Analyzing the Robustness of Nearest Neighbors to Adversarial Examples

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Abstract

Motivated by applications such as autonomous vehicles, test-time attacks via adversarial examples have received a great deal of recent attention. In this setting, an adversary is capable of making queries to a classifier, and perturbs a test example by a small amount in order to force the classifier to report an incorrect label. While a long line of work has explored a number of attacks, not many reliable defenses are known, and there is an overall lack of general understanding about the foundations of designing machine learning algorithms robust to adversarial examples.

In this paper, we take a step towards addressing this challenging question by introducing a new theoretical framework, analogous to bias-variance theory, which we can use to tease out the causes of vulnerability. We apply our framework to a simple classification algorithm: nearest neighbors, and analyze its robustness to adversarial examples. Motivated by our analysis, we propose a modified version of the nearest neighbor algorithm, and demonstrate both theoretically and empirically that it has superior robustness to standard nearest neighbors.

1 Introduction

Machine learning is increasingly being applied in security-critical domains such as automotive systems, healthcare, finance and robotics. For example, much of the technology behind autonomous and driverless vehicle development – a safely critical application – is driven by machine learning. To ensure safe deployment in these applications, there is thus an increasing need to design machine-learning algorithms that can account for the presence of active adversaries and defend against attacks.

A popular and realistic attack paradigm that has received a lot of recent attention is test-time attacks via adversarial examples. In this context, an adversary has no control over the training data or the trained classifier, but instead has only the ability to provide inputs to a classifier and receive outputs; his goal is to perturb a test example by a “small amount” in order to force a classifier to report an incorrect label thus causing malicious
behavior. An example is an adversary that replaces a stop sign by a slightly defaced version in order to force an autonomous vehicle to recognize it as a yield sign. If the perturbation is small enough, the attack is undetectable to the human eye but may turn out to be very dangerous if autonomous cars are around. Like most other work in this line, we also assume for simplicity that the adversary is white box, in the sense that it knows all the details of the classifier used.

A line of recent work has considered adversarial examples in the context of linear classifiers [14] and neural networks [22, 10, 17, 18, 15], much of which has been focussed on developing increasingly sophisticated attacks. How to defend reliably against these attacks, however, is unfortunately less clear. While a number of defenses have been initially proposed [19, 16], these have mostly been attacked and broken by subsequent work [8, 2]. Thus, with a handful of exceptions [7, 23], there is an overall lack of general understanding about the foundations of designing machine learning algorithms that are robust to adversarial examples. In this context, several intriguing questions remain: what makes classifiers vulnerable to adversarial examples? When do robust classifiers exist? What kind of defenses can we employ against these examples and in what situation? This work takes a first step towards addressing these challenging questions.

In this paper, we develop a theoretical framework for learning in a manner that is robust to adversarial examples, with the goal of understanding why a classifier might be vulnerable against these attacks. Our framework is analogous to the traditional bias-variance theory in machine learning [9]. In particular, we identify that a classifier derived from applying a machine-learning algorithm on a training dataset may be robust to adversarial examples because of three reasons. First, it may be distributionally robust – in the sense that the trained classifier will stay robust as the number of training samples increase to infinity; this concept is analogous to bias (or, perhaps more accurately, one minus the bias). Second, even the output of a distributionally robust algorithm may be vulnerable because there are too few training samples – this is characterized by finite sample robustness, just as variance characterizes the effect of finite samples. Finally, different training algorithms might result in classifiers with different degrees of robustness, which we call algorithmic robustness.

We apply our framework to analyze a simple non-parametric classification algorithm: nearest neighbors, and provide bounds on its distributional and finite-sample robustness. Our analysis demonstrates that nearest neighbor classifiers are inherently non-robust when $P(y|x)$ is non-zero for more than one label, even though the classifiers may be quite accurate in these regions. Furthermore, $k$-nearest neighbors, which is considered more stable because of its higher resistance to random classification noise, still suffers from this problem for fixed $k$.

Motivated by our theoretical analysis, we finally propose a modified version of the nearest neighbor classifier, and provide theoretical guarantees to show that our proposed version has higher distributional robustness than standard nearest neighbors under certain conditions. We then implement and evaluate our algorithm empirically on three standard datasets. Our experimental results indicate that our proposed algorithm has higher accuracy on adversarial examples compared with standard nearest neighbors, as well as nearest neighbors that has been subjected to adversarial training – one of the most common and effective defense mechanisms in the literature.

Related Work. Motivated by applications such as autonomous driving, adversarial examples have received a great deal of recent attention [10, 18, 22, 17]. However, most of the work has been empirical in nature, and has largely focussed on developing increasingly
sophisticated attacks [3, 15]. While some recent defenses have been proposed [19, 16], many of them have been attacked and broken by subsequent work [3, 2]. Currently, the only reliable defense that appears to resist adversarial examples successfully is data augmentation – where the classifier is trained on an additional set of adversarial examples in addition to the usual training set.

In terms of theory, [7] is the first work to provide quantitative bounds on the robustness of classifiers; they analyze the robustness of linear and quadratic classifiers when the added perturbation is random as well as semi-random. [23] performs an elegant mathematical analysis of robustness in linear classifiers, and establishes conditions under which these classifiers are highly susceptible to adversarial examples. None of these works however, separate out the causes of vulnerability into distributional and finite sample; moreover, they also do not consider nearest neighbors. [1] provides an attack method for nearest neighbor classifiers, and shows that their robustness decreases with increasing intrinsic dimensionality of the data.

Finally, beginning with the work of Fix and Hodges [8], there has been a long line of work on the convergence and consistency of nearest neighbor classifiers and their many variants [5, 21, 13, 6, 4, 12, 11]; none of these works however have addressed robustness to adversarial examples. In terms of asymptotic results, [5] shows that provided some regularity conditions hold, and provided $k \to \infty$ and $k/n \to 0$ as $n \to \infty$, the error rate of the $k$-nearest neighbor classifier converges to that of the Bayes Optimal classifier. For $k = 1$, the error rate converges to at most twice the error rate of the Bayes Optimal.

There has also been much follow-up work on convergence rates of nearest neighbors [13, 6, 4, 12, 11]; however, the rates have been found to be highly dependent on the underlying data distribution. We also remark that our robust nearest neighbor algorithm is motivated by the algorithm in [12]; however, our robustness analysis is novel.

2 The Setting

2.1 Adversarial Setting and Threat Model

We focus on test-time attacks – that is, the adversary cannot control the training data, and we assume that the adversary is white box – it knows the exact details of the classifier used.

The adversary’s goal is to perturb a test input $x$ so as to force a classifier $f$ to report a label different from $f(x)$. Formally, given a classifier $f$, a test example $x$ and a radius $r$, the adversary’s goal is to find an $x'$ such that $f(x') \neq f(x)$ and $d(x, x') \leq r$. Here $d$ is an application-specific metric – for example, $d$ could be the Euclidean metric, the $L_1$ metric, or for computer vision applications, a perceptual metric [20].

2.2 Robustness

We call a classifier robust if it is not vulnerable to adversarial examples; a formal definition follows.

**Notation.** We assume that unlabeled instances are drawn from an instance space $X$ equipped with a metric $d$, and their labels are drawn from a categorical label space $Y$. There is an underlying data distribution $D$ that generates labeled training and test examples; the marginal over $X$ of $D$ is denoted by $\mu$ and the conditional distribution of the labels given $x$
is denoted by $\eta$. For the rest of this paper, we will assume that $d$ is the Euclidean metric; extensions to other metrics are left as future work.

**Definition 2.1 (Robustness Radius).** The robustness radius of a classifier $f$ at an instance $x \in \mathcal{X}$, denoted by $\rho(f, x)$, is defined as:

$$
\rho(f, x) = \inf_{r > 0} \{ \exists x' \in \mathcal{X} \cap B(x, r) \text{ s.t } f(x) \neq f(x') \}
$$

In other words, $\rho(f, x)$ is the shortest distance between $x$ and an example $x'$ to which $f$ assigns a label different from $f(x)$.

A direct implication is that an adversary who perturbs $x$ by an amount $< \rho(f, x)$ will fail to cause a misclassification. Note that a larger robustness radius implies a more robust classifier.

Fix any radius $r > 0$. It is easy to show that only the constant classifier has robustness radius $r$ at all $x$ when $\mathcal{X}$ is a continuous instance space such as $\mathbb{R}^d$. However, natural inputs rarely span entire continuous spaces – all possible images are not interesting natural images. It is therefore more interesting to consider classifiers that are robust on meaningful instances, which we characterize as instances drawn from an underlying data distribution. This leads to the following definition.

