CERTIFIABLE DISTRIBUTIONAL ROBUSTNESS WITH PRINCIPLED ADVERSARIAL TRAINING

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Paper under double-blind review

ABSTRACT

Neural networks are vulnerable to adversarial examples and researchers have proposed many heuristic attack and defense mechanisms. We take the principled view of distributionally robust optimization, which guarantees performance under adversarial input perturbations. By considering a Lagrangian penalty formulation of perturbation of the underlying data distribution in a Wasserstein ball, we provide a training procedure that augments model parameter updates with worst-case perturbations of training data. For smooth losses, our procedure provably achieves moderate levels of robustness with little computational or statistical cost relative to empirical risk minimization. Furthermore, our statistical guarantees allow us to efficiently certify robustness for the population loss. We match or outperform heuristic approaches on supervised and reinforcement learning tasks.

1 INTRODUCTION

Consider the classical supervised learning problem, in which we minimize the expected loss \( \mathbb{E}_{P_0}[\ell(\theta; Z)] \) over a parameter \( \theta \in \Theta \), where \( Z \sim P_0 \) is a distribution on a space \( Z \) and \( \ell \) is a loss function. In many systems, robustness to changes in the data-generating distribution \( P_0 \) is desirable, either from covariate shifts, changes in the underlying domain (Ben-David et al., 2010), or adversarial attacks (Goodfellow et al., 2015; Kurakin et al., 2016). As deep networks become prevalent in modern performance-critical systems (e.g. perception for self-driving cars, automated detection of tumors), model failure increasingly leads to life-threatening situations; in these systems, it is irresponsible to deploy models whose robustness we cannot certify.

However, recent works have shown that neural networks are vulnerable to adversarial examples; seemingly imperceptible perturbations to data can lead to misbehavior of the model, such as misclassifications of the output (Goodfellow et al., 2015; Kurakin et al., 2016; Moosavi-Dezfooli et al., 2016; Nguyen et al., 2015). Subsequently, many researchers have proposed adversarial attack and defense mechanisms (Rozsa et al., 2016; Papernot et al., 2016a;b;c; Tramèr et al., 2017; Carlini & Wagner, 2017; Madry et al., 2017; He et al., 2017). While these works provide an initial foundation for adversarial training, there are no guarantees on whether proposed white-box attacks can find the most adversarial perturbation and whether there is a class of attacks such defenses can successfully prevent. On the other hand, verification of deep networks using SMT solvers (Katz et al., 2017a;b; Huang et al., 2017) provides formal guarantees on robustness but is NP-hard in general; this approach requires prohibitive computational expense even on small networks.

We take the perspective of distributionally robust optimization and provide an adversarial training procedure with provable guarantees on its computational and statistical performance. We postulate a class \( \mathcal{P} \) of distributions around the data-generating distribution \( Z \sim P_0 \) and consider the problem

\[
\min_{\theta \in \Theta} \sup_{P \in \mathcal{P}} \mathbb{E}_{P}[\ell(\theta; Z)].
\]

The choice of \( \mathcal{P} \) influences robustness guarantees and computability; we develop robustness sets \( \mathcal{P} \) with computationally efficient relaxations that apply even when the loss \( \ell \) is non-convex. We provide an adversarial training procedure that, for smooth \( \ell \), enjoys convergence guarantees similar to non-robust approaches while certifying performance even for the worst-case population loss \( \sup_{P \in \mathcal{P}} \mathbb{E}_{P}[\ell(\theta; Z)] \). On a simple implementation in Tensorflow, our method takes 5–10× as long as stochastic gradient methods for empirical risk minimization (ERM), matching runtimes for other
We show that our procedure—which learns to protect against adversarial perturbations in the training dataset—generalizes, allowing us to train a model that prevents attacks to the test dataset.

Let us overview our approach briefly. Let $c : \mathcal{Z} \times \mathcal{Z} \to \mathbb{R}_+$, where $c(z, z_0)$ represents the “cost” for an adversary to perturb the data point $z_0$ to the point $z$ (we typically use $c(z, z_0) = \|z - z_0\|_p^2$ for some $p \geq 1$). We then consider the robustness region $\mathcal{P} = \{ P : W_e(P, P_0) \leq \rho \}$, a $\rho$-neighborhood of the data generating distribution $P_0$ under the Wasserstein metric $W_e(\cdot, \cdot)$ (see Section 2 for a formal definition). This formulation of problem (1) is still intractable with arbitrary robustness levels $\rho$—at least with deep networks or other complex models—so we instead consider its Lagrangian relaxation for a fixed penalty parameter $\gamma \geq 0$, which results in the reformulation

$$\min_{\theta \in \Theta} \left\{ F(\theta) := \sup_{P} \{ \mathbb{E}_P[\ell(\theta; Z)] - \gamma W_e(P, P_0) \} = \mathbb{E}_P[\phi_\gamma(\theta; Z)] \right\} \quad (2a)$$

where $\phi_\gamma(\theta; z) := \sup_{z \in \mathcal{Z}} \{ \ell(\theta; z) - \gamma c(z, z_0) \}$. (We show the equalities in Proposition 1). That is, we have replaced the usual loss $\ell(\theta; Z)$ by the robust surrogate $\phi_\gamma(\theta; z)$; this surrogate (2b) allows adversarial perturbations of the data $z$, modulated by the magnitude of $\gamma$. We typically solve the penalty problem (2) with $P_0$ replaced by the empirical distribution $\hat{P}_n$, as $P_0$ is unknown (we refer to this as the penalty problem below).

The key feature of the penalty problem (2) is that moderate levels of robustness are achievable at essentially no computational or statistical cost for smooth losses $\ell$. More specifically, for large enough penalty $\gamma$ (by duality, small enough robustness $\rho$), the function $z \mapsto \ell(\theta; z) - \gamma c(z, z_0)$ in the robust surrogate (2b) is strongly concave and hence easy to compute if $\ell(\theta, z)$ is smooth in $z$. As a consequence, the stochastic gradient method applied to problem (2) has similar convergence guarantees as for non-robust methods (ERM). In Section 3 we give a certificate of robustness showing that we are approximately protected against all distributional perturbations satisfying $W_e(P, P_0) \leq \hat{\rho}_n$, where $\hat{\rho}_n$ is the achieved robustness for the empirical objective. We upper-bound the population worst-case scenario $\sup_{P : W_e(P, P_0) \leq \hat{\rho}_n} \mathbb{E}_P[\ell(\theta; Z)]$ by an efficiently computable empirical counterpart. These results suggest advantages of networks with smooth activations rather than ReLUs. We experimentally verify our results in Section 4 and show that, even for non-smooth losses, we are able to match or achieve state-of-the-art performance on a variety of adversarial attacks.

