0}) > C^p \alpha_{i_0}$. Now letting $p \to \infty$ and calculating the limits, we conclude that $W_\infty(\mu, \nu) \leq 2\epsilon$. \hfill \Box

Calculating $W_\infty$ is non-trivial in general. However, in the univariate case the optimal coupling for all $W_p$'s is known to be the degenerate coupling given by the monotone transport map from $\mu$ to $\nu$. This allows us to present a more concrete condition for checking when $D_*(\mu, \nu) = 0$ for measures over $\mathbb{R}$. Our result is contained in the following theorem:

**Theorem 6.** Let $\mu$ and $\nu$ be finite positive measures on $\mathbb{R}$ that are absolutely continuous with respect to the Lebesgue measure with Radon-Nikodym derivatives $f(\cdot)$ and $g(\cdot)$, respectively. The cumulative distribution function (cdf) of $\mu$ is defined as $F(x) = \mu((\infty, x])$, and for $t \in [0, 1]$, the inverse cdf (or quantile function) is defined as $F^{-1}(t) = \inf \{x \in \mathbb{R} : F(x) \geq t\}$. The cdf $G(\cdot)$ and inverse cdf $G^{-1}(\cdot)$ are defined analogously. Suppose that $\mu(\mathbb{R}) = \nu(\mathbb{R}) = U$. Then $D_*(\mu, \nu) = 0$ if and only if $\|F^{-1} - G^{-1}\|_\infty \leq 2\epsilon$.

**Proof.** Consider the monotone transport map from $\mu$ to $\nu$ given by $T(x) = G^{-1}(F(x))$ for $x \in \mathbb{R}$ [36]. We shall show that this map satisfies $|T(x) - x| \leq 2\epsilon$ for all $x \in \mathbb{R}$, and so the optimal transport cost $D_*$ must be 0. To see this, note that
\[
T(x) - x = G^{-1}(F(x)) - x 
\leq F^{-1}(F(x)) + 2\epsilon - x 
= 2\epsilon,
\]
where the last equality is in the $\mu$-almost sure sense. A similar argument shows $x - T(x) \leq 2\epsilon$, and thus $|T(x) - x| \leq 2\epsilon$.

For the converse, suppose that there exists a $t_0 \in (0, 1)$ such that $G^{-1}(t_0) - F^{-1}(t_0) > 2\epsilon$. Equivalently, $G^{-1}(t_0) > F^{-1}(t_0) + 2\epsilon$. Applying the $G$ function on both sides,
\[
t_0 > G(F^{-1}(t_0) + 2\epsilon).
\]
Consider the set $\tilde{A} = (\infty, F^{-1}(t_0)]$. For this set, notice that
\[
\nu(\tilde{A}^{2\epsilon}) = \nu((\infty, F^{-1}(t_0) + 2\epsilon]) = G(F^{-1}(t_0) + 2\epsilon).
\]
Thus, we have
\[
D_*(\mu, \nu) = \sup_{\mathcal{A}} \mu(\mathcal{A}) - \nu(\tilde{A}^{2\epsilon}) 
\geq \mu(\tilde{A}) - \nu(\tilde{A}^{2\epsilon}) 
= t_0 - G(F^{-1}(t_0) + 2\epsilon) > 0.
\]
A similar argument may also be made for the case when $F^{-1}(t_0) - G^{-1}(t_0) > 2\epsilon$. \hfill \Box
The above argument shows that monotone transport maps are optimal when \( D_\epsilon = 0 \). But monotone maps are not always optimal for the cost function \( c(x, y) \). Consider for example the two measures \( \mathcal{N}(0, 1) \) and \( \mathcal{N}(1, 1) \), and \( \epsilon = 0.1 \). The monotone map in this case is \( T(x) = x + 1 \), which gives unit cost of transportation. However, Theorem 3 shows that the optimal transport cost in this example is strictly smaller than 1.

Checking the condition \( \|F^{-1} - G^{-1}\| \leq 2\epsilon \) is not always easy. We identify a simple but useful characterization in the following corollary:

**Corollary 4.1.** Let \( \mu \) and \( \nu \) be as in Theorem 6. Suppose that for every \( x \in \mathbb{R} \), we have \( F(x) \geq G(x) \) and \( F(x) \leq G(x + 2\epsilon) \). Then \( D_\epsilon(\mu, \nu) = 0 \).

**Proof.** Applying the \( G^{-1} \) function to both sides of both inequalities, we arrive at

\[
T(x) \leq x, \quad \text{and} \quad T(x) \geq x + 2\epsilon.
\]

This gives \( |T(x) - x| \leq 2\epsilon \) for all \( x \), which concludes the proof. \( \Box \)

Before we examine the case of Gaussian distributions with identical means but different variances, we define notions of transport for measures with unequal masses.

**Definition 2.** [Optimal transport cost for general measures] Let \( \mu \) and \( \nu \) be as in Theorem 6. Suppose that \( \mu(\mathbb{R}) = U \) and \( \nu(\mathbb{R}) = V \). Let \( \nu' \) be a measure on \( \mathbb{R} \) with Radon-Nikodym derivative \( g' \) such that \( \nu'(\mathbb{R}) = U \). We say \( \nu' \subseteq \nu \), or \( \nu' \) is contained in \( \nu \), if \( g(x) \geq g'(x) \) \( \nu \)-almost surely. Then the optimal transport cost \( D_\epsilon(\mu, \nu) \) is defined as

\[
D_\epsilon(\mu, \nu) = \inf_{\nu' \subseteq \nu} D_\epsilon(\mu, \nu').
\]

Note that the amount of mass being moved is \( \min(U, V) = U \).

**Lemma 4.1.** Let \( \mu \) and \( \nu \) be as in Theorem 6. Assume that \( \mu(\mathbb{R}) = U \) and \( \nu(\mathbb{R}) = V \). Suppose the following conditions hold:

1. The support of \( g \) is \([a, +\infty)\) and the support of \( f \) is \([a + 2\epsilon, +\infty) =: [a', +\infty)\).

2. For all \( x \in \mathbb{R} \), we have \( g(x) \leq f(x + 2\epsilon) \).

Then \( D_\epsilon(\mu, \nu) = 0 \). A similar result holds if the supports of \( g \) and \( f \) are \((-\infty, -a] \) and \((-\infty, -a - 2\epsilon] \), and \( f(-x - 2\epsilon) \geq g(-x) \).

![Figure 4: Figure illustrating the conditions in Lemma 4.1.](image)

**Proof.** Consider the transport map \( T(x) = x + 2\epsilon \) applied to \( \nu \). This map has the effect of “translating” the measure \( \nu \) by \( 2\epsilon \) to the right. Call this translated measure \( \eta \). Since \( f(x) \geq g(x - 2\epsilon) \), it is immediate that \( \eta \subseteq \mu \). Moreover, the transport cost is \( D_\epsilon(\nu, \eta) = 0 \). This shows that \( D_\epsilon(\mu, \nu) = 0 \). \( \Box \)
Lemma 4.2. Let \( \mu \) and \( \nu \) be as in Theorem 6. Assume that \( \mu(\mathbb{R}) = \nu(\mathbb{R}) = U \). Suppose the following conditions hold (see Figure 5 for an illustration):

1. Let \( a, b \in \mathbb{R} \) be such that \( b - a > 2\epsilon \). The support of \( f \) is \([a, b]\) and the support of \( g \) is \([a', b] := [a + 2\epsilon, b]\).

2. There exists \( t \in [a, b] \) such that \( f(x) \geq g(x) \) for \( x \in [a, t] \), and \( f(x) \leq g(x) \) for \( x \in (t, b] \).