**Definition 2.2 (Robustness with respect to a Distribution).** The robustness of a classifier $f$ at a radius $r$ with respect to a distribution $\mu$ over the instance space $\mathcal{X}$, denoted by $R(f, r, \mu)$, is defined as:

$$
R(f, r, \mu) = \Pr_{x \sim \mu} \{ \{x | \rho(f, x) \geq r \}
$$

In other words, $R(f, r, \mu)$ is the fraction of instances drawn from $\mu$ for which the robustness radius is greater than or equal to $r$.

With these definitions in place, we can now talk about three sources of robustness – distributional, finite sample and algorithmic.

**Distributional Robustness.** Let $S_n$ be a labeled sample of size $n$ drawn from an underlying data distribution $D$, with marginal $\mu$ over $\mathcal{X}$. Let $A(S_n, \cdot)$ be a classification rule – for example, the nearest neighbor classifier – trained by applying the classification algorithm $A$ to the training set $S_n$. Then, the distributional robustness of the classification algorithm $A$ at radius $r$ is formally defined as:

$$
\lim_{n \to \infty} \mathbb{E}_{S_n \sim D} [R(A(S_n, \cdot), r, \mu)]
$$

Specifically, this is the expected robustness of the classifier output by $A$ trained on $S_n$ at radius $r$ with respect to the data distribution; the expectation is over samples from $D$.

Note that distributional robustness measures robustness when an infinite number of samples are available to train the classifier, and it depends only on $A$, the robustness radius, and the data distribution, and not on how many samples are available. It is thus analogous to the concept of bias.

**Finite Sample Robustness.** In contrast, when talking about the finite sample robustness, we characterize the behaviour of $R(A(S_n), r, \mu)$ for finite $n$ – usually by putting high probability bounds where the probability is over the training set. Thus, finite sample robustness depends on the training set size $n$, and quantifies how the robustness changes as we vary the sample size.
Algorithmic Robustness. Finally, we observe that robustness also depends on the training algorithm itself, and changing the algorithm may change it for the better or worse; for example, some variants of nearest neighbors may have higher robustness than nearest neighbors itself.

Robustness vs. Accuracy. If robustness were our only concern then it would be trivial to find a solution – simply output the constant classifier; such a solution however has very low classification accuracy. Our goal thus is to design algorithms that produce classifiers which are robust and have high classification performance.

Following [4], we measure classification performance of a predictor $f$ by comparing it with the Bayes Optimal classifier $g(x) = 1(\eta(x) \geq 1/2)$. Thus, we are interested in maximizing the fraction of examples where $f(x)$ is robust, and agrees with $g(x)$.

Definition 2.3 (Robustly Correct and R-accuracy). We say that a classifier $f$ is robustly correct at $x$ at radius $r$ if $f(x) = g(x)$ and $\rho(f,x) \geq r$; in other words, $f$ agrees with the Bayes Optimal classifier $g$ at $x$ and has robustness radius at least $r$.

The R-accuracy of a classifier $f$ with respect to a data distribution $D$ and a robustness radius $r$ is the fraction of examples on which it is robustly correct; formally,

$$ Racc_D(f) = \Pr_{x \sim \mu}(\{x|f(x) = g(x), \rho(f,x) \geq r\}), $$

where $g$ is the Bayes Optimal classifier on $D$ and $\mu$ is the marginal of $D$ on $\mathcal{X}$.

Formally, our goal is to design classifiers that maximize the R-accuracy. In Section 4, we will provide a modified nearest neighbor classifier which achieves this goal in the $n \to \infty$ limit under certain regularity conditions.

2.3 The Nearest Neighbor Classifier

Given a training set $S_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ and a test example $x$, we use the notation $X(i)(x)$ to denote the $i$-th nearest neighbor of $x$ in $S_n$, and $Y(i)(x)$ to denote the label of $X(i)(x)$.

Given a test example $x$, the $k$-nearest neighbor classifier $A_k(S_n, x)$ outputs:

$$ = 1, \text{ if } Y^{(1)}(x) + \ldots + Y^{(k)}(x) \geq k/2 $$

$$ = 0, \text{ otherwise.} $$

3 An Analysis of the Robustness of Nearest Neighbors

We begin with an analysis of the robustness properties of the nearest neighbor classifier for binary classification. For the rest of the section, we assume that the underlying data distribution $\mu$ is absolutely continuous with respect to the Lebesgue measure, and the condition distribution $\eta(x) = \Pr(y = 1|x)$ is also continuous.

Non-robustness of Nearest Neighbors. Our first result shows that if $\mu$ and $\eta$ are continuous and if $\eta(x) = \Pr(y = 1|x) \in (0, 1)$, then the radius of robustness of the classifier $A_1(S_n, \cdot)$ at $x$ tends to 0 as $n \to \infty$. 
Theorem 3.1. Let \( x \in \mathcal{X} \cap \text{supp}(\mu) \) such that (a) \( \mu \) is absolutely continuous with respect to the Lebesgue measure in a neighborhood of \( x \), (b) \( \eta(x) \in (0, 1) \) (c) \( \eta \) is continuous with respect to the Euclidean metric in a neighborhood of \( x \). Then, \( \rho(A_1(S_n, \cdot), x) \) converges in probability to 0.

Theorem 3.1 implies that if \( x \) is a point with \( \eta(x) \in (0, 1) \), then under some continuity conditions, the robustness radius at \( x \) tends to 0 as more and more training samples are obtained! This indicates that unless \( \eta(x) \) is 0 or 1, the 1-nearest neighbor classifier is fundamentally non-robust to adversarial examples.

We show in Theorem 3.2 that a similar result also holds for \( k \)-nearest neighbors for fixed \( k \). This is interesting because \( k \)-nearest neighbor is considered to be a more stable classifier due to its higher resistance to random classification noise. Our results however show that unless \( \eta(x) \) is 0 or 1, it is still not robust to adversarial examples.

Theorem 3.2. Let \( x \in \mathcal{X} \cap \text{supp}(\mu) \) such that (a) \( \mu \) is absolutely continuous with respect to the Lebesgue measure (b) \( \eta(x) \in (0, 1) \) (c) \( \eta \) is continuous with respect to the Euclidean metric in a neighborhood of \( x \). Then, for fixed \( k \), \( \rho(A_k(S_n, \cdot), x) \) converges in probability to 0.

Lower Bound on Robustness. We next consider where the nearest neighbor classifier is actually robust, and show that this happens in the interior of a region where \( \eta(x) = 0 \) or 1. We begin with a precise definition of the notion of interior.

Definition 3.3 \((r, \Delta)\)-Confident Interior. Let \( \mathcal{X} \) be an instance space and \( \eta(x) \) be the conditional distributions of labels given \( x \). Let \( r \) be a target radius of robustness. Then, the \((r, \Delta)\)-confident interior of the \( Y = 1 \) region is defined as:

\[
\mathcal{X}_{r, \Delta}^+ \triangleq \{ x \in \mathcal{X} \mid \eta(x) = \eta(x') = 1, \forall x' \in B(x, 2r + \Delta) \}.
\]

Similarly, the \((r, \Delta)\)-confident interior of the \( Y = 0 \) region is: \( \mathcal{X}_{r, \Delta}^- \triangleq \{ x \in \mathcal{X} \mid \eta(x) = \eta(x') = 0, \forall x' \in B(x, 2r + \Delta) \} \), and the \((r, \Delta)\)-confident interior is defined as: \( \mathcal{X}_{r, \Delta} = \mathcal{X}_{r, \Delta}^+ \cup \mathcal{X}_{r, \Delta}^- \).

Formally, we can now show the following lower bound:

Theorem 3.4. Let \( S_n \) be an i.i.d. sample of size \( n \) drawn from an underlying data distribution \( D \) with marginal \( \mu \) over \( \mathcal{X} \). Then,

\[ E[R(A(S_n, \cdot), r, \mu)] \geq \mu(\mathcal{X}_{r, \Delta}) - d_{\Delta, n}, \tag{1} \]

where \( d_{\Delta, n} = \mathbb{E}_{x \sim \mu}[1 - \mu(B^\Delta(x_0, \Delta))]^n \).

Moreover, with probability at least \( 1 - \delta \), \( R(A(S_n, \cdot), r, \mu) \geq \mu(\mathcal{X}_{r, \Delta}) - \frac{d_{\Delta, n}}{3} \).

Two remarks are in order. Observe that when \( \mu \) is absolutely continuous with respect to the Lebesgue measure, \( \Pr_{x \sim \mu}(\mu(B^\Delta(x_0, \Delta)) = 0) = 0 \) for \( x \) in the support of \( \mu \). This implies that, for fixed \( \Delta > 0 \), as \( n \to \infty \), the second term on the right hand side of (1) goes to zero, and thus the expected robustness tends to the measure of the \((r, \Delta)\)-confident interior. Second, as \( \Delta \to 0 \), \( \mathcal{X}_{r, \Delta} \to \mathcal{X}_{r, 0} \), and thus in the limit, Theorem 3.4 implies that the distributional robustness of the nearest neighbor classifier is at least \( \mu(\mathcal{X}_{r, 0}) \).