**Robust optimization and adversarial training** The standard robust-optimization approach is to minimize losses of the form $\sup_{u \in U} \ell(\theta; z + u)$, where $U$ is some uncertainty set (Ben-Tal et al., 2009; Ratliff et al., 2006; Xu et al., 2009). Unfortunately, this approach is intractable except for specially structured losses, such as the composition of a linear and simple convex function (Ben-Tal et al., 2009; Xu et al., 2009, 2012). Nevertheless, this robust approach underlies recent advances in adversarial training (Szegedy et al., 2013; Goodfellow et al., 2015; Papernot et al., 2016; Carlini & Wagner, 2017; Madry et al., 2017), which consider heuristically perturbing data during a stochastic optimization procedure. One such heuristic uses a locally linearized loss function (proposed with $p = \infty$ as the “fast gradient sign method” (Goodfellow et al., 2015)):

$$\Delta_{\ell_x}(\theta) := \arg\max_{\|\eta\|_p \leq \epsilon} \{ \nabla_x \ell(\theta; x_i, y_i)^T \eta \} \text{ and perturb } x_i \rightarrow x_i + \Delta_{\ell_x}(\theta). \quad (3)$$

One form of adversarial training simply trains on these perturbed losses (Goodfellow et al., 2015; Kurakin et al., 2016), and many others perform iterated variants (Papernot et al., 2016; Tramèr et al., 2017; Carlini & Wagner, 2017; Madry et al., 2017). Madry et al. (2017) observe that these procedures attempt to optimize the objective $\mathbb{E}_{P_0}[\sup_{\|u\|_p \leq \epsilon} \ell(\theta; Z + u)]$, a constrained version of the penalty problem (2). This notion of robustness is typically intractable: the inner supremum is generally non-concave in $u$, so it is unclear whether model-fitting with these techniques converges, and there are possibly worst-case perturbations these techniques do not find. Indeed, when deep networks use ReLU activations, it is NP-hard to find worst-case perturbations, suggesting difficulties for fast and iterated heuristics (see Lemma 2 in Appendix B). Smoothness, which can be obtained in standard deep architectures with exponential linear units (ELU’s) (Clevert et al., 2015), allows us to find Lagrangian worst-case perturbations with low computational cost.

**Distributionally robust optimization** To situate the current work, we review some of the substantial body of work on robustness and learning. The choice of $\mathcal{P}$ in the robust objective (1) affects
both the richness of the uncertainty set we wish to consider as well as the tractability of the resulting optimization problem. Previous approaches to distributional robustness have considered finite-dimensional parametrizations for $\mathcal{P}$, such as constraint sets for moments, support, or directional deviations (Chen et al., 2007; Delage & Ye, 2010; Goh & Sim, 2010), as well as non-parametric distances for probability measures such as $\ell$-divergences (Ben-Tal et al., 2013; Bertsimas et al., 2013; Miyato et al., 2015; Lam & Zhou, 2015; Duchi et al., 2016; Namkoong & Duchi, 2016), and Wasserstein distances (Blanchet et al., 2016; Esfahani & Kuhn, 2015; Shafieezadeh-Abadeh et al., 2015). In contrast to $\ell$-divergences (e.g. $\chi^2$- or Kullback-Leibler divergences) which are effective when the support of the distribution $P_0$ is fixed, a Wasserstein ball around $P_0$ includes distributions $Q$ with different support and allows (in a sense) robustness to unseen data.

Many authors have studied tractable classes of uncertainty sets $\mathcal{P}$ and losses $\ell$. For example, Ben-Tal et al. (2013) and Namkoong & Duchi (2015) use convex optimization approaches for $\ell$-divergence balls. For worst-case regions $\mathcal{P}$ formed by Wasserstein balls, Esfahani & Kuhn (2015), Shafieezadeh-Abadeh et al. (2015) and Blanchet et al. (2016) show how to convert the saddle-point problem (1) to a regularized ERM problem, but this is possible only for a limited class of convex losses $\ell$ and costs $c$. In this work, we treat a much larger class of losses and costs and provide direct solution methods for a Lagrangian relaxation of the saddle-point problem (1).

2 Proposed Approach

Our approach is based on the following simple insight: assume that the function $z \mapsto \ell(\theta; z)$ is smooth, meaning there is some $L$ for which $\nabla \ell(\theta; z)$ is $L$-Lipschitz. Then for any $c : Z \times Z \to \mathbb{R}_+$ strongly convex in its first argument, a Taylor expansion yields

$$\ell(\theta; z') - \gamma c(z', z_0) \leq \ell(\theta; z) - \gamma c(z, z_0) + \langle \nabla_z (\ell(\theta; z) - \gamma c(z, z_0)), z' - z \rangle + \frac{L - \gamma}{2} \|z - z'\|_2^2. \tag{4}$$

For $\gamma \geq L$ this is precisely the first-order condition for concavity of $z \mapsto (\ell(\theta; z) - \gamma c(z, z_0))$. Thus, whenever the loss is smooth enough in $z$ and the penalty $\gamma$ is large enough (corresponding to less robustness), computing the surrogate (26) is a strongly-concave optimization problem.

We leverage the insight (4) to show that as long as we do not require too much robustness, this strong concavity approach (4) provides a computationally efficient and principled approach for robust optimization problems (1). Our starting point is a duality result for the minimax problem (1) and its Lagrangian relaxation for Wasserstein-based uncertainty sets, which makes the connections between distributional robustness and the “lazy” surrogate (26) clear. We then show (Section 2.1) how stochastic gradient descent methods can efficiently find minimizers (in the convex case) or approximate stationary points (when $\ell$ is non-convex) for our relaxed robust problems.

Wasserstein robustness and duality Wasserstein distances define a notion of closeness between distributions. Let $Z \subset \mathbb{R}^m$ be convex, and let $(Z, A, P_0)$ be a probability space. Let the transportation cost $c : Z \times Z \to [0, \infty)$ be nonnegative, continuous, and convex in its first argument and satisfy $c(z, z) = 0$. For example, for a differentiable convex $h : Z \to \mathbb{R}$, the Bregman divergence $c(z, z_0) = h(z) - h(z_0) - \langle \nabla h(z_0), z - z_0 \rangle$ satisfies these conditions. For probability measures $P$ and $Q$ supported on $Z$, let $\Pi(P, Q)$ denote their couplings, meaning measures $M$ on $Z^2$ with $M(A, Z) = P(A)$ and $M(Z, A) = Q(A)$. The Wasserstein distance between $P$ and $Q$ is

$$W_c(P, Q) := \inf_{M \in \Pi(P, Q)} \mathbb{E}_M[c(Z, Z')].$$

For $\rho \geq 0$ and data generating distribution $P_0$, we consider the Wasserstein form of the robust problem (1), with $\mathcal{P} = \{P: W_c(P, P_0) \leq \rho\}$, and its Lagrangian relaxation (2) with $\gamma \geq 0$. The following duality result, which we prove in Appendix C.1 gives the equality (2) and an analogous result for the worst-case problem (1).