3. Let \( \tilde{g}(x) = g(x + 2\epsilon) \). Note that \( \tilde{g} \) is supported on \([a, b - 2\epsilon]\). There exists \( \tilde{t} \in [a, b - 2\epsilon] \) such that \( f(x) \leq \tilde{g}(x) \) for \( x \in [a, \tilde{t}] \), and \( f(x) \geq \tilde{g}(x) \) for \( x \in (\tilde{t}, b - 2\epsilon] \).

Then \( D_\epsilon(\mu, \nu) = 0 \). A mirror image of this result also holds: \( D_\epsilon(\mu, \nu) = 0 \) when the support of \( f \) is \([b, c + 2\epsilon]\), that of \( g \) is \([b, c]\), and \( f(x) \leq g(x) \) for \( x \in [b, t] \) and \( f(x) \geq g(x) \) for \( x \in [t, c + 2\epsilon] \); and for \( \tilde{g}(x) = g(x + 2\epsilon) \) we have \( f(x) \geq \tilde{g}(x) \) for \( x \in [b + 2\epsilon, t] \) and \( f(x) \leq g(x) \) for \( x \in [\tilde{t}, c + 2\epsilon] \).

![Figure 5: Figure illustrating the conditions in Lemma 4.2.](image)

Proof. We first prove \( F(x) \geq G(x) \). To see this, consider \( H(x) = F(x) - G(x) \). Since the derivative of \( H \) is \( f - g \), it must be that \( H \) is increasing from \([a, t]\) and decreasing from \([t, b]\). Also, we have \( H(a) = H(b) = 0 \), and so the function \( H \) must be non-negative in \([a, b]\). Equivalently, we must have \( F(x) \geq G(x) \) for \( x \in \mathbb{R} \). We now prove \( F(x) \leq G(x + 2\epsilon) \). Consider \( \tilde{H}(x) = F(x) - \tilde{G}(x) \). By condition (3), the derivative of this function is negative from \([a, \tilde{t}]\) and positive from \([\tilde{t}, b]\). Thus, the function \( \tilde{H} \) decreases on the interval \([a, \tilde{t}]\) and increases on the interval \([\tilde{t}, b]\). Note that since \( \tilde{H}(a) = \tilde{H}(b) = 0 \), the function \( \tilde{H} \) must be non-positive in the interval \([a, \tilde{t}]\). Thus, we have \( F(x) \leq G(x + 2\epsilon) \). Applying Corollary 4.1 concludes the proof.

Our next lemma is specific to Gaussian pdfs:

Lemma 4.3. Let \( f \) and \( g \) be Gaussian pdfs corresponding to \( \mathcal{N}(\mu_1, \sigma_1^2) \) and \( \mathcal{N}(\mu_2, \sigma_2^2) \), respectively. Assume \( \sigma_1^2 > \sigma_2^2 \). Then the equation \( f(x) - g(x) = 0 \) has exactly two solutions \( s_1 < \mu_2 < s_2 \).

Proof. By scaling and translating, we may set \( \mu_2 = 0 \) and \( \sigma_2^2 = 1 \). Solving \( f(x) - g(x) = 0 \) is equivalent to solving the quadratic equation

\[
\frac{x^2}{2} - \frac{(x - \mu_1)^2}{2\sigma_1^2} = \log \sigma_1.
\]
Simplifying, we wish to solve
\[ x^2(\sigma_1^2 - 1) + 2\mu_1 x - (\mu_1^2 + 2\sigma_1^2 \log \sigma_1) = 0. \]
Since \( \sigma_1 > 1 \), the above quadratic has two distinct roots: one negative and one positive. This proves the claim.

We shall call the two points where \( f \) and \( g \) intersect as the left and right intersection points.

**Theorem 7.** Let \( \mu \) and \( \nu \) be the Gaussian measures \( \mathcal{N}(0, \sigma_1^2) \) and \( \mathcal{N}(0, \sigma_2^2) \), respectively. Assume \( \sigma_1^2 > \sigma_2^2 \) without loss of generality. Let \( m > 0 \) be such that \( f(m + \epsilon) = g(m - \epsilon) \). Let \( A = (-\infty, -m] \cup [m, +\infty) \). Then the optimal transport cost between \( \mu \) and \( \nu \) is given by

\[ D_\epsilon(\mu, \nu) = \mu(A^{-\epsilon}) - \nu(A^\epsilon) = 2Q \left( \frac{m + \epsilon}{\sigma_1} \right) - 2Q \left( \frac{m - \epsilon}{\sigma_2} \right). \]

The corresponding robust risk is

\[ R^*_\epsilon = \frac{1 - \mu(A^{-\epsilon}) + \nu(A^\epsilon)}{2}. \]

Moreover, if \( \mu \) corresponds to hypothesis 1, the optimal robust classifier decides 1 on the set \( A \).

**Proof.** We shall propose a map that transports \( \mu \) to \( \nu \). (See Figure 6 for an illustration.) Consider \( r \in (0, m - \epsilon) \) whose value will be provided later. First, we partition \( \mathbb{R} \) into the five regions for \( \mu \) and \( \nu \), as shown in Table 1. For \( \mu \), these partitions are \((-\infty, -m - \epsilon], (-m - \epsilon, -r], (-r, +r], [r, m + \epsilon), [m + \epsilon, \infty)\). Let \( \mu \) restricted to these intervals be \( \mu_{-}, \mu_{-}, \mu_{0}, \mu_{+}, \) and \( \mu_{++} \), respectively. The measure \( \nu \) is also partitioned five ways, but the intervals used in this case are slightly modified to be \((-\infty, -m + \epsilon], (-m + \epsilon, -r], (-r, r], [r, m - \epsilon), [m - \epsilon, +\infty)\). Call \( \nu \) restricted to these intervals \( \nu_{-}, \nu_{-}, \nu_{0}, \nu_{+}, \) and \( \nu_{++}, \) respectively.

The transport plan from \( \mu \) to \( \nu \) will consist of five maps transporting \( \mu_{--} \rightarrow \nu_{--} \), \( \mu_{-} \rightarrow \nu_{-} \), \( \mu_{0} \rightarrow \nu_{0} \), \( \mu_{+} \rightarrow \nu_{+} \), and \( \mu_{++} \rightarrow \nu_{++} \). In each case, we plan to show that \( D_\epsilon(\mu_{s}, \nu_{s}) = 0 \), where * ranges over all possible subscripts. Note that these measures do not necessarily have identical masses, and thus by Definition 2, we are transporting a quantity of mass equal to the minimum mass among the two measures. For this reason, even though the transport cost is \( D_\epsilon(\mu_{s}, \nu_{s}) = 0 \), it does not mean \( D_\epsilon(\mu, \nu) = 0 \).

Consider \( \mu_{++} \) and \( \nu_{++} \). We have \( f(m + \epsilon) = g(m - \epsilon) \) by the choice of \( m \). We argue that for any \( t \geq 0 \), we must have \( f(m + \epsilon + t) \geq g(m - \epsilon + t) \). This is because any two Gaussian pdfs can intersect in at most two points. By Lemma 4.3, the \( \epsilon \)-shifted Gaussian pdfs \( f(x + \epsilon) \) and \( g(x - \epsilon) \) have \( m \) as their right intersection point, and there are no additional points of intersection to the right of \( m \).
Since the tail of $f$ is heavier, it means that $f(m + \epsilon + t) \geq g(m - \epsilon + t)$ for all $t \geq 0$. By Lemma 4.1, we can now conclude $D_\epsilon(\mu_+, \nu_+) = 0$. A similar argument also shows $D_\epsilon(\mu_-, \nu_-) = 0$.