Finally, we remark that the entire analysis in Theorem 3.4 also applies to R-accuracy. This leads to the following corollary:

Corollary 3.5. Let \( S_n \) be an i.i.d. sample of size \( n \) drawn from an underlying data distribution \( D \) with marginal \( \mu \) over \( \mathcal{X} \). Then, \( \mathbb{E}_{S_n \sim D}[\text{Racc}_D(A_1(S_n, \cdot))] \geq \mu(\mathcal{X}_{r, \Delta}) - d_{\Delta, n}, \)

where \( d_{\Delta, n} = \mathbb{E}_{x \sim \mu}[1 - \mu(B^\Delta(x_0, \Delta))]^n \).
4 A More Robust Nearest Neighbor Classifier

Motivated by the analysis in Section 3, we now provide a modified nearest neighbor classification algorithm that achieves robustness and classification accuracy.

4.1 Algorithm

Our algorithm is motivated by the following observation. Suppose we are given a test case \( x \in \mathcal{X} \) and a training sample \( S_{\text{labeled}} \); also suppose that \( g \) is the Bayes Optimal classifier.

**Lemma 4.1.** If there exists a training point \((x_0, y_0)\) such that 1) \( g(x) = y_0 \) and 2) for all \((x_i, y_i) \in S_{\text{labeled}}, y_i \neq g(x)\) implies \( d(x_0, x_i) > 2r + 2d(x, x_0) \), then \( A_1(S_{\text{labeled}}, \cdot) \) is robustly correct at radius \( r \) at \( x \).

Lemma 4.1 implies that a 1-NN classifier is robust if differently labeled points in the training set are far apart. This observation suggests that we could improve robustness by training a 1-NN classifier on a subset \( S \) of \( S_{\text{labeled}} \) with this property.

To ensure accuracy, the subset \( S \) should also satisfy an additional condition – a random test example \( x \sim \mu \) should be close to some point in \( S \). This can be ensured by making sure that the union of balls of some small radius \( \Delta \) around each point in \( S \) has high probability mass with respect to the data distribution. Of course, the true data distribution is not available to us, but we can estimate the probability mass covered using an independently drawn, unlabeled, validation sample. Putting these components together gives us the full algorithm.

**Definitions.** Before we state the algorithm formally, we need some definitions.

**Definition 4.2 (\( \Delta \)-cover).** The \( \Delta \)-cover induced by a set \( S \) of points is defined as:

\[
\text{Cover}(S, \Delta) = \bigcup_{x \in S} B(x, \Delta).
\]

**Definition 4.3 (\( r \)-separated set).** A set \( A = \{(x_1, y_1), \ldots, (x_m, y_m)\} \) of labeled examples is said to be \( r \)-separated if for all pairs \((x_i, y_i), (x_j, y_j) \in A, d(x_i, x_j) \leq r \) implies \( y_i = y_j \).

We are interested in the set of all \( r \)-separated subsets of a set of labeled samples \( S_{\text{labeled}} \). We denote this quantity by \( \Sigma(r, S_{\text{labeled}}) \).

**Algorithm.** We are now ready to state the algorithm formally; this is done in Algorithm 1.

The algorithm takes four inputs – a robustness radius \( r \), a user-specified tolerance parameter \( \Delta \), a training set \( S_{\text{labeled}} \) of labeled examples, and a validation set \( S_{\text{valid}} \) of unlabeled examples. It then iterates over all \((2r + 2\Delta)\)-separated subsets \( S \) of \( S_{\text{labeled}} \), and picks the one which has the highest value of \(|\text{Cover}(S, \Delta) \cap S_{\text{valid}}|\). Finally, it returns the nearest neighbor classifier with the selected subset as training set. The formal algorithm is stated in Algorithm 1.

4.2 Performance Guarantees

We begin by showing a fundamental upper bound on the R-accuracy of any classifier.
Algorithm 1 RobustNN($S_{labeled}$, $S_{valid}$, $r$, $\Delta$)

\[
S_{max} = \emptyset \\
\text{for } S \in \Sigma(2r + 2\Delta, S_{labeled}) \text{ do} \\
\quad \text{if } |\text{Cover}(S, \Delta) \cap S_{valid}| \geq |S_{max} \cap S_{valid}| \text{ then} \\
\quad \quad S_{max} = S \\
\quad \text{end if} \\
\text{end for} \\
\text{return } A_1(S_{max}, \cdot)
\]

A Fundamental Upper Bound on R-accuracy. Consider the Bayes optimal classifier $g$. To state our bound, we need to extend the definition of $r$-separated set to those with respect to the Bayes optimal classifier $g$.

Definition 4.4 ($r$-separated set with respect to the Bayes optimal classifier). Given a Bayes optimal classifier $g$ over the instance space $\mathcal{X}$ and a metric $d$, a set $V \subseteq \mathcal{X}$ is said to be $r$-separated if $\forall x, x' \in V$, $d(x, x') \leq r$ implies $g(x) = g(x')$.

Let $\Sigma(r, \mathcal{X}, g)$ denote the set of all $r$-separated subsets of $\mathcal{X}$ with respect to the Bayes optimal classifier $g$. We are interested in the $r$-separated subset that has the most probability over the distribution $\mu$, and we use

\[
V_{max}(r) = \arg \max_{V \in \Sigma(r, \mathcal{X}, g)} \mu(V)
\]

(2)

to denote such a set. Then

Theorem 4.5. For any classifier $f$, $Racc_D(f, r) \leq \mu(V_{max}(2r))$.

R-accuracy Lower Bound. We show the following lower bound on the R-accuracy of Algorithm [1]. Let $A_1^{\text{robust}}(\cdot)$ denote the output of Algorithm [1] on $S_{labeled}$ of size $n$, $S_{valid}$ of size $m$, a tolerance parameter $\Delta$ and a robustness radius $r$.

Theorem 4.6. Consider an underlying data distribution $D$ with marginal $\mu$ over $\mathcal{X}$ and $\delta \in (0, 1]$. If $\mu$ is absolutely continuous with respect to Lebesgue measure, then

\[
\mathbb{E}_{S_{labeled}} \mathbb{E}_{S_{valid}} [Racc_D(A_1^{\text{robust}}(\cdot), r)] \geq \mu(V_{max}(2r + 2\Delta)) - [\epsilon(n, m, \delta) + c_{\Delta, \mu}(n) + 2\delta] - (1 - \mu(\mathcal{X}_0, \Delta)),
\]

(3)

where $c_{\Delta, \mu}(n) = \int_{V_{max}(2r + 2\Delta)} \left[1 - \frac{1}{2} \mu(B(x, \Delta)]^n d\mu(x)$, $\epsilon(n, m, \delta) = \sqrt{\frac{2 \log(1/\delta) + n}{2m}}$ and $\mathcal{X}_0, \Delta$ is the $(0, \Delta)$-confident interior. Moreover, with probability at least $1 - 3\delta$,

\[
Racc_D(A_1^{\text{robust}}(\cdot), r) \geq \mu(V_{max}(2r + 2\Delta)) - \left[\epsilon(n, m, \delta) + \frac{c_{\Delta, \mu}(n)}{\delta}\right] - (1 - \mu(\mathcal{X}_0, \Delta)).
\]

(4)

Corollary 4.7.
\[
\mathbb{E}_{S_{labeled}} \mathbb{E}_{S_{valid}} [R(A_1^{\text{robust}}(\cdot), r, \mu)] \geq \mu(V_{max}(2r + 2\Delta)) - [\epsilon(n, m, \delta) + c_{\Delta, \mu}(n) + 2\delta]
\]

Corollary 4.8. If $\mu(\mathcal{X}_0, \Delta) = 1$, then
\[
\mathbb{E}_{S_{labeled}} \mathbb{E}_{S_{valid}} [Racc_D(A_1^{\text{robust}}(\cdot), r)] \geq \mu(V_{max}(2r + 2\Delta)) - [\epsilon(n, m, \delta) + c_{\Delta, \mu}(n) + 2\delta]
\]
Three remarks are in order. First, note that when \(\mu(X_0, \Delta) = 1, \delta \to 0, \Delta \to 0, m \to \infty, n \to \infty\) and \(\frac{1}{m} \to 0, \Delta \to 0, m \to \infty, n \to \infty\), then \(E[Racc(D(A_1^{robust}(.), r)) \to \mu(V_{\text{max}}(2r))\), which is the optimal R-accuracy. As we see in Appendix C, even when \(\mu(X_0, \Delta) = 1\), nearest neighbor may not attain optimal R-accuracy. Second, while this upper bound is achieved assuming \(\mu(X_0, \Delta) = 1\), RobustNN may still outperform standard NN when \(\eta \in (0, 1)\) under certain condition; Appendix C presents an example to illustrate why. Third, the user-specified parameter \(\Delta\) controls the trade-off between asymptotic performance and the convergence rate with respect to sample sizes; a smaller \(\Delta\) leads to better asymptotic performance but requires larger training samples.