**Proposition 1.** Let $\ell : \Theta \times Z \to \mathbb{R}$ and $c : Z \times Z \to \mathbb{R}_+$ be continuous. Let $\phi_c(\theta; z_0) = \sup_{z \in Z} \{\ell(\theta; z) - \gamma c(z, z_0)\}$ be the robust surrogate (26). For any distribution $Q$ and any $\rho > 0$, the following duality result, which we prove in Appendix C.1 gives the equality (2) and an analogous result for the worst-case problem (1).

$$\sup_{P: W_c(P, Q) \leq \rho} \mathbb{E}_P[\ell(\theta; Z)] = \inf_{\gamma \geq 0} \{\sup_{P: W_c(P, Q) \leq \rho} \mathbb{E}_P[\ell(\theta; Z)] - \gamma W_c(P, Q)\}, \tag{5}$$

and for any $\gamma \geq 0$, we have

$$\sup_{P} \{\mathbb{E}_P[\ell(\theta; Z)] - \gamma W_c(P, Q)\} = \mathbb{E}_Q[\phi_c(\theta; Z)]. \tag{6}$$
Algorithm 1  Distributionally robust optimization with adversarial training

INPUT: Sampling distribution $P_0$, constraint sets $\Theta$ and $Z$, stepsize sequence $\{\alpha_t > 0\}_{t=0}^{T-1}$
for $t = 0, \ldots, T - 1$ do
Sample $z_t^* \sim P_0$ and find an $\epsilon$-approximate maximizer $\tilde{z}_t^*$ of $\ell(\theta_t^*; z) - \gamma c(z, z_t^*)$
$\theta_{t+1} \leftarrow \text{Proj}_\Theta(\theta_t^* - \alpha_t \nabla_\theta \ell(\theta_t^*; \tilde{z}_t^*))$

Leveraging the insight (4), we give up the requirement that we wish a prescribed amount $\rho$ of robustness (solving the worst-case problem (1) for $P = \{P : W_c(P, P_0) \leq \rho\}$) and focus instead on the Lagrangian penalty problem (2) and its empirical counterpart

$$
\text{minimize}_{\theta \in \Theta} \left\{ F_n(\theta) := \sup_P \left\{ \mathbb{E}[\ell(\theta; Z)] - \gamma W_c(P, \hat{P}_n) \right\} = \mathbb{E}_{\hat{P}_n} [\phi_\gamma(\theta; Z)] \right\}, \quad (7)
$$

2.1 OPTIMIZING THE ROBUST LOSS BY STOCHASTIC GRADIENT DESCENT

We now develop stochastic gradient-type methods for the relaxed robust problem (7), developing a number of results that make clear the computational benefits of relaxing the strict robustness requirements of formulation (5). We begin with the assumptions we require for our development, which roughly quantify the amounts of robustness we can provide.

Assumption A. The function $c : Z \times Z \to \mathbb{R}_+$ is continuous. For each $z_0 \in Z$, $c(\cdot, z_0)$ is 1-strongly convex with respect to the norm $\|\cdot\|$.

To guarantee that the robust formulation (2b) is tractably computable, we also require a few smoothness assumptions. Let $\|\cdot\|_\Theta$ be the dual norm to $\|\cdot\|$; we abuse notation by using the same norm $\|\cdot\|$ on $\Theta$ and $Z$, though the specific norm is clear from context.

Assumption B. The loss $\ell : \Theta \times Z \to \mathbb{R}$ satisfies the Lipschitzian smoothness conditions

$$
\| \nabla_\theta \ell(\theta; z) - \nabla_\theta \ell(\theta'; z) \|_{\|\cdot\|_\Theta} \leq L_{\theta \theta} \| \theta - \theta' \|, \quad \| \nabla_z \ell(\theta; z) - \nabla_z \ell(\theta'; z) \|_{\|\cdot\|_Z} \leq L_{\theta z} \| z - z' \|, \\
\| \nabla_\theta \ell(\theta; z) - \nabla_\theta \ell(\theta'; z) \|_{\|\cdot\|_\Theta} \leq L_{\theta \theta} \| \theta - \theta' \|, \quad \| \nabla_z \ell(\theta; z) - \nabla_z \ell(\theta'; z) \|_{\|\cdot\|_Z} \leq L_{\theta z} \| \theta - \theta' \| .
$$

These properties are enough to guarantee both (i) the well-behavedness of the robust surrogate $\phi_\gamma$ and (ii) its efficient computability. Making point (i) precise, the following lemma shows (more generically) that if $\gamma$ is large enough and Assumptions A and B hold, the surrogate $\phi_\gamma$ is still smooth.

Lemma 1. Let $f : \Theta \times Z \to \mathbb{R}$ be differentiable and $\lambda$-strongly concave in $z$ with respect to the norm $\|\cdot\|$, and define $\overline{f}(\theta) = \sup_{z \in Z} f(\theta, z)$. Let $g_\theta(z, \theta) = \nabla_\theta f(\theta, z)$ and $g_z(z, \theta) = \nabla_z f(\theta, z)$, and assume $g_\theta$ and $g_z$ satisfy the Lipschitz conditions of Assumption B. Then $\tilde{f}$ is differentiable, and letting $z^*(\theta) = \arg\max_{z \in Z} f(\theta, z)$, we have $\nabla \tilde{f}(\theta) = g_\theta(\theta, z^*(\theta))$. Moreover,

$$
\| z^*(\theta_1) - z^*(\theta_2) \| \leq \frac{L_{z \theta}}{\lambda} \| \theta_1 - \theta_2 \| \quad \text{and} \quad \| \nabla \tilde{f}(\theta) - \nabla \tilde{f}(\theta') \|_{\|\cdot\|_Z} \leq \left( L_{\theta \theta} + \frac{L_{\theta z} L_{z \theta}}{\lambda} \right) \| \theta - \theta' \| .
$$

See Section [2] for the proof. Focusing on the $\ell_2$-norm case, an immediate application of Lemma 1 shows that if Assumption B holds, then $\phi_\gamma$ has $L = L_{\theta \theta} + \frac{L_{\theta z} L_{z \theta}}{\gamma - L_{z z}^+}$-Lipschitz gradients, and

$$
\nabla_\theta \phi_\gamma(\theta; z_0) = \nabla_\theta v(\theta; \gamma c(z, z_0)) \quad \text{where} \quad z^*(z_0, \theta) = \arg\max_{z \in Z} \{ \ell(\theta; z) - \gamma c(z, z_0) \}.
$$

This motivates Algorithm 1 a stochastic-gradient approach for the penalty problem (7). The benefits of Lagrangian relaxation become clear here: for $\ell(\theta; z)$ smooth in $z$ and $\gamma$ large enough, gradient ascent on $\ell(\theta^*; z) - \gamma c(z, z^*)$ in $z$ converges linearly and we can compute (approximate) $\tilde{z}^*$ efficiently.