Before we consider $\mu_-$ and $\nu_-$, we first define $r$ as follows: Pick $r > 0$ such that $\mu([-m-\epsilon, -r)) = \nu([-m+\epsilon, -r))$. To see that such an $r$ must exist, consider the functions $a(t) := \mu([-m-\epsilon, t))$ and $b(t) := \nu([-m+\epsilon, t))$ as $t$ ranges over $(-m+\epsilon, 0)$. When $t = -m + \epsilon$, we have $a(t) > b(t) = 0$. When $t = 0$, we have $a(t) = 1/2 - \mu_-(\mathbb{R}) < b(t) = 1/2 - \nu_-(\mathbb{R})$. Thus, there must exist a $t_0 \in (-m + \epsilon, 0)$ such that $a(t_0) = b(t_0)$. Pick the smallest (i.e., the leftmost) such $t_0$, and set $-r = t_0$. Call $f(\cdot)$ restricted to $[-m - \epsilon, -r)$ and $g(\cdot)$ restricted to $[-m + \epsilon, -r)$ as $f_-$ and $g_-$, respectively, and their corresponding cdfs $F_-$ and $G_-$, respectively. We claim that $\mu_-$ and $\nu_-$ satisfy all three conditions from Lemma 4.2. Since the supports of $f_-$ and $g_-$ are $[-m - \epsilon, -r)$ and $[-m + \epsilon, -r)$, condition (1) is immediately verified. To check condition (2), we break up the interval $[-m - \epsilon, -r)$ into two parts: $[-m - \epsilon, -s)$ and $[-s, -r)$, where $s$ is such that $f(-s) = g(-s)$. Observe that $f_- \geq g_-$ on $[-m - \epsilon, -s)$, whereas $f_- \leq g_-$ on $[-s, -r)$. This shows that condition (2) is satisfied. We have $g_-(-m + \epsilon) = f_-(-m - \epsilon)$. Again, using Lemma 4.3 the 2$\epsilon$-shifted Gaussian pdf $f(x - 2\epsilon)$ and $g(x)$ have $-m + \epsilon$ as their left intersection point, and the right intersection point is to the right of 0. Thus, we have $f(x - 2\epsilon) \leq g(x)$ for all $x \in [-m + \epsilon, 0] \supseteq [-m + \epsilon, r)$. Using this domination, we conclude that $f_- \leq g_-$ in the interval $[-m - \epsilon, -r - 2\epsilon)$ and $f_- \geq g_- = 0$ in the interval $(-r - 2\epsilon, -r)$, and so condition (3) is satisfied. Applying Lemma 4.2, we conclude $D_\epsilon(\mu_-, \nu_-) = 0$. An essentially identical argument may be used to show $D_\epsilon(\mu_+, \nu_+) = 0$. The minor difference being that $r$ is chosen to satisfy $\mu((r, m + \epsilon)) = \nu((r, m - \epsilon))$, and the mirror image of Lemma 4.2 is applied.

Finally, consider the interval $(-r, +r)$. In this interval, $f(x) \leq g(x)$ for every point. Hence, a transport map from $\mu_0$ to $\nu_0$ is obtained by simply considering the identity function. Any remaining mass in $\mu$ is moved to $\nu$ arbitrarily, incurring a cost of at most 1 per unit mass. The total cost of transport is then upper-bounded by

$$D_\epsilon(\mu, \nu) \leq 1 - [\min(\mu_-, \nu_-) + \min(\mu_+, \nu_+) + \min(\mu_0, \nu_0) + \min(\mu_-, \nu_0) + \min(\mu_0, \nu_-) + \min(\mu_0, \nu_+) + \min(\mu_+, \nu_0) + \min(\mu_+, \nu_+)]$$

$$= 1 - [\nu_- + \mu_+ + \mu_0 + \nu_+]$$

$$= 1 - \mu([-m - \epsilon, m + \epsilon]) - 2\nu([m - \epsilon, \infty))$$

$$= \mu(A^{-\epsilon}) - \nu(A^\epsilon)$$

$$= 2Q\left(\frac{m + \epsilon}{\sigma_1}\right) - 2Q\left(\frac{m - \epsilon}{\sigma_2}\right).$$

where for brevity we have denoted $\mu_* (\mathbb{R})$ as $\mu_*$. However, we also have

$$D_\epsilon(\mu, \nu) \geq \mu(A^{-\epsilon}) - \nu(A^\epsilon).$$

The lower and upper bounds match and this concludes the proof. The robust risk $R_*^\epsilon$ is given by Theorem 2. The robust risk of the classifier that decides 1 on the set $A$ is easily seen to be $R_*^\epsilon$. \[\square\]

We now extend the above proof strategy to demonstrate the optimal coupling for Gaussians with arbitrary means and arbitrary variances. Our main result is the following:

**Theorem 8.** Let $\mu$ and $\nu$ be Gaussian measures $\mathcal{N}(\mu_1, \sigma_1^2)$ and $\mathcal{N}(\mu_2, \sigma_2^2)$ respectively. Assume $\sigma_1^2 > \sigma_2^2$ without loss of generality. Let $m_1, m_2 > 0$ be such that $f(-m_1 - \epsilon) = g(-m_1 + \epsilon)$ and $f(m_2 + \epsilon) = g(m_2 - \epsilon)$. Let $A = (-\infty, -m_1] \cup [m_2, \infty)$. Then the optimal transport cost between $\mu$ and $\nu$ is given by

$$D_\epsilon(\mu, \nu) = \mu(A^{-\epsilon}) - \nu(A^\epsilon).$$

16
Figure 6: Optimal transport coupling for centered Gaussian distributions $\mu$ and $\nu$. As in the proof of Theorem 7, we divide the real line into five regions. The transport plan from $\mu$ to $\nu$ consists of five maps transporting $\mu_{-} \rightarrow \nu_{-}$ (blue regions to the left), $\mu_{-} \rightarrow \nu_{-}$ (orange regions to the left), $\mu_{0} \rightarrow \nu_{0}$ (green regions in the middle), $\mu_{+} \rightarrow \nu_{+}$ (orange regions to the right), and $\mu_{++} \rightarrow \nu_{++}$ (blue regions to the right).

Consequently, the robust risk is given by

$$R^*_\epsilon = \frac{1}{2} (1 - \mu(A^-) + \nu(A^+) )$$

If $\mu$ corresponds to hypothesis 1, the optimal robust classifier decides 1 on the set $A$.

Proof. As in the proof of Theorem 7, we shall divide the real line into five regions as shown in Table 2 where we define $r_1$ and $r_2$ shortly. Using an identical strategy as in Theorem 7, we conclude $D_\epsilon(\mu_{-}, \nu_{-}) = D_\epsilon(\mu_{0+}, \nu_{0+}) = 0$. Define $r_1$ as the leftmost point where $\mu([-m_1 - \epsilon, r_1]) = \nu([-m_1 + \epsilon, r_1])$. Similarly, define $r_2$ to be the rightmost point such that $\mu([r_2, m_2 + \epsilon]) = \nu([r_2, m_2 - \epsilon])$. We shall now prove $D_\epsilon(\mu_{-}, \nu_{-}) = 0$ by using Lemma 4.2. Verifying conditions (1) and (2) is exactly as in that of Theorem 7. The novel component of this proof is verifying condition (3), since the domination used in the proof of Theorem 7 does not work in this case due to the asymmetry. Consider the pdfs $f_{-}(x)$ and $g_{-}(x + 2\epsilon)$. These two pdfs, being restrictions of Gaussian pdfs to suitable intervals, may only intersect in at most two points. One of these points of intersection is $-m_1 - \epsilon$ by the choice of $m_1$, so there can be at most one other point of intersection in the interval $[-m_1 - \epsilon, -r_1 - 2\epsilon]$. Note that there may be no point of intersection in this interval. However, the key observation is that in both cases, condition (3) continues to be satisfied. To see this, suppose that there is a point of interaction $\tilde{t}$. In this case, $f_{-} \leq g_{-}$ in $[-m_1 - \epsilon, \tilde{t})$, and $f_{-} \geq g_{-}$ in $(\tilde{t}, -r_1]$. If there is no point of intersection, then $f_{-} \leq g_{-}$ in $[-m_1 - \epsilon, -r_1 - 2\epsilon)$, and $f_{-} \geq g_{-} = 0$ in $(-r_1 - 2\epsilon, -r_1]$. This verifies condition (3). Using Lemma 4.2, we conclude $D_\epsilon(\mu_{-}, \nu_{-}) = 0$. An identical approach gives $D_\epsilon(\mu_{+}, \nu_{+}) = 0$. Since $f(x) \leq g(x)$ for all points in the interval $(-r_1, r_2)$, the identity map may be used to conclude $D_\epsilon(\mu_{0}, \nu_{0}) = 0$.