5 Experiments

In this section, we validate the result of Section 3 and Section 4 through experiments. Specifically, we investigate the following questions:

1. Can the robust nearest neighbor classifier achieve higher performance in the adversarial setting compared to the standard 1-NN classifier?

2. How does the knowledge of the magnitude \(r\) of adversarial perturbation affect performance?

3. How does our algorithm’s performance compare with nearest neighbors trained with data augmentation using adversarial examples - a common robustness-enhancing method?

These questions will be considered in the context of three datasets - (a) the halfmoon dataset, which is a standard benchmark for nearest neighbor algorithms, (b) a subset of the Abalone dataset and (c) a subset of the MNIST dataset.

We begin with a description of the experimental methodology.

A Practical Heuristic Robust NN Algorithm. Algorithm RobustNN in Section 4 is computationally expensive as it iterates over all \((2r + 2\Delta)\)-separated subsamples of \(S_{\text{labeled}}\). For our experiments, we propose a more tractable approximate version called RobustNNApprox.

Given a training set \(S_{\text{labeled}}\) and a robustness radius \(r\), robustNNApprox finds the \(2r\)-separated subset of training sample \(S_{\text{labeled}}\) of maximum cardinality. The intuition is that if \(S_{\text{labeled}}\) is representative, then the cover induced by this subset should approximately cover the high probability mass with respect to the data distribution. The procedure is similar to finding the margin-regularized nearest neighbor classifier in [12]. First, a collision graph is built: each point in \(S_{\text{labeled}}\) is a vertex, and an edge exists between two vertices if 1) they are \(\leq 2r\) apart and 2) they have different labels. The set of points to remove from \(S_{\text{labeled}}\) is then the minimum vertex cover of the collision graph. In binary classification, the problem can be reduced to finding the maximum matching in a bipartite graph, which has a polynomial time solution.

Attack Method. We use the attack method of [1]. The inputs are a test example \(x \in \mathcal{X}\), a perturbation magnitude \(r\) and a NN classifier \(A_1(S_{\text{labeled}}, \cdot)\) trained on \(S_{\text{labeled}}\). The attack algorithm finds an \(x' \in S_{\text{labeled}}\) that is closest to \(x\) but has a different label, and then returns the adversarial example \(x_{\text{adv}} = x + r \frac{x - x'}{|x - x'|_2}\).
Algorithm 2 RobustNNApprox($S_{labeled}$, $r$)

$$E = \emptyset$$

for $((x, y), (x', y')) \in S_{labeled} \times S_{labeled}$ do
  if $d(x, x') \leq 2r$ and $y \neq y'$ then
    $E = E \cup \{(x, y), (x', y')\}$
  end if
end for

$S' = S_{labeled} \backslash \text{MinVertexCover}(S_{labeled}, E)$

return $A_1(S', \cdot)$

Baselines. We compare the following algorithms. Our first baseline is the standard 1-NN algorithm, denoted by StdNN. Next, we have the Adversarially-Trained NN (ATNN), which is nearest neighbors on a training set augmented as follows: for each $(x, y) \in S_{labeled}$, we create an adversarial example $x_{adv}$ and add the point $(x_{adv}, y)$ to the training set. The perturbation magnitude of ATNN is the same as the perturbation magnitude used to create $x_{adv}$. Finally, we have two versions of our algorithm, RobustNN and AdaptiveNN. Both versions use Algorithm 2. For AdaptiveNN, the robustness parameter $r$ is set to the exact magnitude of the adversarial perturbation. For RobustNN, $r$ is set to the maximum magnitude of adversarial perturbations used in the experiment.

Procedure. We compare the effectiveness of each algorithm against adversarial examples; this is done by generating an adversarial example for each example in the test set, and then measuring if it is correctly classified. While attacking StdNN, we pick the point $x'$ closest to the test example $x$ from the training set; for ATTN, from the training set augmented by the adversarial examples, and for both versions of our algorithm, from the labeled data set $S'$ obtained at the end of Algorithm 2. For the halfmoon dataset, a training set of size 2000 and a test set of size 1000 with standard deviation $\sigma = 0.2$ is generated, and the reported accuracy is averaged over 20 data generations. Additionally, the perturbation magnitude varies from 0 to 0.2 with step size 0.01, and ATNN is trained with a perturbation magnitude of $r = 0.1$. For MNIST, the training data contains 1000 images of Digits 1 and Digit 7, while the test set contains 500 images from each class. The perturbation magnitude varies from 0 to 4 with step size 0.2, and the ATNN is trained with perturbation magnitude $r = 2$. Finally, for the Abalone dataset, 1000 out of the 1307 random instances of female abalone are used for training and the rest for testing. The classification task is to determine if the abalone is younger than 12.5 years old. The experiment is repeated 20 times for different random division of training and test sets, and the average accuracy is reported. The perturbation magnitude varies from 0 to 0.04 with step size 0.004, and the ATNN is trained with perturbation magnitude $r = 0.02$.

Results. Figure 1 shows the results. We observe that AdaptiveNN always performs better than StdNN and ATNN; therefore, if the perturbation magnitude is known, then our algorithm provides an effective defense, and is more robust than both standard nearest neighbors and nearest neighbors trained with data augmentation. This addresses our Questions 1 and 3. An interesting feature of the results is the ineffectiveness of ATNN; we believe this is because contrary to our algorithm, data augmentation decreases the distance between oppositely labeled training examples, and hence makes it easier to find a oppositely labeled training
Figure 1: Plot of classification accuracy of adversarial examples v.s. perturbation magnitude on 1) the halfmoon dataset, 2) MNIST 1 v.s. 7 and 3) the Abalone dataset. On all three datasets, AdaptiveNN outperforms StdNN, and RobustNN has the best performance when perturbation magnitude is large enough to full StdNN most of the time.

point in the vicinity of an adversarial example.

To address Question 2, we observe that RobustNN’s classification accuracy is lower than StdNN on MNIST when the perturbation magnitude is small but becomes higher with increasing perturbation magnitude. This is expected because RobustNN removes more training points than necessary for small perturbations. While knowing the perturbation magnitude is generally helpful, we observe that on the Abalone dataset, RobustNN outperforms both AdaptiveNN and StdNN; a plausible reason is that this dataset is very noisy, and RobustNN achieves better performance for small perturbations because it removes noisy points close to the decision boundary.

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A Proof for Standard NN in Section 3

Proof. (Of Theorem 3.1) To show convergence in probability, we need to show that for all \( \epsilon, \delta > 0 \), there exists an \( n(\epsilon, \delta) \) such that \( \Pr(\rho(A_1(S_n), x) \geq \epsilon) \leq \delta \) for \( n \geq n(\epsilon, \delta) \).

The proof proceeds in two stages. First, we show in Lemma A.1 that if the conditions in the statement of Theorem 3.1 hold, then there exists some \( n(\epsilon, \delta) \) such that for \( n \geq n(\epsilon, \delta) \), with probability \( \geq 1 - \delta \), there are two points \((x_0, y_0)\) and \((x_1, y_1)\) in \( B(x, \epsilon) \cap S_n \) such that (a) \( x_0 \neq x_1 \) (b) \( y_0 \neq y_1 \).

In the second step, let \((x', y')\) be the nearest neighbor of \( x \) in \( S_n \). \( x' \) is distinct from at least one of \( \{x_0, x_1\} \). Moreover, either \( y_0 = y' \) or \( y_1 = y' \); assume that \( y_0 = y' \). Then, \( x_1 \) is an example in \( B(x, \epsilon) \) that \( A_1(S_n) \) classifies as \( y_1 \), while \( A_1(S_n) \) classifies \( x \) as \( y_0 \), which implies that the robustness radius \( \rho(A_1(S_n), x) \leq \epsilon \).

\[ \square \]

Lemma A.1. If the conditions in the statement of Theorem 3.1 hold, then there exists some \( n(\epsilon, \delta) \) such that for \( n \geq n(\epsilon, \delta) \), with probability \( \geq 1 - \delta \), there are two points \((x_0, y_0)\) and \((x_1, y_1)\) in \( B(x, \epsilon) \cap S_n \) such that (a) \( x_0 \neq x_1 \) (b) \( y_0 \neq y_1 \).

Proof. Let \( c_1(n) \) denote the number of points in \( B(x, \epsilon) \cap S_n \) with label 1, and \( c_0(n) \) denote the number of points in \( B(x, \epsilon) \cap S_n \) with label 0. We define the following two bad events:

1. \( \exists x_i, x_j \in S_n \) such that \( x_i = x_j \), and
2. \( c_1(n) < 1 \) or \( c_0(n) < 1 \). If none of the bad events occur, then there exist two points \((x_0, y_0), (x_1, y_1)\) in \( B(x, \epsilon) \cap S_n \) such that \( x_0 \neq x_1 \) and \( y_0 \neq y_1 \). We show that for any sample size \( n \), the probability of the first bad event is 0 and for large enough \( n \), the probability of the second bad event is at most \( \delta \). Lemma A.1 then follows by taking a union bound over these two bad events.