Convergence properties of Algorithm 1 depend on the loss $\ell$. When $\ell$ is convex in $\theta$ and $\gamma$ is large enough that $z \mapsto (\ell(\theta; z) - \gamma c(z, z_0))$ is concave for all $(\theta, z_0) \in \Theta \times Z$, we have a stochastic monotone variational inequality, which is efficiently solvable [Juditsky et al., 2011; Chen et al., 2014] with convergence rate $1/\sqrt{T}$. When the loss $\ell$ is nonconvex in $\theta$, the following theorem guarantees convergence to a stationary point of problem (7) at the same rate when $\gamma \geq L_{z z}^+$. Recall that $F(\theta) = \mathbb{E}_{P_0}[\phi_\gamma(\theta; Z)]$ is the robust surrogate objective for the Lagrangian relaxation (2).
Our main result in this section is a data-dependent upper bound for the worst-case population objective. Second, we show in Section 3.2 that adversarial perturbations by solving (7). Our bound is efficiently computable and hence \( \rho \) allows us to prevent attacks on the test set. Our subsequent results hold uniformly over the space of parameters \( \theta \in \Theta \), including \( \theta_{\text{WDM}} \), the output of the stochastic gradient descent procedure in Section 2.1. Our first main result, presented in Section 3.1, gives a data-dependent upper bound on the population worst-case objective \( \sup_{P:W_{c}(P,P_0)\leq \rho} \mathbb{E}_{P}[\ell(\theta;Z)] \) for any arbitrary level of robustness \( \rho \); this bound is optimal for \( \rho = \hat{\rho}_n \), the level of robustness achieved for the empirical distribution by solving (7). Our bound is efficiently computable and hence certifies a level of robustness for the worst-case population objective. Second, we show in Section 3.2 that adversarial perturbations on the training set (in a sense) generalize: solving the empirical penalty problem (7) guarantees a similar level of robustness as directly solving its population counterpart (2).

3 ROBUSTNESS CERTIFICATE AND GENERALIZATION

From results in the previous section, Algorithm 1 provably learns to protect against adversarial perturbations of the form (7) on the training dataset. Now, we show that such procedures generalize, allowing us to prevent attacks on the test set. Our subsequent results hold uniformly over the space of parameters \( \theta \in \Theta \), including \( \theta_{\text{WDM}} \), the output of the stochastic gradient descent procedure in Section 2.1. Our first main result, presented in Section 3.1, gives a data-dependent upper bound on the population worst-case objective \( \sup_{P:W_{c}(P,P_0)\leq \rho} \mathbb{E}_{P}[\ell(\theta;Z)] \) for any arbitrary level of robustness \( \rho \); this bound is optimal for \( \rho = \hat{\rho}_n \), the level of robustness achieved for the empirical distribution by solving (7). Our bound is efficiently computable and hence certifies a level of robustness for the worst-case population objective. Second, we show in Section 3.2 that adversarial perturbations on the training set (in a sense) generalize: solving the empirical penalty problem (7) guarantees a similar level of robustness as directly solving its population counterpart (2).

3.1 Robustness Certificate

Our main result in this section is a data-dependent upper bound for the worst-case population objective: \( \sup_{P:W_{c}(P,P_0)\leq \rho} \mathbb{E}_{P}[\ell(\theta;Z)] \leq \gamma \rho + \mathbb{E}_{P_{\rho}[\delta_{\star}(\theta;Z) + O(1/\sqrt{n}) \text{ for all } \theta \in \Theta \text{ with high probability. To make this rigorous, fix } \gamma > 0 \text{, and consider the worst-case perturbation, typically called the transportation map or Monge map (Villani 2009).}}

\[
T_{\gamma}(\theta; z_0) := \arg\max_{z \in \mathbb{R}} \{\ell(\theta; z) - \gamma c(z, z_0)\}.
\]

Under our assumptions, it is easy to compute \( T_{\gamma} \) whenever \( \gamma \geq L_{zz} \). Letting \( \delta_{\star} \) denote the point mass at \( z \), Proposition 1 (or Kantorovich duality (Villani 2009, Chs. 9–10)) shows the empirical maximizers of the Lagrangian formulation (5) are attained by

\[
P_{\rho}^n(\theta) := \arg\max_{P} \left\{ \mathbb{E}_{P}[\ell(\theta; Z)] - \gamma W_{c}(P, \hat{P}_n) \right\} = \frac{1}{n} \sum_{i=1}^{n} \delta_{T_{\gamma}(\theta; Z_i)} \text{ and } \hat{\rho}_n(\theta) := W_{c}(P_{\rho}^n(\theta), \hat{P}_n) = \mathbb{E}_{\hat{P}_n}[c(T_{\gamma}(\theta; Z), Z)].
\]

Our results will imply, in particular, that the empirical worst-case objective \( \mathbb{E}_{P_{\rho}^n}[\ell(\theta; Z)] \) gives a certificate of robustness to (population) Wasserstein perturbations of up to level \( \hat{\rho}_n \). The equalities (9) show that \( \mathbb{E}_{P_{\rho}^n}[\ell(\theta; Z)] \) is efficiently computable, thereby providing a data-dependent performance guarantee for the worst-case population loss.
Our bound relies on the usual covering numbers for the model class \( \{ \ell(\theta; \cdot) : \theta \in \Theta \} \) as the notion of complexity (e.g., [van der Vaart & Wellner 1996]), so, despite the infinite-dimensional problem \( \mathbf{7} \), we retain the same uniform convergence guarantees typical of empirical risk minimization. Recall that for a set \( V \), a collection \( v_1, \ldots, v_N \) is an \( \varepsilon \)-cover of \( V \) in norm \( \| \cdot \| \) if for each \( v \in V \), there exists \( v_i \) such that \( \| v - v_i \| \leq \varepsilon \). The covering number of \( V \) with respect to \( \| \cdot \| \) is

\[
N(V, \varepsilon, \| \cdot \|) := \inf \{ N \in \mathbb{N} \mid \text{there is an } \varepsilon\text{-cover of } V \text{ with respect to } \| \cdot \| \}.
\]

For \( \mathcal{F} := \{ \ell(\theta, \cdot) : \theta \in \Theta \} \) equipped with the \( L^\infty(\mathcal{Z}) \) norm \( \| f \|_{L^\infty(\mathcal{Z})} := \sup_{z \in \mathcal{Z}} |f(z)| \), we state our results in terms of \( \| \|_{L^\infty(\mathcal{Z})} \) covering numbers of \( \mathcal{F} \). To ease notation, we let

\[
e_{n,1}(t) := \gamma b_1 \sqrt{\frac{M_1}{n}} \int_0^1 \sqrt{\log N(\mathcal{F}, M_\ell, \| \cdot \|_{L^\infty(\mathcal{Z})})} \, d\ell + b_2 M_\ell \sqrt{\frac{t}{n}}
\]

where \( b_1, b_2 \) are numerical constants. See Section C.3 for its proof.