Any remaining mass in $\mu$ is moved to $\nu$ arbitrarily, incurring a cost of at most 1 per unit mass.
shows the optimal coupling for the case when the real line into several regions for Proof sketch of Theorem 9. Like in the proof for Theorem 7, we prove Theorem 9 by partitioning \( \mu \) where for brevity we have denoted \( \mu^*(\mathbb{R}) \) as \( \mu^* \). The rest of the proof is identical to that of Theorem 7.

\[ D_\epsilon(\mu, \nu) \leq 1 - [\min(\mu_-, \nu_-) + \min(\mu_-, \nu_-) + \min(\mu_0, \nu_0) + \min(\mu_+, \nu_+) + \min(\mu_+, \nu_+)] \]
\[ = 1 - [\nu_- + \mu_- + \mu_0 + \mu_+ + \nu_+] \]
\[ = 1 - \mu([-m_1 - \epsilon, m_2 + \epsilon]) - \nu((-\infty, -m_1 + \epsilon)) - \nu([m_2 - \epsilon, \infty]) \]
\[ = \mu(A^{-\epsilon}) - \nu(A^\epsilon), \]

where for brevity we have denoted \( \mu^*(\mathbb{R}) \) as \( \mu^* \). The rest of the proof is identical to that of Theorem 7.

\[ \text{Table 2: The real line is partitioned into five regions for } \mu \text{ and } \nu \text{ as shown in the table.} \]

\[
\begin{array}{|c|c|c|}
\hline
\mu_- & (-\infty, -m_1 - \epsilon) & \nu_- & (-\infty, -m_1 + \epsilon) \\
\mu_0 & (-m_1 - \epsilon, -r_1] & \nu_0 & (-m_1 + \epsilon, -r_1] \\
\mu_+ & [r_2, m_2 + \epsilon) & \nu_+ & [r_2, m_2 - \epsilon) \\
\mu_{++} & [m_2 + \epsilon, \infty) & \nu_{++} & [m_2 - \epsilon, \infty) \\
\hline
\end{array}
\]

The total cost of transport is then upper-bounded by

\[ D_\epsilon(\mu, \nu) \leq 1 - [\min(\mu_-, \nu_-) + \min(\mu_-, \nu_-) + \min(\mu_0, \nu_0) + \min(\mu_+, \nu_+) + \min(\mu_+, \nu_+)] \]

where for brevity we have denoted \( \mu^*(\mathbb{R}) \) as \( \mu^* \). The rest of the proof is identical to that of Theorem 7.

**4.3 Beyond Gaussian examples**

The coupling strategy for Gaussian random variables can also be applied to other univariate examples that share some similarities with the Gaussian case. To illustrate, we describe the optimal classifier and optimal coupling for uniform distributions and triangular distributions. The precise proof details in these cases may be reconstructed from the proofs of Theorems 7 and 8.

**Theorem 9 (Uniform distributions).** Let \( \mu \) and \( \nu \) be uniform measures on closed intervals \( I \) and \( J \) respectively. Without loss of generality, we assume \( |I| \leq |J| \). Then the optimal robust risk is \( \nu(I^{2\epsilon}) \) and the optimal classifier is given by \( A = I^\epsilon \).

**Proof sketch of Theorem 9.** Like in the proof for Theorem 7, we prove Theorem 9 by partitioning the real line into several regions for \( \mu \) and \( \nu \), and transporting mass between these regions. Figure 7 shows the optimal coupling for the case when \( I^{2\epsilon} \subseteq J \).

We first prove a lower bound. Choose the set \( A = I \), we have that

\[ D_\epsilon(\mu, \nu) \geq \mu(A) - \nu(A^{2\epsilon}) = 1 - \nu(I^{2\epsilon}). \]

To establish the upper bound, we need to find a coupling that transports \( \mu \) to \( \nu \) such that the cost of transportation is bounded above by \( 1 - \nu(I^{2\epsilon}) \). Let \( I = [i_1, i_2] \) and \( J = [j_1, j_2] \). As shown in Figure 7, we pick \( t_1 \in [i_1, i_2] \) such that \( \nu([i_1 - 2\epsilon, t_1]) = \mu([i_1, t_1]) \). Similarly, pick \( t_2 \in [t_1, i_2] \) such that \( \mu([t_2, i_2]) = \nu([t_2, i_2 + 2\epsilon]) \).

We now present a plan to transport \( \nu \) to \( \mu \). This plan consists of four mini-plans:

1. First, transport the mass \( \nu([i_1 - 2\epsilon, t_1]) \) to \( \mu([i_1, t_1]) \) using a monotone transport map.
2. Then transport the mass from \( \nu([t_2, i_2 + 2\epsilon]) \) to \( \mu([t_2, i_2]) \) using a monotone transport map.
3. Keep any mass in \([t_1, t_2]\) in its place.
4. Move any remaining mass in \( \nu \) arbitrarily to the necessary places in \( \mu \).
Figure 7: Optimal coupling for two uniform distributions. The region shaded in green is kept in place (at no cost). The two regions shaded in orange are transported monotonically from either side at a cost not exceeding $2\epsilon$ per unit mass. The remaining region in blue is moved at the cost of 1 per unit mass.

The key point to note is that in maps (1) and (2), the total distance moved by every unit of mass is at most $2\epsilon$. The proof of this part is along similar lines to that of Theorem 8. Thus, the transport cost in steps (1) and (2) is 0. Naturally, the transport cost in (3) is 0. This means that all the mass in the interval $[i_1 - 2\epsilon, i_2 + 2\epsilon]$ can be transported into $\mu$ for zero cost. The total cost of transportation is therefore at most $1 - \nu([i_1 - 2\epsilon, i_2 + 2\epsilon])$, which matches our lower bound. It is easily checked that the error attained by the proposed classifier also matches the bound, which completes the proof.

**Theorem 10** (Triangular distributions). Denote a triangular distribution with support $[m-\delta, \mu+\delta]$ as $\Delta(m, \delta)$. Let $\mu$ and $\nu$ correspond to the triangular distributions $\Delta(m_1, \delta_1)$ and $\Delta(\mu_2, \delta_2)$ with pdfs $f$ and $g$ respectively. Without loss of generality, assume $\delta_1 < \delta_2$. Let $l < m_1 < r$ be such that $f(l + \epsilon) = g(l - \epsilon)$ and $f(r - \epsilon) = g(r + \epsilon)$. (In case of multiple such points, pick $l$ to be the largest among all such points, and $r$ to smallest.) Let $A$ be the closed set $[l, r]$. Then $D_\epsilon(\mu, \nu) = \mu(A^-) - \nu(A^\epsilon)$, the robust risk is

$$R^- = \frac{1 - \mu(A^-) + \nu(A^\epsilon)}{2},$$

and if $\mu$ corresponds to hypothesis 1, then the optimal robust classifier decides 1 on $A$.

**Proof sketch for Theorem 10.** We omit all proof details and point to Figure 8 which shows the coupling in a special case.