Since \( \mu \) is absolutely continuous with respect to Lebesgue measure, for any two i.i.d. drawn points \((x_i, y_i)\) and \((x_j, y_j)\) in \( S_n \), \( \Pr(x_i = x_j) = 0 \). Taking union bound over all yet finitely many pairs of points in \( S_n \), we see that the probability of seeing two points in \( S_n \) with identical \( x \), i.e. the first bad event, is 0.

Next, we find a threshold value such that for all \( n \) larger than the threshold, the probability of the second bad event is at most \( \delta \). Similar to [4], we extend the definition of \( \eta \) to measurable sets \( A \subset X \) with \( \mu(A) > 0 \) as

\[ \eta(A) = \frac{1}{\mu(A)} \int_A \eta(x) d\mu(x), \]

which is the probability of \( Y = 1 \) for a point \( X \) randomly drawn from \( \mu \) given \( X \) lies in \( A \).

Let \( p = \mu(B(x, \epsilon) \cap X) \) and \( q = \eta(B(x, \epsilon) \cap X) \). For \( x \in \text{supp}(\mu) \), we have \( p > 0 \) because \( \mu(x) > 0 \), \( \mu \) is absolutely continuous in the neighborhood of \( x \) and \( B(x, \epsilon) \cap X \neq \emptyset \). Since \( p > 0 \), \( q \) is well defined. Meanwhile, \( 0 < q < 1 \) because \( \eta(x) \in (0, 1) \) and \( \eta \) is continuous in the neighborhood of \( x \).

For a random sample \((X, Y)\) drawn from the underlying distribution \( D \), \( pq \) is the probability that \( X \in B(x, \epsilon) \) and \( Y = 1 \). Similarly, \( p(1 - q) \) is the probability that \( X \in B(x, \epsilon) \) and \( Y = 0 \). By Hoeffding’s inequality,

\[ \Pr[c_1(n) \leq (pq - \epsilon_1)n] \leq \exp(-2\epsilon_1^2n) \]

for some constant \( \epsilon_1 \leq pq \). Substitute \( \epsilon_1 = \frac{1}{2}pq \) into the formula, we obtain

\[ \Pr[c_1(n) \leq \frac{1}{2}pqn] \leq \exp(-\frac{1}{2}p^2q^2n), \]

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which implies for all $n \geq \max \left(\frac{2}{\rho q}, \frac{2\log(2/\delta)}{p^2 q^2} \right)$, with probability at least $1 - \frac{1}{2}\delta$, $c_1(n) \geq 1$. Similarly, for all $n \geq \max \left(\frac{2}{\rho q}, \frac{2\log(2/\delta)}{p^2 q^2}, \frac{2}{p(1-q)}, \frac{2\log(2/\delta)}{p^2(1-q)^2} \right)$, with probability at least $1 - \frac{1}{2}\delta$, $c_0(n) \geq 1$. Therefore, for $n \geq \max \left(\frac{2}{\rho q}, \frac{2\log(2/\delta)}{p^2 q^2}, \frac{2}{p(1-q)}, \frac{2\log(2/\delta)}{p^2(1-q)^2} \right)$, with probability at least $1 - \delta$, $c_1(n) \geq 1$ and $c_0(n) \geq 1$, i.e. there are two points $(x_0, y_0)$ and $(x_1, y_1)$ such that $y_0 \neq y_1$. □

Proof. (Of Theorem 3.2) To show convergence in probability, we need to show that for all $\epsilon, \delta > 0$, there exists an $n(\epsilon, \delta)$ such that $Pr(\rho(A_k(S_n), x) \geq \epsilon) \leq \delta$ for $n \geq n(\epsilon, \delta)$.

The proof will again proceed in two stages. First, we show in Lemma A.2 that if the conditions in the statement of Theorem 3.2 hold, then there exists some $n(\epsilon, \delta)$ such that for $n \geq n(\epsilon, \delta)$, with probability at least $1 - \delta$, there exists two points $x_+$ and $x_-$ in $B(x, \epsilon)$ such that (a) all $k$ nearest neighbors of $x_+$ have label 1, (b) all $k$ nearest neighbors of $x_-$ have label 0, and (c) $x_+ \neq x_-$. Next we show that if the event stated above happens, then $\rho(A_k(S_n, x)) \leq \epsilon$. This is because $A_k(S_n, x) = 1$ and $A_k(S_n, x) = 0$. No matter what $A_k(S_n, x)$ is, we can always find a point $x'$ that lies in $\{x_+, x_-\} \subset B(x, \epsilon)$ such that the prediction at $x'$ is different from $A_k(S_n, x)$. □

**Lemma A.2.** If the conditions in the statement of Theorem 3.2 hold, then there exists some $n(\epsilon, \delta)$ such that for $n \geq n(\epsilon, \delta)$, with probability at least $1 - \delta$, there are two points $x_+$ and $x_-$ in $B(x, \epsilon)$ such that (a) all $k$ nearest neighbors of $x_+$ have label 1, (b) all $k$ nearest neighbors of $x_-$ have label 0, and (c) $x_+ \neq x_-$. 

Proof. (Of Lemma A.2) The proof consists of two major components. First, for large enough $n$, with high probability there are many disjoint balls in the neighborhood of $x$ such that each ball contains at least $k$ points in $S_n$. Second, with high probability among these balls, there exists a ball such that the $k$ nearest neighbors of its center all have label 1. Similarly, there exists a ball such that the $k$ nearest neighbor of its center all have label 0.

Since $\mu$ is absolutely continuous with respect to Lebesgue measure in the neighborhood of $x$ and $\eta$ is continuous, then for any $m \in \mathbb{Z}^+$, we can always find $m$ balls $B(x_1, r_1), \ldots, B(x_m, r_m)$ such that (a) all $m$ balls are disjoint, and (b) for all $i \in \{1, \ldots, m\}$, we have $x_i \in B(x, \epsilon)$, $\mu(B(x_i, r_i)) > 0$ and $\eta(x) \in (0, 1)$ for $x \in B(x_i, r_i)$. For simplicity, we use $B_i$ to denote $B(x_i, r_i)$ and $c_i(n)$ to denote the number of points in $B_i \cap S_n$. Also, let $\mu_{\min} = \min_{i \in \{1, \ldots, m\}} \mu(B_i)$. Then by Hoeffding’s inequality, for each ball $B_i$ and for any $n > \frac{k+1}{\mu_{\min}}$, \[Pr[c_i(n) < k] \leq \exp\left(-2n\mu_{\min}^2/(k+1)^2\right),\]where the randomness comes from drawing sample $S_n$. Then taking the union bound over all $m$ balls, we have \[Pr[\exists i \in \{1, \ldots, m\} \text{ such that } c_i(n) < k] \leq m \exp\left(-2n\mu_{\min}^2/(k+1)^2\right),\]which implies that when $n > \max \left(\frac{k+1}{\mu_{\min}}, \frac{\log m - \log(\delta/3)(k+1)^2}{\mu_{\min}^2}\right)$, with probability at least $1 - \delta/3$, each of $B_1, \ldots, B_m$ contains at least $k$ points in $S_n$. An important consequence of the above result is that with probability at least $1 - \delta/3$, the set of $k$ nearest neighbors of each center $x_i$ of $B_i$ is completely different from another center $x_j$'s, so the labels of $x_i$'s $k$ nearest neighbors are independent of the labels of $x_j$'s $k$ nearest neighbors.
Now let $\eta_{\min,+} = \min_{x \in B_1 \cup \cdots \cup B_m} \eta(x)$ and $\eta_{\min,-} = \min_{x \in B_1 \cup \cdots \cup B_m} (1 - \eta(x))$. Both $\eta_{\min,+}$ and $\eta_{\min,-}$ are greater than 0 by the construction requirements of $B_1, \cdots, B_m$. For any $x_i$, 

\[
\Pr[x_i\,Si\,k\,\text{nearest neighbors all have label } 1] \geq \eta_{\min,+}^k
\]

Then, 

\[
\Pr[\exists i \in \{1, \cdots, m\} \text{ s.t. } x_i\,Si\,k\,\text{ nearest neighbor all have label } 1] \geq 1 - (1 - \eta_{\min,+}^k)^m,
\]

which implies when $m \geq \frac{\log \delta/3}{\log (1 - \eta_{\min,+}^k)}$, with probability at least $1 - \delta/3$, there exists an $x_i$ s.t. its $k$ nearest neighbors all have label 1. This $x_i$ is our $x_+$. 