**Theorem 3.** Assume that \( |\ell(\theta; z)| \leq M_\ell \) for all \( \theta \in \Theta \) and \( z \in \mathcal{Z} \). Then, for a fixed \( t > 0 \) and numerical constants \( b_1, b_2 > 0 \), with probability at least \( 1 - e^{-t} \), simultaneously for all \( \theta \in \Theta \), \( \eta \geq 0 \), and \( \rho \geq 0 \),

\[
\sup_{P:W_c(P,P_0) \leq \rho} \mathbb{E}_P[\ell(\theta; Z)] \leq \eta \rho + \mathbb{E}_{\widehat{P}_n}[\phi_\eta(\theta; Z)] + e_{n,1}(t). \tag{10}
\]

In particular, if \( \rho = \widehat{\rho}_n \) then with probability at least \( 1 - e^{-t} \), for all \( \theta \in \Theta \)

\[
\sup_{P:W_c(P,P_0) \leq \widehat{\rho}_n(\theta)} \mathbb{E}_P[\ell(\theta; Z)] \leq \sup_{P:W_c(P,P_0) \leq \widehat{\rho}_n(\theta)} \mathbb{E}_P[\ell(\theta; Z)] + e_{n,1}(t). \tag{11}
\]

A key consequence of Theorem 3 is that setting \( \eta = \gamma \) in the bound \( \mathbf{10} \), \( \gamma \rho + \mathbb{E}_{\widehat{P}_n}[\phi_\gamma(\theta; Z)] \) certifies robustness for the worst-case population objective at any level \( \rho \). When \( \rho = \widehat{\rho}_n(\theta) \), duality shows that \( \eta = \gamma \) minimizes the right hand side of the bound \( \mathbf{10} \), and

\[
\mathbb{E}_{\widehat{P}_n}[\phi_\gamma(\theta; Z)] + \gamma \widehat{\rho}_n(\theta) = \sup_{P:W_c(P,P_0) \leq \widehat{\rho}_n(\theta)} \mathbb{E}_P[\ell(\theta; Z)] = \mathbb{E}_P[\ell(\theta; Z)]. \tag{12}
\]

(See Section C.3 for a proof of these equalities.) The bound \( \mathbf{11} \) gives a tight bound on performance for the \( \widehat{\rho}_n \)-robustness of the population loss, and the certificate \( \mathbf{12} \) is easy to compute via expression \( \mathbf{9} \): the transportation mappings \( T(\theta, Z_i) \) are efficiently computable for large enough \( \gamma \), as noted in Section 2.1, and \( \widehat{\rho}_n = W_c(P^*_n, P^n) = \mathbb{E}_{\widehat{P}_n}[c(T(\theta, Z), Z)] \).

When the parameter set \( \Theta \) is finite dimensional (\( \Theta \subset \mathbb{R}^d \)), Theorem 3 provides a robustness guarantee scaling with \( d \) in spite of the infinite-dimensional Wasserstein penalty. Assuming there exist \( \theta_0 \in \Theta, M_{\theta_0} < \infty \) such that such that \( |\ell(\theta_0; z)| \leq M_{\theta_0} \) for all \( z \in \mathcal{Z} \), we have the following corollary (see Section C.3 for a proof).

**Corollary 1.** Let \( \ell(\cdot; z) \) be \( L \)-Lipschitz with respect to some norm \( \| \cdot \| \) for all \( z \in \mathcal{Z} \). Assume that \( \Theta \subset \mathbb{R}^d \) satisfies \( \text{diam}(\Theta) = \sup_{\theta, \theta' \in \Theta} \| \theta - \theta' \| < \infty \). Then, the bounds \( \mathbf{10} \) and \( \mathbf{11} \) hold with

\[
e_{n,1}(t) = b_1 \sqrt{d (L \text{diam}(\Theta) + M_{\theta_0})} + b_2 (L \text{diam}(\Theta) + M_{\theta_0}) \sqrt{t/n}
\]

for some numerical constants \( b_1, b_2 > 0 \).

### 3.2 Generalization of Adversarial Examples

We can also show that the level of robustness on the training set generalizes. Our starting point is Lemma 1 which shows that \( T_\gamma(\cdot; z) \) is smooth under Assumptions A and B

\[
\| T_\gamma(\theta_1; z) - T_\gamma(\theta_2; z) \| \leq \frac{L_{zz}}{\gamma - L_{zz}} \| \theta_1 - \theta_2 \| \tag{13}
\]

for all \( \theta_1, \theta_2 \), where we recall that \( L_{zz} \) is the Lipschitz constant of \( \nabla_z \ell(\theta; z) \). Leveraging this smoothness, we show that \( \widehat{\rho}_n(\theta) = \mathbb{E}_{\widehat{P}_n}[c(T_\gamma(\theta; Z), Z)] \), the level of robustness achieved for the empirical problem, concentrates uniformly around its population counterpart.
Theorem 4. Let $Z \subset \{z \in \mathbb{R}^m : \|z\| \leq M_z\}$ so that $\|Z\| \leq M_z$ almost surely and assume either that (i) $c(\cdot, \cdot)$ is $L_c$-Lipschitz over $Z$ with respect to the norm $\|\|$ in each argument, or (ii) that $\ell(\theta, z) \in [0, M_\ell]$ and $z \mapsto \ell(\theta, z)$ is $\gamma L_c$-Lipschitz for all $\theta \in \Theta$. If Assumptions A and B hold, then with probability at least $1 - e^{-1}$,

$$
sup_{\theta \in \Theta} |E_{P_\theta}[c(T_\gamma(\theta; Z), Z)] - E_{P_\theta}[c(T_\gamma(\theta; Z), Z)]| \leq 4D \sqrt{\frac{1}{n} \left(t + \log N \left(\Theta, \frac{\gamma - L_c}{4L_c L_{z\theta}^\ell} \|\|\right)\right)},$$

where $B = L_c M_z$ under assumption (i) and $B = M_\ell / \gamma$ under assumption (ii).

See Section C.5 for the proof. For $\Theta \subset \mathbb{R}^d$, we have $\log N(\Theta, \epsilon, \|\|) \leq d \log(1 + \frac{\text{diam}(\Theta)}{\epsilon})$ so that the bound (14) gives the usual $\sqrt{d/n}$ generalization rate for the distance between adversarial perturbations and natural examples. Another consequence of Theorem 4 is that the bound (14) is positive as long as the loss $\ell$ is not completely invariant to data. To see this, note from the optimality conditions for $T_\gamma(\theta; Z)$ that $E_{P_\theta}[c(T_\gamma(\theta; Z), Z)] = 0$ iff $\nabla z \ell(\theta; z) = 0$ almost surely, and hence for large enough $n$, we have $\hat{\rho}_n(\theta) > 0$ by the bound (14).

4 Experiments

Our technique for distributionally robust optimization with adversarial training extends beyond supervised learning. To that end, we present empirical evaluations on supervised and reinforcement learning tasks where we compare performance with empirical risk minimization (ERM) and, where appropriate, models trained with the fast-gradient method (FGM) (Goodfellow et al. 2015), its iterated variant (IFGM) (Kurakin et al. 2016), and the projected-gradient method (PGM) (Madry et al. 2017). PGM augments stochastic gradient steps for the parameter $\theta$ with projected gradient ascent over $x \mapsto \ell(\theta; x, y)$, iterating (for data point $x_i, y_i$)

$$
\Delta x_{i+1}^t(\theta) := \arg\max_{\|\eta\|_p \leq \epsilon} \{\nabla x \ell(\theta; x_i^t, y_i)^T \eta\} \quad \text{and} \quad x_{i+1}^t := \Pi_{B_{c,p}(x_i)} \{x_i^t + \alpha_t \Delta x_i^t(\theta)\}
$$

for $t = 1, \ldots, T_{\text{adv}}$, where $\Pi$ denotes projection onto $B_{c,p}(x_i) := \{x : \|x - x_i\|_p \leq \epsilon\}$. We use the squared Euclidean cost $c(z, z') := \|z - z'\|^2$ for WRM and $p = 2$ for FGM, IFGM, PGM training in all experiments; we test against adversarial perturbations with respect to the norms $p = 2, \infty$. We use $T_{\text{adv}} = 15$ iterations for all iterative methods (IFGM, PGM, and WRM) in training and attacks. Larger adversarial budgets correspond to smaller $\gamma$ for WRM and larger $\epsilon$ for other models.