5 **Some results for continuous loss functions**

It is natural to ask if the results for 0–1 loss may be generalized for continuous losses. In this section, we present adversarial risk bounds in regression-like settings with continuous losses, and investigate Questions 1 and 2 in light of these bounds. Throughout this section, we shall assume that parameters and data are real-valued vectors; i.e., $\mathcal{W} \subseteq \mathbb{R}^{\dim(\mathcal{W})}$ and $\mathcal{Z} \subseteq \mathbb{R}^{\dim(\mathcal{Z})}$. Note that the adversary’s perturbation ball around $x$ is according to a metric $d(\cdot, \cdot)$, which need not be the same as the $L_2$ metric.
As in the proof of Theorem 8, we divide the real line into five regions. The transport plan from $\mu$ to $\nu$ consists of five maps transporting $\mu_- \to \nu_-$ (blue regions to the left), $\mu_- \to \nu_0$ (green regions in the middle), $\mu_0 \to \nu_0$ (green regions in the middle), $\mu_+ \to \nu_+$ (orange regions to the right), and $\mu_{++} \to \nu_{++}$ (blue regions to the right).

5.1 Optimal adversarial risk

In this section, we prove a lower bound on optimal adversarial risk for the data perturbing adversary and an upper bound optimal adversarial risk for the distribution perturbing adversary. As noted earlier, the lower bound is also valid for distribution perturbing adversary and the upper bound is also valid for data perturbing adversary.

For the lower bound, we consider loss functions that are convex with respect to the input $x$, as defined below.

Definition 3 (Convex loss function). We say that the loss function $\ell : \mathcal{Z} \times \mathcal{W} \to \mathbb{R}^+$ is convex with respect to the input if it satisfies the following condition.

$$\ell((x', y), w) - \ell((x, y), w) \geq \langle \nabla_x \ell(z, w), x' - x \rangle.$$  

(11)

Theorem 11. The adversarial risk for a loss function satisfying (11) is bounded as follows.

$$R_*^\epsilon \geq R_0^\epsilon + \inf_{w \in \mathcal{W}} \mathbb{E}_z \left[ \sup_{d(x, x') \leq \epsilon} \langle \nabla_x \ell((x, y), w), x' - x \rangle \right].$$  

(12)

In the special case when the distance function $d$ corresponds to the norm $\|\cdot\|_{\text{adv}}$, i.e. $d(x, x') = \|x - x'\|_{\text{adv}}$, we can further tighten the result of Theorem 11 as follows.

Corollary 5.1. In the setting of Theorem 11, if $d(x, x') = \|x - x'\|_{\text{adv}}$ for $x, x' \in \mathcal{X}$, then the following bound holds:

$$R_*^\epsilon \geq R_0^\epsilon + \epsilon \inf_{w \in \mathcal{W}} \mathbb{E}_z \|\nabla_x \ell((x, y), w)\|_{\text{adv}^*},$$  

(13)

where $\|\cdot\|_{\text{adv}^*}$ is the dual norm of $\|\cdot\|_{\text{adv}}$. 

20
Proof of Theorem 11. Since \(w^*_\epsilon\) is sub-optimal for minimizing standard risk, we have
\[
\mathbb{E}_z[\ell((x, y), w^*_\epsilon)] \geq \mathbb{E}_z[\ell((x, y), w^*_0)].
\]

Hence,
\[
R^*_\epsilon - R^*_0 = \mathbb{E}_z \left[ \sup_{d(x, x') \leq \epsilon} \ell((x', y), w^*_\epsilon) - \mathbb{E}_z[\ell((x, y), w^*_0)] \right]
\geq \mathbb{E}_z \left[ \sup_{d(x, x') \leq \epsilon} \ell((x', y), w^*_\epsilon) - \mathbb{E}_z[\ell((x, y), w^*_\epsilon)] \right]
= \mathbb{E}_z \left[ \sup_{d(x, x') \leq \epsilon} \ell((x', y), w^*_\epsilon) - \ell((x, y), w^*_\epsilon) \right]
\geq \mathbb{E}_z \left[ \sup_{d(x, x') \leq \epsilon} \langle \nabla_x \ell((x, y), w^*_\epsilon), x' - x \rangle \right],
\geq \inf_{w \in W} \mathbb{E}_z \left[ \sup_{d(x, x') \leq \epsilon} \langle \nabla_x \ell((x, y), w^*_\epsilon), x' - x \rangle \right].
\]

Proof of Corollary 5.1. From the proof of Theorem 11, we have
\[
R^*_\epsilon - R^*_0 \geq \mathbb{E}_z \left[ \sup_{d(x, x') \leq \epsilon} \langle \nabla_x \ell((x', y), w^*_\epsilon), x' - x \rangle \right].
\]

Under the condition that \(d(x, x') = \|x - x'\|_{\text{adv}}\),
\[
\sup_{d(x, x') \leq \epsilon} \langle \nabla_x \ell((x', y), w^*_\epsilon), x' - x \rangle
= \sup_{\|\delta\|_{\text{adv}} \leq \epsilon} \langle \nabla_x \ell((x', y), w^*_\epsilon), \delta \rangle
= \epsilon \|\nabla_x \ell((x', y), w^*_\epsilon)\|_{\text{adv}^*}.
\]

Now, we prove an upper bound for the adversarial risk for a distribution perturbing adversary. As noted earlier, this upper bound also holds for the data perturbing adversary. We make the following assumption on the loss function:

Definition 4 \((L_x(w))-\text{Lipschitz loss function}\). We say that the loss function \(\ell : Z \times W \rightarrow \mathbb{R}^+\) is \(L_x(w))-\text{Lipschitz with respect to the input if it satisfies the following condition.}
\[
|\ell((x', y), w) - \ell((x, y), w)| \leq L_x(w)\|x' - x\|.
\]

Theorem 12. The adversarial risk for a distribution perturbing adversary satisfies \(\hat{R}^*_\epsilon \leq R^*_0 + \epsilon L_x(w^*_0)\). Naturally, we also have \(R^*_\epsilon \leq R^*_0 + \epsilon L_x(w^*_0)\).

The proof of this result uses an optimal transport idea from [34].
Proof of Theorem 12. Suppose that the infimum in in equation (3) is attained at \( \hat{w}_e^* \), and the corresponding maximizer in equation (2) is \( \rho^*_e \). Then
\[
\hat{R}_e^* - R_0^* = \mathbb{E}_{Z \sim \rho^*_{e}} \ell(Z, \hat{w}_e^*) - \mathbb{E}_{Z' \sim \rho_0} \ell(Z', w_0^*) \\
\leq (a) \mathbb{E}_{Z \sim \rho^*_{e}} \ell(Z, \hat{w}_0^*) - \mathbb{E}_{Z' \sim \rho_0} \ell(Z', w_0^*) \\
\leq (b) \mathbb{E}_{(Z, Z') \sim \Pi(\rho^*_{e}, \rho_0)} \ell(Z', w_0^*) - \ell(Z, w_0^*) \\
\leq (c) \mathbb{E}_{(Z, Z') \sim \Pi(\rho^*_{e}, \rho_0)} d(Z, Z') \cdot L w_0^*.
\]
Here, (a) follows from the definition of \( \hat{w}_e^* \), (b) follows from linearity of expectation since \( \Pi(\rho^*_{e}, \rho_0) \) is a coupling of \( (X, Z') \) that preserves the marginals, and (c) follows from the Lipschitz assumption. Picking the optimal possible coupling corresponding to the Wasserstein distance between \( \rho_0 \) and \( \rho^*_e \), we conclude that
\[
\hat{R}_e^* - R_0^* \leq \epsilon L_x(w_0^*).
\]
\( \square \)

5.2 Optimal adversarial classifier

In Sections 3 and 5.1, we looked at Question 1 and showed that the adversarial risk can be strictly lower-bounded as a function of adversarial budget \( \epsilon \). In this section, we tackle Question 2 and analyze how \( w_0^* \) or \( \hat{w}_e^* \) may deviate from \( w_0^* \) with \( \epsilon \). For the case of 0-1 loss, the optimal classifier can change drastically even with small change in the adversarial budget \( \epsilon \). For instance, consider the setting of Theorem 3. When \( \epsilon \) changes from being less than \( \frac{|\mu_0 - \mu_1|}{2} \) to greater than \( \frac{|\mu_0 - \mu_1|}{2} \), the optimal classifier changes from a halfspace to a constant classifier. Studying the 0-1 loss is hard because closed sets are not parametrized easily. Hence we focus on the case of convex loss functions to derive bounds in this section.