Similarly, 

\[
\Pr[\exists i \in \{1, \cdots, m\} \text{ s.t. } x_i\,Si\,k\,\text{ nearest neighbor all have label } 0] \geq 1 - (1 - \eta_{\min,-}^k)^m,
\]

and when $m \geq \frac{\log \delta/3}{\log (1 - \eta_{\min,-}^k)}$, with probability at least $1 - \delta/3$, there exists an $x_i$ s.t. its $k$ nearest neighbors all have label 0. This $x_i$ is our $x_-$. 

Combining the results above, we show that for $n > \max \left( \frac{k+1}{\mu_{\min}}, \frac{\log m - \log (\delta/3)(k+1)^2}{\mu_{\min}} \right)$, 

\[
m \geq \max \left( \frac{\log \delta/3}{\log (1 - \eta_{\min,+}^k)}, \frac{\log \delta/3}{\log (1 - \eta_{\min,-}^k)} \right),
\]

with probability at least $1 - \delta$, the statement in Lemma A.3 is satisfied. 

\[\square\]

**Lemma A.3.** Let $x_0 \in X$. If $x_0 \in X_{r,\Delta}$ and if $\exists x \in S_n$ such that $d(x_0, x) < \Delta$, then $\rho(A_1(S_n, \cdot), x_0) \geq r$. Moreover, $A_1(S_n, \cdot)$ reports the correct label for $x_0$. 

\[\text{Proof. (Of Lemma A.3)}\]

Let $x'$ be any point in $S_n$ whose label is different from that of $x_0$. If $x_0 \in X_{r,\Delta}$, then by definition, $d(x_0, x') \geq 2r + \Delta$. Now if $\exists x \in S_n$ s.t. $d(x_0, x) < \Delta$, then again by the definition of $X_{r,\Delta}$, $x$ and $x_0$ will have the same label. 

Let $x'_0 = x_0 + x_{adv}$ denote any test case obtained from adversarially perturbing $x_0$, with $||x_{adv}||_2 \leq r$. Then by triangle inequality, $d(x'_0, x) \leq d(x'_0, x_0) + d(x_0, x) < \Delta + r$, and similarly $d(x'_0, x') \geq d(x'_0, x) - d(x_0, x_0) \geq \Delta + r$. Therefore $A_1(S_n, x'_0) = A_1(S_n, x_0)$, leading to the first part of the lemma. For the second part, observe that any $x'' \in B(x_0, \Delta)$ also lies in $X_{r,\Delta}$, which implies that $A_1(S_n, x_0)$ reports the correct label for $x_0$. The lemma follows. 

\[\square\]

\[\text{Proof. (Of Theorem 3.3)}\]

The contrapositive of Lemma A.3 says that if $\rho(A_1(S_n, \cdot), x_0) < r$, then either $x_0 \notin X_{r,\Delta}$ or $\exists x \in S_n$ s.t. $d(x_0, x) < \Delta$, i.e. $d(x_0, S_n) \geq \Delta$. By union bound, we have 

\[
\mathbb{1}(\rho(A_1(S_n, \cdot), x_0) < r) \leq \mathbb{1}(x_0 \notin X_{r,\Delta}) + \mathbb{1}(\exists x \in S_n \text{ s.t. } d(x_0, x) < \Delta)
\]

(6)

Now let $BAD(x_0, S_n)$ be the event that $\mathbb{1}(d(x_0, S_n) \geq \Delta)$. Taking expectation over $x_0 \sim \mu$ on both sides of (6), we obtain 

\[
\Pr(\{x_0|\rho(A_1(S_n, \cdot), x_0) < r\}) \leq (1 - \mu(X_{r,\Delta})) + \mathbb{E}_{x_0 \sim \mu}BAD(x_0, S_n)
\]

(7)

Recall that by definition, $R(A_1(S_n, \cdot), r, \mu) = \Pr(\{x_0|\rho(A_1(S_n, \cdot), x_0) \geq r\}$, therefore $\Pr(\{x_0|\rho(A_1(S_n, \cdot), x_0) < r\}) = 1 - R(A_1(S_n, \cdot), r, \mu)$, and thus for a fixed training sample $S_n$, (7) can be rewritten as: 

\[
R(A_1(S_n, \cdot), r, \mu) \geq \mu(X_{r,\Delta}) - \mathbb{E}_{x_0 \sim \mu}BAD(x_0, S_n).
\]

(8)
For the rest of the proof, we will provide an upper bound on the quantity $E_{S_n} \sim D \mathbb{E}_{x,y} \mu BAD(x_0, S_n)$; observe that since $\mu(\mathcal{X}, \Delta)$ does not depend on the training sample $S_n$, this will give us a lower bound on $E_{S_n} \sim D [R(A_1(S_n, \cdot), r, \mu)]$.

For any $x_0$, we have
\begin{equation}
E_{S_n} \sim D BAD(x_0, S_n) = E_{S_n} \sim D 1(d(x_0, S_n) \geq \Delta) = \Pr_{S_n} \sim D [d(x_0, S_n) \geq \Delta] = [1 - \mu(B^o(x_0, \Delta))]^n,
\end{equation}
which is the probability that none of sample points in $S_n$ is in $B(x_0, \Delta)$. Then,
\begin{equation}
E_{S_n} \sim D E_{x_0} \sim \mu BAD(x_0, S_n) = E_{x_0} \sim \mu E_{S_n} \sim D BAD(x_0, S_n) = E_{x_0} [1 - \mu(B^o(x_0, \Delta))]^n = d_{\mu, n^n}
\end{equation}
Moreover, by Markov’s inequality, with probability at least $1 - \delta$, $E_{x_0} \sim \mu BAD(x_0, S_n) < d_{\mu, n^n}/\delta$, which leads to the high probability bound in Theorem 3.4.

### B Proofs for Robust NN in Section 4

**Lemma B.1.** If for $x, x' \in \mathcal{X}$, $g(x) \neq g(x')$ and $d(x, x') \leq 2r$, then no classifier $f$ can be robustly correct at radius $r$ at both $x$ and $x'$.

**Proof.** Consider the mid-point $x_{\text{mid}}$ between $x$ and $x'$. If $f(x_{\text{mid}}) = g(x)$, then $x_{\text{mid}}$ is an adversarial example for $x'$, and vice versa. □

**Proof.** (Of Theorem 4.5) We shall prove by contradiction. Suppose $Racc_D(f, r) > \mu(V_{\text{max}}(2r))$. Let $V \subseteq \mathcal{X}$ be the set of points where $f$ is robustly correct at radius $r$. By definition, $Racc_D = \mu(V)$. By Lemma B.1, any two points $x, x' \in V$ where $g(x) \neq g(x')$ has to be more than $2r$ apart. Therefore $V$ should be a $2r$-separated set with respect to $g$. By the definition of $V_{\text{max}}$ in Eq. 2, $Racc_D = \mu(V) \leq \mu(V_{\text{max}}(2r))$, contradicting to our initial assumption. Therefore $Racc_D(f, r) \leq \mu(V_{\text{max}}(2r))$. □

**Proof.** (Of Lemma 4.1) Let $\Delta = d(x, x_0)$. First, $x_0$ is closer to $x$ than any $x_i$ in the training sample whose label $y_i$ is different from $g(x)$. Therefore, $A_1(S_{\text{labeled}}, x) = y_0 = g(x)$. Second, by triangle inequality, $d(x, x_i) \geq d(x_0, x_i) - d(x, x_0) > 2r + \Delta$. Then for all $x_{\text{adv}}$ such that $d(x, x_{\text{adv}}) \leq r$, by triangle inequality we have $d(x_{\text{adv}}, x_0) \leq r + \Delta < d(x_{\text{adv}}, x_i)$. As a result, $A_1(S_{\text{labeled}}, x_{\text{adv}})$ still equals to $y_0$. Hence, $A_1(S_{\text{labeled}}, \cdot)$ is robustly correct at radius $r$ at $x$. □

Before we prove Theorem 4.6, we establish a sufficient condition for a classifier to be robustly correct at a point $x \in \mathcal{X}$. Consider running the RobustNN algorithm on a labeled set $S_{\text{labeled}}$ of size $n$, an unlabeled validation set $S_{\text{valid}}$ of size $m$, a tolerance parameter $\Delta$ and a robustness parameter $r$. Let $A^{\text{robust}}_r(\cdot)$ be the classifier returned by RobustNN and $S_{\text{max}}$ be the subset of $S_{\text{labeled}}$ selected by RobustNN for training. Also, let $\mathcal{X}_{0, \Delta}$ represent the $(0, \Delta)$-confident interior. Then we have the following observation.

**Lemma B.2.** $A^{\text{robust}}_r(\cdot)$ is robustly correct at radius $r$ at all $x \in \text{Cover}(S_{\text{max}}, \Delta) \cap \mathcal{X}_{0, \Delta}$.