In Section 4.1, we visualize differences between our approach and ad-hoc methods to illustrate the benefits of certified robustness. In Section 4.2, we consider a supervised learning problem for MNIST where we adversarially perturb the test data. Finally, we consider a reinforcement learning problem in Section 4.3, where the Markov decision process used for training differs from that for testing.

4.1 Visualizing the benefits of certified robustness

For our first experiment, we generate synthetic data $Z = (X, Y) \sim P_0$ by $X_i \overset{i.i.d.}{\sim} \mathcal{N}(0, I_2)$ with labels $Y_i = \text{sign}(\|X\|_2 - \sqrt{2})$, where $X \in \mathbb{R}^2$ and $I_2$ is the identity matrix in $\mathbb{R}^2$. Furthermore, to create a wide margin separating the classes, we remove data with $\|X\|_2 \in (\sqrt{2}/1.3, 1.3\sqrt{2})$. We train a small neural network with 2 hidden layers of size 4 and 2 and either all ReLU or all ELU activations between layers, comparing our approach (WRM) with ERM and the 2-norm FGM. For our approach, we use $\gamma = 0.5$ and to make fair comparisons with FGM, we use

$$
e^2 = \hat{\rho}_n(\theta_{\text{WRM}}) = W_c(P_{c,n}(\theta_{\text{WRM}}), \hat{P}_n) = E_{P_\theta} [c(T(\theta_{\text{WRM}}, Z), Z)],$$

for the fast-gradient perturbation magnitude $\epsilon$, where $\theta_{\text{WRM}}$ is the output of Algorithm 1.

Figure 1 illustrates the classification boundaries for the three training procedures over the ReLU-activated (Figure 1(a)) and ELU-activated (Figure 1(b)) models. Since 70% of the data are of the...
ELU model

where $\hat{\theta}$ represents the neighborhood of the nominal input, which ensures stability of the model. Figure 3(a) shows that $\hat{\theta}$ provides robustness to $\infty$-norm and $2$-norm fast gradient attacks. We provide further evidence in Appendix A.1.

Next we study stability of the loss surface with respect to perturbations to inputs. First, consider the test-time penalty for the robustness levels ($\epsilon$ and $\gamma$) used for training the adversarial models.

It is thus important to distinguish the methods’ abilities to combat attacks. We first test performance against gradient-exploiting attacks by reducing the magnitudes of gradients near the nominal input. In Figure 3(b) we provide a qualitative picture by adversarially perturbing a single test datapoint against gradient-exploiting attacks by reducing the magnitudes of gradients near the nominal input. Specifically, we again consider WRM attacks and we decrease $\gamma$ by WRM (16). In the figures, we scale the budgets $1/\gamma_{\text{adv}}$ and $\epsilon_{\text{adv}}$ for the adversary with $C := \mathbb{E}_{\hat{P}_n} [||X||_p]$. All methods achieve at least 99% test-set accuracy, implying there is little test-time penalty for the robustness levels ($\epsilon$ and $\gamma$) used for training the adversarial models.

Next we study stability of the loss surface with respect to perturbations to inputs. First, consider the distance to adversarial examples under the models $\theta = \theta_{\text{ERM}}, \theta_{\text{FGM}}, \theta_{\text{IFGM}}, \theta_{\text{PGM}}, \theta_{\text{WRM}}$.

$$\hat{\rho}_{\text{test}}(\theta) := \mathbb{E}_{\hat{P}_{\text{test}}} [c(T_{\gamma_{\text{adv}}}(\theta, Z), Z)],$$

where $\hat{P}_{\text{test}}$ is the test distribution, $c(z, z') := ||x - x'||_2^2$ as usual, and $T_{\gamma_{\text{adv}}}(\theta, Z) = \arg\max_z \{\ell(\theta; z) - \gamma_{\text{adv}}c(z, Z)\}$ is the adversarial perturbation of $Z$ (Monge map) for the model $\theta$. We note that small values of $\hat{\rho}_{\text{test}}(\theta)$ correspond to small magnitudes of $\nabla_z \ell(\theta; z)$ in a neighborhood of the nominal input, which ensures stability of the model. Figure 3(a) shows that $\hat{\rho}_{\text{test}}(\theta)$ differs by orders of magnitude between the training methods; the trend is nearly uniform over all $\gamma_{\text{adv}}$, with $\theta_{\text{WRM}}$ being the most stable. Thus, we see that our adversarial-training method defends against gradient-exploiting attacks by reducing the magnitudes of gradients near the nominal input.

In Figure 3(b) we provide a qualitative picture by adversarially perturbing a single test datapoint until the model misclassifies it. Specifically, we again consider WRM attacks and we decrease $\gamma_{\text{adv}}$.

blue class ($||X||_2 \leq \sqrt{2}/1.3$), distributional robustness favors pushing the classification boundary outwards; intuitively, adversarial examples are most likely to come from pushing blue points outwards across the boundary. ERM and FGM suffer from sensitivities to various regions of the data, as evidenced by the lack of symmetry in their classification boundaries. For both activations, WRM pushes the classification boundaries further outwards than ERM or FGM. However, WRM with ReLU’s still suffers from sensitivities (e.g. asymmetry in the classification surface) due to the lack of robustness guarantees. WRM with ELUs provides a certified level of robustness, yielding an axisymmetric classification boundary that hedges against adversarial perturbations in all directions.

### 4.2 Learning a More Robust Classifier

We now consider a standard benchmark—training a neural network classifier on the MNIST dataset. The network consists of $8 \times 8$, $6 \times 6$, and $5 \times 5$ convolutional filter layers with ELU activations followed by a fully connected layer and softmax output. We train our method (WRM) with $\gamma = \frac{3}{10} \mathbb{E}_{\hat{P}_n} [||X||_2]$, and for the other methods we choose $\epsilon$ as the level of robustness achieved by WRM (16). In the figures, we scale the budgets $1/\gamma_{\text{adv}}$ and $\epsilon_{\text{adv}}$ for the adversary with $C := \mathbb{E}_{\hat{P}_n} [||X||_p]$. All methods achieve at least 99% test-set accuracy, implying there is little test-time penalty for the robustness levels ($\epsilon$ and $\gamma$) used for training the adversarial models.

For this $\gamma$, $\phi_{\gamma}(\theta_{\text{WRM}}; z)$ is strongly concave for 98% of the training data.

For the standard MNIST dataset, $C_2 := \mathbb{E}_{\hat{P}_n} [||X||_2] = 1.24$ and $C_\infty := \mathbb{E}_{\hat{P}_n} [||X||_\infty] = 0.52$. In Figure 1, we provide a qualitative picture by adversarially perturbing a single test datapoint.
Figure 2. PGM attacks on the MNIST dataset. (a) and (b) show test misclassification error vs. the adversarial perturbation level \( \epsilon_{\text{adv}} \) for the PGM attack with respect to Euclidean and \( \infty \) norms respectively. The vertical bar in (a) indicates the perturbation level used for training the FGM, IFGM, and PGM models as well as the estimated radius \( \sqrt{\hat{\rho}(\theta_{\text{WRM}})} \). For MNIST, \( C_2 = 1.24 \) and \( C_\infty = 0.52 \).