Since our proof technique uses the upper and lower bounds for adversarial losses obtained in Section 5.1, the bounds for deviation of \( w_0^* \) and \( \hat{w}_e^* \) are identical. Now, we prove a theorem on how much the optimal classifier can change in the presence of an adversary.

Theorem 13. For a loss function \( \ell \) that satisfies (14), the following result holds for sufficiently small \( \epsilon \):
\[
\|w_e^* - w_0^*\| \leq \sqrt{\frac{\epsilon L_x(w_0^*)}{\lambda_{\text{min}}(\nabla^2 w_0 R_0(\ell, w_0^*))}}.
\]

With regards to Theorem 13, we note that if \( \ell \) is strongly convex with respect to \( w \), then (15) holds for any \( \epsilon \). For instance, if \( \ell_2 \) regularization is used, then the overall loss function will naturally be strongly convex with respect to \( w \).

Proof of Theorem 13. We take the Taylor expansion of \( R_0(\ell, w) \) at \( w_0^* \).
\[
R_0(\ell, w_e^*) = R_0(\ell, w_0^*) + \nabla_w R_0(\ell, w_0^*)^T (w_e^* - w_0^*) \\
+ (w_e^* - w_0^*)^T \nabla^2 w_0 R_0(\ell, w_0^*) (w_e^* - w_0^*) \\
+ O (\|w_e^* - w_0^*\|^3).
\]
Now, $\nabla_w R_0(\ell, w_0^*) = 0$ since $w_0^*$ is the minimizer of $R_0(\ell, w_0^*)$. Therefore for small enough $\epsilon$, we have the following.

$$
\epsilon L_x(w_0^*) \geq R_0^* - R_0^0

\geq R_0(\ell, w_{\epsilon}) - R_0(\ell, w_0^*)

\geq (w_{\epsilon}^* - w_0^*)^T \nabla^2_w R_0(\ell, w_0^*)(w_{\epsilon}^* - w_0^*)

\geq \lambda_{\text{min}}(\nabla^2_w R_0(\ell, w_0^*)) \|w_{\epsilon}^* - w_0^*\|^2.
$$

Here, (a) follows from Theorem 12, (b) follows from the fact that $w_{\epsilon}^*$ is sub-optimal for minimizing $R_0(\ell, w)$, and (c) follows from the Taylor expansion presented above (for small enough $\epsilon$).

\[\Box\]

6 Experiments

In this section, we present lower bounds on the optimal adversarial risk for empirical distributions derived from several real-world datasets.

For the case of empirical distributions, the computation of the optimal transport cost in (6) can be formulated as a linear program and solved efficiently. Moreover, when the number of data points in the two empirical distributions is the same, the problem of finding the optimal coupling between the two distributions is reduced to an assignment problem (see Proposition 2.11 in [29]), wherein the task is to optimally match each data point from the first distribution to a distinct data point from the second distribution. Using this methodology, we evaluate the optimal risk for $\ell_2$ and $\ell_\infty$ adversaries for classes 3 and 5 in CIFAR10, MNIST, Fashion-MNIST, and SVHN datasets. The results for other pairs of classes are very similar, and are therefore omitted for brevity. For MNIST, Fashion-MNIST, and SVHN datasets, we evaluate the optimal adversarial risk given in Theorem 2 by randomly sampling 5000 data points from each class. The results are showing in Figure 9 with the legend $\sigma = 0$.

Since a major fraction of the data points in the empirical distributions are well-separated in $\ell_2$ and $\ell_\infty$ metrics, the optimal risk bound remains 0 even for high $\epsilon$. For instance, for CIFAR10 dataset, the optimal risk remains 0 for $\epsilon$ as high as $40/255$ for $\ell_\infty$. Similar results were also obtained in Bhagoji et al. [4]. However, the optimal risk bounds for the true distributions may not be 0 for high $\epsilon$, as it is unreasonable to expect a perfectly robust optimal classifier under very strong adversarial perturbations. In addition, a common technique while training for a classifier is to augment the dataset with Gaussian perturbed samples for robustness and generalization [23, 19]. Motivated by this, we also compute optimal risk lower bounds on Gaussian mixture distribution with the data points as the centers with scaled identity covariances. $\sigma = 0$ corresponds to the empirical distribution of the data points from the two classes. As $\sigma$ increases, the overlap in the probability mass between the two classes increases. This allows for the cost of optimal coupling that achieves $D_\epsilon$ to decrease, thus leading to a higher, possibly non-trivial bound for $R_\epsilon^*$.

To compute the optimal risk lower bound for Gaussian mixture, we use a coupling between the mixture distributions in two steps. In the first step, we solve for the optimal coupling that gives the exact optimal risk for the empirical distributions. This gives a pairwise matching of data points between the two empirical distributions. In the second step, we use the optimal coupling for multidimensional Gaussians from Theorem 4 to transport the mass in the Gaussians within each pair. Overall, this transport map gives an upper bound on the $D_\epsilon$ optimal transport cost between the two mixture distributions. Using this, we obtain the lower bounds on adversarial risk shown in Figure 9.
Figure 9 shows the lower bounds for various values of the variance $\sigma$ used for the Gaussian mixture, where $\sigma^*$ is half of the mean distance between data points from the two distributions. As explained previously, we see in Figure 9 that the lower bound curves for higher values of $\sigma$ are above those for lower values. For instance, the optimal risk for CIFAR10 dataset under $\ell_2$ perturbation with $\epsilon = 3$ is 0.25 for $\sigma = \sigma^*$. That is, the adversarial error rate for CIFAR10 with $\epsilon = 3$ for any algorithm cannot be less than 0.25 even when trained with Gaussian data augmentation (with $\sigma = \sigma^*$). In comparison, the lower bound obtained in Bhagoji et al. [4] (which is equivalent to the case of $\sigma = 0$) is 0 for $\epsilon = 3$. Computation of non-trivial lower bounds for higher values of $\epsilon$ on adversarial error rate as in Figure 9 is made possible by our analysis on the optimal coupling to achieve $D_\epsilon$ between multivariate Gaussians in section 4.1.

7 Discussion

In this paper, we have analyzed two notions of adversarial risk - one resulting from a distribution perturbing adversary ($\hat{R}_\epsilon^*$) and the other from a data perturbing adversary ($R_\epsilon^*$). We have introduced the $D_\epsilon$ optimal transport distance between probability distributions. Through an application of duality in the optimal transport cost formulation (via Strassen’s theorem), we have shown that $D_\epsilon$ completely characterizes the optimal adversarial risk $R_\epsilon^*$ for the case of binary classification under $0-1$ loss function. For general loss functions, we give lower bounds on $R_\epsilon^*$ and upper bounds on $\hat{R}_\epsilon^*$ in terms of the smoothness properties of the loss function. Our analysis raises several interesting questions: How big is the gap between $\hat{R}_\epsilon^*$ and $R_\epsilon^*$ for different kinds of loss functions? Is it possible to directly lower bound $\hat{R}_\epsilon^*$ without appealing to its dependence on $R_\epsilon^*$? Does there exist an optimal transport distance akin to $D_\epsilon$ that characterizes $\hat{R}_\epsilon^*$? As evidenced by experiments, our bounds for general loss functions are not particularly tight. Furthermore, we need fairly strong assumptions such as convexity and Lipschitz property for the loss function to state these bounds. It would be interesting to study if these conditions may be relaxed and if tighter bounds could be obtained.