**Proof.** Consider any $x \in \text{Cover}(S_{\text{max}}, \Delta) \cap \mathcal{X}_{0, \Delta}$. Since $x \in \text{Cover}(S_{\text{max}}, \Delta)$, there exists a training point $(x, y_0) \in S_{\text{max}}$ such that $d(x, x_0) \leq \Delta$. Meanwhile, since $x \in \mathcal{X}_{0, \Delta}$ and $d(x, x_0) \leq \Delta$, by the definition of confident interior, $\eta(x) = \eta(x_0) = 0$ or $1$. As a result, $y_0 = g(x)$. □
Now suppose there exists a training point \((x_1, y_1) \in S_{\text{max}}\) such that \(d(x, x_1) \leq 2r + \Delta\), then by triangle inequality, \(d(x_0, x_1) \leq 2r + 2\Delta\). Since \(S_{\text{max}}\) is \(2r + 2\Delta\) separated, we must have \(y_0 = y_1\). In other words, \(y_0 \neq y_1\) implies \(d(x, x_1) > 2r + 2\Delta\). Therefore by Lemma \ref{lem:robust-cover}, \(A_{\text{robust}}(\cdot)\) is robustly correct at \(x\).

**Proof.** (Proof to Theorem \ref{thm:robust-cover}) By Lemma \ref{lem:robust-cover}, \(A_{\text{robust}}(\cdot)\) is robustly correct at radius \(r\) at \(x \in \text{Cover}(S_{\text{max}}, \Delta) \cap X_0,\Delta\). The main ingredient of the proof is to find a lowerbound for the expected value of \(\mu(\text{Cover}(S_{\text{max}}, \Delta))\), where the expectation is taken over the randomness of both the labeled training sample \(S_{\text{labeled}}\) and the unlabeled \(S_{\text{valid}}\). The rest follows from \(\mu(\text{Cover}(S_{\text{max}}, \Delta) \cap X_0,\Delta) \geq \mu(\text{Cover}(S_{\text{max}}, \Delta)) + \mu(X_0,\Delta) - 1\).

The proof of the lowerbound of \(\mathbb{E}_{S_{\text{labeled}}} \mathbb{E}_{S_{\text{valid}}} [\mu(\text{Cover}(S_{\text{max}}, \Delta))])\) consists of two parts. First, as the size of \(S_{\text{labeled}}\) increases, we will likely see some \((2r + 2\Delta)\)-separated subset of \(S_{\text{labeled}}\) such that its \(\Delta\)-cover almost contains \(V_{\text{max}}(2r + 2\Delta)\). By Lemma \ref{lem:max-cover}, there exists such a \((2r + 2\Delta)\)-separated subset \(S\) of \(S_{\text{labeled}}\) that

\[
\mu(V_{\text{max}}(2r + 2\Delta)) - \mathbb{E}_{S_{\text{labeled}}} [\mu(\text{Cover}(S, \Delta))] \leq c_{\Delta, \mu}(n). \tag{11}
\]

Second, \(\mu(\text{Cover}(S_{\text{max}}, \Delta))\) should not be much smaller than \(\mu(\text{Cover}(S, \Delta))\) since the empirical estimation of \(\mu(\text{Cover}(S_{\text{max}}, \Delta))\) is larger than that of \(\mu(\text{Cover}(S, \Delta))\). By Lemma \ref{lem:robust-cover} for the same \((2r + 2\Delta)\)-separated subset \(S\) of \(S_{\text{labeled}}\) constructed in Lemma \ref{lem:max-cover}:

\[
\mathbb{E}_{S_{\text{valid}}} [\mu(\text{Cover}(S, \Delta))] - \mathbb{E}_{S_{\text{valid}}} [\mu(\text{Cover}(S_{\text{max}}, \Delta))] \leq \epsilon(n, m, \delta) + 2\delta. \tag{12}
\]

Notice that Formula \ref{eq:lower-bound} is independent of \(S_{\text{valid}}\) as the construction of \(S\) only involves \(S_{\text{labeled}}\). Meanwhile, Formula \ref{eq:upper-bound} applies to any fixed \(S_{\text{labeled}}\). Therefore, assembling these two results together gives

\[
\mathbb{E}_{S_{\text{labeled}}} \mathbb{E}_{S_{\text{valid}}} [\mu(\text{Cover}(S_{\text{max}}, \Delta))] \geq \mu(V_{\text{max}}(2r + 2\Delta)) - \left[c_{\Delta, \mu}(n) + \epsilon(n, m, \delta) + 2\delta\right].
\]

The rest follows from \(\mu(\text{Cover}(S_{\text{max}}, \Delta) \cap X_0,\Delta) \geq \mu(\text{Cover}(S_{\text{max}}, \Delta)) + \mu(X_0,\Delta) - 1\). The high probability finite sample result is obtained by taking the union bound over the high probability results in Lemma \ref{lem:max-cover} and Lemma \ref{lem:robust-cover}.

**Lemma \ref{lem:max-cover}.** Let \(V_{\text{max}}(2r + 2\Delta)\) be the \((2r + 2\Delta)\)-separated subset of \(X\) as defined in \ref{lem:robust-cover}, and let \(S\) be a \((2r + 2\Delta)\)-separated subset of \(S_{\text{labeled}}\) such that \(S = \{(x, y) | (x, y) \in S_{\text{labeled}} \cap V_{\text{max}}(2r + 2\Delta) \land y = g(x)\}\). If \(|S_{\text{labeled}}| = n\), then

\[
\mu(V_{\text{max}}(2r + 2\Delta)) - \mathbb{E}_{S_{\text{labeled}}} [\mu(\text{Cover}(S, \Delta))] \leq c_{\Delta, \mu}(n), \tag{13}
\]

where \(c_{\Delta, \mu}(n) = \int_{V_{\text{max}}(2r + 2\Delta)} [1 - \frac{1}{2} \mu(B(x, \Delta))] \, d\mu(x)\). Moreover, with probability at least \(1 - \delta\),

\[
\mu(V_{\text{max}}(2r + 2\Delta)) - \mu(\text{Cover}(S, \Delta)) \leq \frac{c_{\Delta, \mu}(n)}{\delta}. \tag{14}
\]

**Proof.** (Of Lemma \ref{lem:max-cover}) For simplicity, we use \(V\) to denote \(V_{\text{max}}(2r + 2\Delta)\). A point \(x \in X\) is in \(\text{Cover}(S, \Delta)\) iff \(d(x, S) \leq \Delta\), where \(d(x, S) = \min_{x' \in S} d(x, x')\). Therefore,

\[
\mu(\text{Cover}(S, \Delta)) = \mathbb{E}_{x \sim \mu} 1[d(x, S) \leq \Delta]
\]
and
\[
1 - \mu(\text{Cover}(S, \Delta)) = \mathbb{E}_{x \sim \mu} \mathbb{I}[d(x, S) > \Delta]
\]
\[
= \int_{X \setminus V} \mathbb{I}[d(x, S) > \Delta]d\mu(x) + \int_{V} \mathbb{I}[d(x, S) > \Delta]d\mu(x)
\]
\[
\leq 1 - \mu(V) + \int_{V} \mathbb{I}[d(x, S) > \Delta]d\mu(x),
\]
which can be re-arranged into
\[
\mu(V) - \mu(\text{Cover}(S, \Delta)) \leq \int_{V} \mathbb{I}[d(x, S) > \Delta]d\mu(x).
\] (15)

Taking expectation of both sides of (15) with respect to the random sample \( S_{\text{labeled}} \), we obtain
\[
\mu(V) - \mathbb{E}_{S_{\text{labeled}}} \mu(\text{Cover}(S, \Delta)) \leq \mathbb{E}_{S_{\text{labeled}}} \left[ \int_{V} \mathbb{I}[d(x, S) > \Delta]d\mu(x) \right].
\]

Moreover,
\[
\mathbb{E}_{S_{\text{labeled}}} \left[ \int_{V} \mathbb{I}[d(x, S) > \Delta]d\mu(x) \right]
\]
\[
= \int_{V} \mathbb{E}_{S_{\text{labeled}}} \left[ \mathbb{I}[d(x, S) > \Delta] \right]d\mu(x)
\]
\[
= \int_{V} \text{Pr}[\forall (x', y') \in S_{\text{labeled}}, x' \not\in B(x, \Delta) \vee g(x') \neq y']d\mu(x)
\]
\[
\leq \int_{V} \left[ 1 - \frac{1}{2} \mu(B(x, \Delta)) \right]^{n}d\mu(x) = c_{\Delta, \mu}(n).
\]
The second equation follows from the observation that for \( x \in V, d(x, S) > \Delta \) iff no points in \( S_{\text{labeled}} \) are in \( B(x, \Delta) \) or the labels of points in \( B(x, \Delta) \cap S_{\text{labeled}} \) do not agree with the Bayes optimal classifier. The inequality in the last line holds because 1) all the sample points are independently drawn, and 2) for each sample point \((x', y')\), the probability of \( x' \in B(x, \Delta) \) and \( y' = g(x') \) is at least \( \frac{1}{2} \mu(B(x, \Delta)) \). Notice that by Markov’s inequality, with probability at least \( 1 - \delta \), \( \int_{V} \mathbb{I}[d(x, S) > \Delta]d\mu(x) \leq \frac{c_{\Delta, \mu}(n)}{\delta} \) and therefore
\[
\mu(V) - \mu(\text{Cover}(S, \Delta)) \leq \frac{c_{\Delta, \mu}(n)}{\delta}.
\]