Figure 3. Stability of the loss surface. In (a), we show the average distance of the perturbed distribution \( \hat{\rho}_{\text{test}} \) for a given \( \gamma_{\text{adv}} \), an indicator of local stability to inputs for the decision surface. The vertical bar in (a) indicates the \( \gamma \) we use for training WRM. In (b) we visualize the smallest WRM perturbation (largest \( \gamma_{\text{adv}} \)) necessary to make a model misclassify a datapoint. More examples are in Appendix A.2.

until each model misclassifies the input. The original label is 8, whereas on the adversarial examples IFGM predicts 2, PGM predicts 0, and the other models predict 3. WRM’s “misclassifications” appear consistently reasonable to the human eye (see Appendix A for examples with other digits); WRM defends against gradient-based exploits by learning a representation that makes gradients point towards inputs of other classes. Together, Figures 3(a) and (b) depict our method’s defense mechanisms to gradient-based attacks: creating a more stable loss surface by reducing the magnitude of gradients and improving their interpretability.

4.3 ROBUST MARKOV DECISION PROCESSES

For our final experiments, we consider distributional robustness in the context of Q-learning, a model-free reinforcement learning technique. We consider Markov decision processes (MDPs) \((\mathcal{S}, \mathcal{A}, P_{sa}, r)\) with finite state space \( \mathcal{S} \), action space \( \mathcal{A} \), state-action transition probabilities \( P_{sa} \), and rewards \( r : \mathcal{S} \to \mathbb{R} \). The goal of a reinforcement-learning agent is to maximize (discounted) cumulative rewards \( \sum_t \lambda^t E[r(s^t)] \) (with discount factor \( \lambda \)); this is the analogue of minimizing \( \mathbb{E}_P[\ell(\theta; Z)] \) in supervised learning. A robust MDP considers an ambiguity set \( \mathcal{P}_{sa} \) for the state-action transitions, and the goal is to maximize the worst-case realization \( \inf_{P \in \mathcal{P}_{sa}} \sum_t \lambda^t \mathbb{E}_P[r(s^t)] \); this is the analogue of problem (1).

In a standard MDP, Q-learning learns a quality function \( Q : \mathcal{S} \times \mathcal{A} \to \mathbb{R} \) via the iterations

\[
Q(s^t, a^t) \leftarrow Q(s^t, a^t) + \alpha_t \left( r(s^{t+1}) + \max_a Q(s^{t+1}, a) - Q(s^t, a^t) \right)
\]

such that \( \arg\max_a Q(s, a) \) is (eventually) the optimal action to take in state \( s \) to maximize cumulative reward. In scenarios where the underlying environment has a continuous state-space, we can
easily modify the update (18) to include distributional robustness by an adversarial state perturbation. Namely, we draw the nominal state-transition update $\hat{s}_{t+1} \sim p_{sa}(s^t, a^t)$, and proceed with the update (18) using the its adversarial perturbation

$$s_{t+1} \leftarrow \text{argmin}_s \{ r(s) + \gamma c(s, \hat{s}_{t+1}) \}.$$  

(19)

Since the underlying state-space is continuous, we can solve problem (19) efficiently using gradient descent. This procedure provides robustness to uncertainties in state-action transitions.

We test this formulation of adversarial training in the classic cart-pole environment, where the goal is to balance a pole on a cart by moving the cart left or right. The environment caps episode lengths to 400 steps and ends the episode prematurely if the pole falls too far from the vertical or the cart translates too far from its origin. We use the reward $r(\beta) := \exp\{-|\beta|\}$, where $\beta$ is the angle of the pole form the vertical. Furthermore, we use a simple tabular representation for Q with 30 discretized states for $\beta$ and 15 for its time-derivative $\dot{\beta}$. The action space is binary: push the cart left or right with a fixed force. Due to the nonstationary, policy-dependent effective radius for the Wasserstein ball, an analogous $\epsilon$ for the fast-gradient method (or other variants) is not well-defined. Thus, we only compare with an agent trained on the nominal MDP. We test the models with various perturbations to the physical parameters. Namely, we consider reducing/magnifying the pole’s mass by 2, reducing/magnifying the pole’s length by 2, and reducing/magnifying the strength of gravity $g$ by 5. The dynamics of the system are such that the heavy, short, and strong-gravity cases are more physically unstable than the original environment, whereas their counterparts are less unstable.

Table 1 shows the performance of the trained models over the original MDP and all of the perturbed MDPs. Both models perform similarly over easier environments, but the robust model greatly outperforms in harder environments. Interestingly, as shown in Figure 4, the robust model also learns more efficiently than the nominal model in the original MDP. We hypothesize that a potential side-effect of robustness is that adversarial perturbations encourage better exploration of the environment.

### 5 Conclusion

Explicit distributional robustness of the form (5) is intractable except in limited cases. We provide a method for efficiently guaranteeing distributional robustness with a simple form of adversarial data perturbation. Using only assumptions about the smoothness of the loss function $\ell$, we prove that our method enjoys strong statistical guarantees and fast optimization rates for a large class of problems. The NP-hardness of certifying robustness for ReLU networks, coupled with our empirical success and theoretical certificates for smooth networks in deep learning, suggest that using smooth networks may be preferrable if we wish to guarantee robustness. Empirical evaluations indicate that our methods are in fact robust to perturbations in the data, and they outperform less-principled adversarial training techniques. The major benefit of our approach is its simplicity and wide applicability across many models and machine-learning scenarios.

---

For tabular Q-learning, we can then round $s_{t+1}^{\epsilon}$ as usual. Since the update (19) simply modifies the state-action transitions (independent of Q), all standard results on convergence for tabular Q-learning (e.g. Szepesvári & Littman (1999)) apply under these adversarial dynamics.
REFERENCES


A ADDITIONAL EXPERIMENTS

A.1 MNIST ATTACKS

We repeat Figure 2 using FGM (Figure 5) and IFGM (Figure 6) attacks. The same trends are evident as in Figure 2.

Figure 5. Fast-gradient attacks on the MNIST dataset. (a) and (b) show test misclassification error vs. the adversarial perturbation level $\epsilon_{adv}$ for the FGM attack with respect to the Euclidean and $\infty$ norms respectively. The vertical bar in (a) indicates the perturbation level that was used for training the FGM, IFGM, and PGM models and the estimated radius $\sqrt{\hat{\rho}_n}\left(\theta_{WRM}\right)$.

Figure 6. Iterated fast-gradient attacks on the MNIST dataset. (a) and (b) show test misclassification error vs. the adversarial perturbation level $\epsilon_{adv}$ for the IFGM attack with respect to the Euclidean and $\infty$ norms respectively. The vertical bar in (a) indicates the perturbation level that was used for training the FGM, IFGM, and PGM models and the estimated radius $\sqrt{\hat{\rho}_n}\left(\theta_{WRM}\right)$.