In analysing the adversarial risk for $0-1$ loss functions, we give a novel coupling strategy based on monotone mappings that solves the $D_\epsilon$ optimal transport problem for symmetric unimodal distributions like Gaussian, triangular, and uniform distributions. Employing the duality in the optimal transport, we also obtain the adversarially optimal classifier under these settings. Our coupling analysis calls for an interesting open question: Is there a general coupling strategy, akin to the maximal coupling strategy to achieve the total variation transport cost, that works for a broader class of distributions? If yes, this gives us a handle on analyzing the nature of optimal decision boundaries in the adversarial setting. Optimal transport between measures with unequal mass has received attention in recent work [7]. We plan to investigate if the version of transport from Definition 2 is useful in other contexts, and whether computational methods as in [29] may be used to compute it in practice.

Our analysis for $0-1$ loss reveals how the optimal risk smoothly changes from Bayes risk as the data perturbing budget $\epsilon$ is increased. Somewhat more surprisingly, our analysis shows that in some cases, the optimal classifier can change abruptly in the presence of an adversary even for small changes in $\epsilon$. It remains to be seen if these observations on optimal risk and optimal classifier also hold for the distribution perturbing adversary.

Using our characterization of $R_\epsilon^*$ in terms of $D_\epsilon$, we obtain the optimal risk attainable for classification of real-world datasets like CIFAR10, MNIST, Fashion-MNIST and SVHN. Moreover, leveraging our optimal coupling strategy for Gaussian distributions, we also obtain lower bounds on optimal risk for Gaussian mixtures based on these datasets. These lower bounds have implications
Lemma A.1. Let the input statement provided below is as in Villani [36, Corollary 1.28]: as a linear program. In addition, our bounds are efficiently computable for empirical/mixture distributions via reformulation bounds on adversarial risk are classifier agnostic, and only depend on the data distributions. In addition, our bounds are efficiently computable for empirical/mixture distributions via reformulation. We note that our optimal transport cost \( c_{\ast} \) is discontinuous and does not satisfy triangle inequality. This makes it hard to analyze Strassen’s theorem is a special case for the Kantorovich duality in the case of a 0 \(-\) 1 loss. The optimal transport cost \( c_{\ast}(x, x') = \mathbb{1}\{d(x, x') > 2\epsilon\} \) is discontinuous and does not satisfy triangle inequality. This makes it hard to analyze.

Finally, we remark that analyzing the \( D_{\epsilon} \) optimal transport cost may be interesting in itself. The optimal transport cost \( c_{\ast}(x, x') = \mathbb{1}\{d(x, x') > 2\epsilon\} \) is discontinuous and does not satisfy triangle inequality. This makes it hard to analyze using standard techniques in optimal transport literature. For instance, it would be interesting to see how fast \( D_{\epsilon} \) between empirical distributions converges to \( D_{\epsilon} \) between the true data-generating distributions. This may be used to obtain finite-sample lower bounds for adversarial error.

A Proofs for Section 3

A.1 Strassen’s theorem

Strassen’s theorem is a special case for the Kantorovich duality in the case of a 0 \(-\) 1 loss. The statement provided below is as in Villani [36, Corollary 1.28]:

**Lemma A.1.** Let the input \( X \) be drawn from a Polish space \( \mathcal{X} \). Let \( \Pi(p_0, p_1) \) be the set of all probability measures on \( \mathcal{X} \times \mathcal{X} \) with marginals \( p_0 \) and \( p_1 \). Then for \( \epsilon \geq 0 \) and \( A \subseteq \mathcal{X} \),

\[
\inf_{\pi \in \Pi(p_0, p_1)} \pi[\{d(x, x') > \epsilon\}] = \sup_{A \text{ closed}} \{p_0(A) - p_1(A^c)\}.
\]

A.2 Proof of Lemma 3.1

Let \( A \) be a closed set and let \( B \) be the closed ball of radius \( \epsilon \). Let \( \{z_i\}_{i \geq 1} \) be a sequence of points in \( A^c \) converging to a limit \( z \). We shall show that \( z \in A^c \) as well. Note that every \( z_i \) admits an expression \( z_i = a_i + b_i \), where \( a_i \in A \) and \( b_i \in B \). Since \( B \) is a compact set, there exists a subsequence among the \( \{b_i\} \) sequence that converges to \( b^* \in B \). Call the subsequence \( \{\tilde{b}_i\}_{i \geq 1} \) such that \( \tilde{b}_i \to b^* \) and \( |\tilde{b}_i - b^*| < \delta \) for some small \( \delta > 0 \). Since \( z = \tilde{a}_i + \tilde{b}_i = \tilde{a}_i + \tilde{b}_i - b^* + b^* \). Thus, we see that \( \tilde{a}_i \) is also bounded within a ball of radius \( \delta \) around \( z - b^* \), and so there exists a convergence subsequence within the \( \{\tilde{a}_i\} \) sequence. Let that subsequence converge to \( a^* \). We must have \( a^* \in A \) and \( b^* \in B \) since \( A \) and \( B \) are closed. This means \( z = a^* + b^* \) must lies in \( A^c \), which shows that \( A^c \) is closed.

Recall that \( A^{-\epsilon} = (A^\epsilon)^c \). Since \( A^\epsilon \) is an open set, it is enough to show that \( C^\epsilon \) is open if \( C \) is open. Let \( z \in C^\epsilon \). We know that \( z = c + b \) for some \( c \in C \) and \( b \in B \). Consider a small open ball of radius \( \delta \) around \( c \), called \( N_\delta(c) \) that lies entirely in \( C \). This is possible since \( C \) is assumed to be open. Now observe that \( N_\delta(z) \subseteq C^\epsilon \), since \( N_\delta(z) = N_\delta(c) + b \). This shows that every point \( z \in C^\epsilon \) admits a small ball around it that is contained in \( C^\epsilon \), or equivalently, \( C^\epsilon \) is open. This completes the proof.

A.3 Proof of Lemma 3.2

Notice that a point \( x \in A^{-\epsilon} \) if and only if \( N_\epsilon(x) \) (which is the ball of radius \( \epsilon \) centered at \( x \)) lies entirely in \( A \). If this were not the case, then we could find a \( y \in A^c \) such that \( d(x, y) \leq \epsilon \), and so \( x \in (A^\epsilon)^c \), which implies \( x \not\in ((A^\epsilon)^c)^c = A^{-\epsilon} \). This observation implies that \( (A^{-\epsilon})^c \subseteq A \).

Similarly, a point \( x \in (A^\epsilon)^{-\epsilon} \) if and only if \( N_\epsilon(x) \in A^c \). By definition of \( A^\epsilon \), every point \( x \in A \) satisfies \( N_\epsilon(x) \in A^c \). Thus, if \( x \in A \) then \( x \in (A^\epsilon)^{-\epsilon} \). Equivalently, \( A \subseteq (A^\epsilon)^{-\epsilon} \).
References

[1] Shafahi A., W. R. Huang, S. Studer, S. Feizi, and T. Goldstein. Are adversarial examples inevitable? *International Conference on Learning Representations*, 2019.

[2] A. Athalye, N. Carlini, and Wagner D. A. Obfuscated gradients give a false sense of security: Circumventing defenses to adversarial examples. In *International Conference on Machine Learning*, 2018.