\textbf{Lemma B.4.} Suppose \( |S_{\text{labeled}}| = n \) and \( |S_{\text{valid}}| = m \). Let \( S \) be the same \((2r+2\Delta)\)-separated subset of \( S_{\text{labeled}} \) constructed in Lemma \textit{B.3}. Then for any constant \( \delta \in (0, 1)\),
\[
\mathbb{E}_{S_{\text{valid}}} [\mu(\text{Cover}(S, \Delta))] - \mathbb{E}_{S_{\text{valid}}} [\mu(\text{Cover}(S_{\text{max}}, \Delta))] \leq \epsilon(n, m, \delta) + 2\delta,
\] (16)

where \( \epsilon(n, m, \delta) = \sqrt{\frac{2 \log(1/\delta) + n}{2m}} \). Moreover, with probability at least \( 1 - 2\delta \),
\[
\mu(\text{Cover}(S, \Delta)) - \mu(\text{Cover}(S_{\text{max}}, \Delta)) \leq \epsilon(n, m, \delta).
\] (17)
Proof. (Of Lemma 4) Let \( \bar{\mu}(\text{Cover}(S_{\text{max}}, \Delta)) \) denote the empirical estimation of \( \mu(\text{Cover}(S_{\text{max}}, \Delta)) \) on \( S_{\text{valid}} \), and let \( \mu(\text{Cover}(S, \Delta)) \) denote that of \( \mu(\text{Cover}(S, \Delta)) \). Notice that \( S \) is fixed regardless of \( S_{\text{valid}} \), therefore by Hoeffding’s inequality, with probability at least \( 1 - \delta \),

\[
\mu(\text{Cover}(S, \Delta)) - \bar{\mu}(\text{Cover}(S, \Delta)) \leq \sqrt{\frac{\log(1/\delta)}{2m}}.
\]

Meanwhile, there are \( 2^n \) possible subsets of \( S_{\text{labeled}} \). By Hoeffding’s inequality, for all \( S' \subseteq S_{\text{labeled}} \), with probability at least \( 1 - \delta \),

\[
\mu(\text{Cover}(S', \Delta)) - \bar{\mu}(\text{Cover}(S', \Delta)) \leq \sqrt{\frac{\log(1/\delta) + n}{2m}}.
\]

The dependence on \( n \) arises from taking the union bound over all \( 2^n \) subsets of \( S_{\text{labeled}} \). Since \( S_{\text{max}} \) is also a subset of \( S_{\text{labeled}} \), with probability at least \( 1 - \delta \),

\[
\bar{\mu}(\text{Cover}(S_{\text{max}}, \Delta)) - \mu(\text{Cover}(S_{\text{max}}, \Delta)) \leq \sqrt{\frac{\log(1/\delta) + n}{2m}}.
\]

Since \( \bar{\mu}(\text{Cover}(S, \Delta)) \leq \bar{\mu}(\text{Cover}(S_{\text{max}}, \Delta)) \) by how \( S_{\text{max}} \) is chosen, with probability at least \( 1 - 2\delta \),

\[
\mu(\text{Cover}(S, \Delta)) - \mu(\text{Cover}(S_{\text{max}}, \Delta)) \leq \sqrt{\frac{2\log(1/\delta) + n}{2m}} = \epsilon(n, m, \delta),
\]

which implies

\[
\mathbb{E}_{S_{\text{valid}}} \left[ \mu(\text{Cover}(S, \Delta)) \right] - \mathbb{E}_{S_{\text{valid}}} \left[ \mu(\text{Cover}(S_{\text{max}}, \Delta)) \right] \leq \epsilon(n, m, \delta) + 2\delta
\]

\( \Box \)

C A Schematic Illustration of the Benefits of RobustNN

In Section 4, we saw that \( A^*_1(\cdot) \) obtained by Algorithm 1 can reach the fundamental R-accuracy upper bound assuming \( \mu(\mathcal{X}_0, \Delta) = 1 \). The assumption implies \( \Pr_{x \sim \mu}(\eta(x) \in \{0, 1\}) = 1 \). In this section, we will see a schematic illustration of when \( A^*_1(\cdot) \) can perform better than standard 1-NN both with and without the assumption.

When \( \eta(x) \in (0, 1) \), we have shown in Section 3 that standard 1-NN is inherently non-robust as the sample size \( n \to \infty \). The left hand side of Figure 2 illustrates the cause. The Bayes optimal classifier \( g \) predicts 1 in the entire blue block, and block is far away from where \( g(x) = 0 \). Even so, there will always be training points with label 0 in the block, and the adversary can create an adversarial examples by moving the test case towards the nearest training point with label 0.

RobustNN only uses a subset of training sample that are \( (2r + 2\Delta) \)-separated. When \( \eta(x) = \Pr(y = 1|x) \) is above \( 1/2 \) by a margin, for example \( \eta(x) = 0.6 \), then the training points with label 0 are very likely the minority compared to those with label 1, and therefore RobustNN will only keep the training points with label 1, as the right hand side of Figure 2 shows. In this case, all test cases in the interior will be classified in a manner consistent with the Bayes Optimal and also robustly.
Figure 2: An illustration of what RobustNN does. The blue block represents a region where $g(x) = 1$. Noisy training points whose labels are different from the Bayes optimal’s prediction are removed. The 1-NN trained on such a subset is robustly correct in the blue block.

Figure 3: A pathological case of standard 1-NN. The points in the figure are training points. Points drawn from the blue block all have label 1 and those drawn from the orange region all have label 0. $\mu$(blue block) = 0.9, $\mu$(orange block) = 0.1, $\eta(x) = 1$ for $x$ in the blue dotted line and $\eta(x) = 0$ in the orange dotted line. The margin between the dotted line and the filled region is $\Delta$. Although in this case $\mu(X_{0,\Delta}) = 1$, the R-accuracy of standard 1-NN is still 0 because all test cases in the blue block are within distance $r$ of some training points in the orange block and vice versa. RobustNN can achieve R-accuracy of 0.9 instead.

When $\mu(X_{0,\Delta}) = 1$, RobustNN can asymptotically approach the fundamental R-accuracy upper bound. However, even in this case we can find pathological examples as shown in Figure 3 where standard 1-NN has almost no robustness. On the left hand side, all points in the blue block are within distance $r$ to some training point with label 0, and all point in the orange block are within distance $r$ to some training point with label 1, therefore standard 1-NN is not robust. RobustNN will remove these training points in the orange block from its training set and still be robustly correct in the blue block. Notice that this does not mean RobustNN always outputs a constant classifier; Figure 3 shows another pathological case for standard 1-NN, while this time RobustNN does not return a constant classifier.

D Visualization of Experiment Related Results.

Training subset selected by RobustNNApprox. Figure 5 shows the training set selected by RobustNNApprox on a halfmoon training set of size 2000. On the original training set, we see a noisy region between the two halfmoons where both red and blue points appear. RobustNNApprox cleans training points in this region so as to create a gap between the red and blue halfmoons, and the gap width increases with robustness parameter $r$.

Adversarial examples created on the MNIST dataset. Figure 6 shows a subset of original MNIST test images and their adversarial examples created with perturbation
Figure 4: Another pathological case for standard 1-NN when $\mu(\mathcal{X}_{0,\Delta}) = 1$. $\mu(\text{big blue block}) = \mu(\text{big orange block}) = 0.45$, $\mu(\text{small blue block}) = \mu(\text{small orange block}) = 0.05$, and other settings are identical to Figure 3. The distance between the small blue block and the small orange block is much greater than $r$. In this case, the R-accuracy of standard 1-NN is also 0. RobustNN will remove training points in small blue and small orange block, and return a classifier with R-accuracy 0.9.

Figure 5: Visualization of the halfmoon dataset. 1) Training sample of size $n = 2000$, 2) subset selected by robustNNApprox with $r = 0.1$, 3) subset selected by robustNNapprox with $r = 0.2$. 
magnitude $r = 3$. At $r = 3$, the digits in some adversarial examples of Digit 1 become ambiguous even by human perception. The adversarial examples of Digit 7 still look like 7 most of the time, but signs of artifacts can be identified. These observations suggest that at $r = 3$, the adversarial examples can already be close to the boundary of human perception. Therefore, the robust nearest neighbor classifiers in our experiment are successful as they still have non-trivial classification accuracy at such perturbation magnitude.