[3] I. Attias, A. Kontorovich, and Y. Mansour. Improved generalization bounds for robust learning. *Algorithmic Learning Theory*, 2018.

[4] A. N. Bhagoji, D. Cullina, and P. Mittal. Lower bounds on adversarial robustness from optimal transport. *Conference on Neural Information Processing Systems*, 2019.

[5] J. Blanchet, Y. Kang, and K. Murthy. Robust Wasserstein profile inference and applications to machine learning. *arXiv preprint arXiv:1610.05627*, 2016.

[6] N. Carlini and D. Wagner. Adversarial examples are not easily detected: Bypassing ten detection methods. In *Proceedings of the 10th ACM Workshop on Artificial Intelligence and Security*, pages 3–14. ACM, 2017.

[7] L. Chizat, G. Peyr´e, B. Schmitzer, and F-X. Vialard. Scaling algorithms for unbalanced optimal transport problems. *Mathematics of Computation*, 87(314):2563–2609, 2018.

[8] M. Cisse, P. Bojanowski, E. Grave, Y. Dauphin, and N. Usunier. Parseval networks: Improving robustness to adversarial examples. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pages 854–863. JMLR. org, 2017.

[9] J.M. Cohen, E. Rosenfeld, and J. Z. Kolter. Certified adversarial robustness via randomized smoothing. In *International Conference on Machine Learning*, 2019.

[10] D. Cullina, A. N. Bhagoji, and P. Mittal. PAC-learning in the presence of adversaries. In *Conference on Neural Information Processing Systems*, pages 230–241, 2018.

[11] D. I. Diochnos, S. Mahloujifar, and M. Mahmoody. Adversarial risk and robustness: General definitions and implications for the uniform distribution. In *Conference on Neural Information Processing Systems*, 2018.

[12] D. I. Diochnos, S. Mahloujifar, and M. Mahmoody. Lower bounds for adversarially robust pac learning. *arXiv preprint arXiv:1906.05815*, 2019.

[13] P. M. Esfahani and D. Kuhn. Data-driven distributionally robust optimization using the wasserstein metric: Performance guarantees and tractable reformulations. *Mathematical Programming*, 171(1-2):115–166, 2018.

[14] A. Fawzi, H. Fawzi, and O. Fawzi. Adversarial vulnerability for any classifier. In *Conference on Neural Information Processing Systems*, 2018.

[15] R. Gao, X. Chen, and A. J. Kleywegt. Wasserstein distributional robustness and regularization in statistical learning. *arXiv preprint arXiv:1712.06050*, 2017.

[16] R. Gao and A. J. Kleywegt. Distributionally robust stochastic optimization with wasserstein distance. *arXiv preprint arXiv:1604.02199*, 2016.
[17] J. Gilmer, L. Metz, F. Faghri, S. S. Schoenholz, M. Raghunathan, M. Wattenberg, and I. Goodfellow. Adversarial spheres. *arXiv preprint arXiv:1801.02774*, 2018.

[18] C. R. Givens and R. M. Shortt. A class of Wasserstein metrics for probability distributions. *The Michigan Mathematical Journal*, 31(2):231–240, 1984.

[19] I. Goodfellow, Y. Bengio, and A. Courville. *Deep learning*. MIT press, 2016.

[20] I. J. Goodfellow, J. Shlens, and C. Szegedy. Explaining and harnessing adversarial examples. *arXiv preprint arXiv:1412.6572*, 2014.

[21] P. Gourdeau, V. Kanade, M. Kwiatkowska, and J. Worrell. On the hardness of robust classification. *arXiv preprint arXiv:1909.05822*, 2019.

[22] M. Hein and M. Andriushchenko. Formal guarantees on the robustness of a classifier against adversarial manipulation. In *Advances in Neural Information Processing Systems*, pages 2266–2276, 2017.

[23] L. Holmstrom and P. Koistinen. Using additive noise in back-propagation training. *IEEE transactions on Neural Networks*, 3(1):24–38, 1992.

[24] J. Khim and P-L. Loh. Adversarial risk bounds for binary classification via function transformation. *arXiv preprint arXiv:1810.09519*, 2018.

[25] A. Madry, A. Makelov, L. Schmidt, D. Tsipras, and A. Vladu. Towards deep learning models resistant to adversarial attacks. *International Conference on Learning Representations*, 2018.

[26] S. Mahloujifar, D. I. Diochnos, and M. Mahmoody. The curse of concentration in robust learning: Evasion and poisoning attacks from concentration of measure. *Thirty-Third Conference on Artificial Intelligence (AAAI)*, 2019.

[27] S-M. Moosavi-Dezfooli, A. Fawzi, J. Uesato, and P. Frossard. Robustness via curvature regularization, and vice versa. *arXiv preprint arXiv:1811.09716*, 2018.

[28] N. Papernot, P. McDaniel, X. Wu, S. Jha, and A. Swami. Distillation as a defense to adversarial perturbations against deep neural networks. In *2016 IEEE Symposium on Security and Privacy (SP)*, pages 582–597. IEEE, 2016.

[29] G. Peyré and M. Cuturi. Computational optimal transport. *Foundations and Trends® in Machine Learning*, 11(5-6):355–607, 2019.

[30] A. Raghunathan, J. Steinhardt, and P. Liang. Certified defenses against adversarial examples. *International Conference on Learning Representations*, 2018.

[31] A. Sinha, H. Namkoong, and J. C. Duchi. Certifying some distributional robustness with principled adversarial training. In *International Conference on Learning Representations*, 2017.

[32] D. Su, H. Zhang, H. Chen, J. Yi, P-Y. Chen, and Y. Gao. Is robustness the cost of accuracy—a comprehensive study on the robustness of 18 deep image classification models. In *Proceedings of the European Conference on Computer Vision (ECCV)*, pages 631–648, 2018.

[33] C. Szegedy, W. Zaremba, I. Sutskever, J. Bruna, D. Erhan, I. Goodfellow, and R. Fergus. Intriguing properties of neural networks. *arXiv preprint arXiv:1312.6199*, 2013.
[34] A. Tovar-Lopez and V. Jog. Generalization error bounds using Wasserstein distances. In 2018 IEEE Information Theory Workshop (ITW), pages 1–5. IEEE, 2018.

[35] D. Tsipras, S. Santurkar, L. Engstrom, A. Turner, and A. Madry. Robustness may be at odds with accuracy. arXiv preprint arXiv:1805.12152, 2018.

[36] C. Villani. Topics in optimal transportation. American Mathematical Soc., 2003.

[37] T-W. Weng, H. Zhang, P-Y. Chen, J. Yi, D. Su, Y. Gao, C-J. Hsieh, and L. Daniel. Evaluating the robustness of neural networks: An extreme value theory approach. International Conference on Learning Representations, 2018.

[38] D. Wozabal. Robustifying convex risk measures for linear portfolios: A nonparametric approach. Operations Research, 62(6):1302–1315, 2014.

[39] D. Yin, K. Ramchandran, and P. Bartlett. Rademacher complexity for adversarially robust generalization. International Conference on Machine Learning, 2019.

[40] H. Zhang, T-W. Weng, P-Y. Chen, C-J. Hsieh, and L. Daniel. Efficient neural network robustness certification with general activation functions. In Advances in Neural Information Processing Systems, pages 4944–4953, 2018.

[41] B. Zhu, J. Jiao, and J. Steinhardt. Generalized resilience and robust statistics. arXiv preprint arXiv:1909.08755, 2019.
Figure 9: Lower bounds on adversarial risk computed using Theorem 2. The curves with $\sigma = 0$ gives the exact optimal risk for empirical distributions, while the other curves give lower bounds on the optimal risk for Gaussian mixtures based on the empirical distributions using the coupling in Theorem 4.