A.2 MNIST STABILITY OF LOSS SURFACE

In Figure 7, we repeat the illustration in Figure 3(b) for more digits. WRM’s “misclassifications” are consistently reasonable to the human eye, as gradient-based perturbations actually transform the original image to other labels. Other models do not exhibit this behavior with the same consistency (if at all). Reasonable misclassifications correspond to having learned a data representation that makes gradients interpretable.

A.3 MNIST EXPERIMENTS WITH VARIED $\gamma$

In Figure 8 we choose a fixed WRM adversary (fixed $\gamma_{adv}$) and perturb WRM models trained with various penalty parameters $\gamma$. We note that as the bound (10) with $\eta = \gamma$ suggests, even when the adversary has more budget than that used for training ($1/\gamma < 1/\gamma_{adv}$), degradation in performance is still smooth. Further, as we decrease the penalty $\gamma$, we see that the amount of achieved robustness—measured here by test error on adversarial perturbations with $\gamma_{adv}$—has diminishing gains; this is
Figure 7. Visualizing stability over inputs. We illustrate the smallest WRM perturbation (largest $\gamma_{\text{adv}}$) necessary to make a model misclassify a datapoint.

Figure 8. (a) Stability and (b) test error for a fixed adversary. We train WRM models with various levels of $\gamma$ and perturb them with a fixed WRM adversary ($\gamma_{\text{adv}}$ indicated by the vertical bar).

again consistent to our theory which says that the inner problem (2b) is not efficiently computable for small values of $\gamma$. 
B FINDING WORST-CASE PERTURBATIONS WITH ReLU’S IS NP-HARD

We show that computing worst-case perturbations \( \sup_{u \in \mathcal{U}} \ell(\theta; z + u) \) is NP-hard for a large class of feedforward neural networks with ReLU activations. This result is essentially due to Katz et al. (2017a). In the following, we use polynomial time mean polynomial growth with respect to \( m \), the dimension of the inputs \( z \).

An optimization problem is NPO (NP-Optimization) if (i) the dimensionality of the solution grows polynomially, (ii) the language \( \{ u \in \mathcal{U} \} \) can be recognized in polynomial time (i.e. a deterministic algorithm can decide in polynomial time whether \( u \in \mathcal{U} \)), and (iii) \( \ell \) can be evaluated in polynomial time. We restrict analysis to feedforward neural networks with ReLU activations such that the corresponding worst-case perturbation problem is NPO. Furthermore, we impose separable structure on \( \mathcal{U} \), that is, \( \mathcal{U} := \{ v \leq u \leq w \} \) for some \( v < w \in \mathbb{R}^m \).

**Lemma 2.** Consider feedforward neural networks with ReLU’s and let \( \mathcal{U} := \{ v \leq u \leq w \} \), where \( v < w \) such that the optimization problem \( \max_{u \in \mathcal{U}} \ell(\theta; z + u) \) is NPO. There exist \( \theta \) such that this optimization problem is also NP-hard.

**Proof** First, we introduce the decision reformulation of the problem: for some \( b \), we ask whether there exists some \( u \) such that \( \ell(\theta; z + u) \geq b \). The decision reformulation for an NPO problem is in NP, as a certificate for the decision problem can be verified in polynomial time. By appropriate scaling of \( \theta, v \), and \( w \), Katz et al. (2017a) show that 3-SAT Turing-reduces to this decision problem: given an oracle \( D \) for the decision problem, we can solve an arbitrary instance of 3-SAT with a polynomial number of calls to \( D \). The decision problem is thus NP-complete.

Now, consider an oracle \( O \) for the optimization problem. The decision problem Turing-reduces to the optimization problem, as the decision problem can be solved with one call to \( O \). Thus, the optimization problem is NP-hard. \( \square \)

C PROOFS

C.1 PROOF OF PROPOSITION 1

We provide a slightly more general duality result, for which Proposition 1 is an immediate special case. Recalling Rockafellar & Wets (1998) Def. 14.27 and Prop. 14.33, we say that a function \( g : X \times Z \to \mathbb{R} \) is a normal integrand if for each \( \alpha \), the mapping

\[
z \mapsto \{ x \mid g(x, z) \leq \alpha \}
\]

is closed-valued and measurable. We recall that if \( g \) is continuous, then \( g \) is a normal integrand (Rockafellar & Wets 1998 Cor. 14.34); therefore, \( g(x, z) = \gamma c(x, z) - \ell(\theta; x) \) is a normal integrand.

**Theorem 5.** Let \( f, c \) be such that for any \( \gamma \geq 0 \), the function \( g(x, z) = \gamma c(x, z) - f(x) \) is a normal integrand. (For example, continuity of \( f \) and closed convexity of \( c \) is sufficient.) For any \( \rho > 0 \) we have

\[
\sup_{P : W_c(P, Q)} \int f(x) dP(x) = \inf_{\gamma \geq 0} \left\{ \int_{x \in X} f(x) - \gamma c(x, z) dQ(z) + \gamma \rho \right\}.
\]

**Proof** First, the mapping \( P \mapsto W_c(P, Q) \) is convex in the space of probability measures. As taking \( P = Q \) yields \( W_c(P, Q) = 0 \), Slater’s condition holds and we may apply standard (infinite dimensional) duality results (Luenberger 1969) Thm. 8.7.1 to obtain

\[
\sup_{P : W_c(P, Q)} \int f(x) dP(x) = \sup_{P : W_c(P, Q)} \inf_{\gamma \geq 0} \left\{ \int f(x) dP(x) - \gamma W_c(P, Q) + \gamma \rho \right\}
= \inf_{\gamma \geq 0} \sup_{P : W_c(P, Q)} \left\{ \int f(x) dP(x) - \gamma W_c(P, Q) + \gamma \rho \right\}.
\]

Note that \( z, u \in \mathbb{R}^m \), so trivially the dimensionality of the solution grows polynomially.
Now, noting that for any \( M \in \Pi(P,Q) \) we have \( \int f dP = \int f(x) dM(x,z) \), we have that the rightmost quantity in the preceding display satisfies

\[
\int f(x) dP(x) - \gamma \inf_{M \in \Pi(P,Q)} \int c(x,z) dM(x,z) = \sup_{M \in \Pi(P,Q)} \left\{ \int [f(x) - \gamma c(x,z)] dM(x,z) \right\}.
\]

That is, we have

\[
\sup_{P,W_{c}(P,Q)} \int f(x) dP(x) = \inf_{\gamma \geq 0} \sup_{P,M \in \Pi(P,Q)} \left\{ \int [f(x) - \gamma c(x,z)] dM(x,z) + \gamma \rho \right\}.
\]

(20)

Now, we note a few basic facts. First, because we have a joint supremum over \( P \) and measures \( M \in \Pi(P,Q) \) in expression (20), we have that

\[
\sup_{P,M \in \Pi(P,Q)} \int [f(x) - \gamma c(x,z)] dM(x,z) \leq \int \sup_{x} [f(x) - \gamma c(x,z)] dQ(z).
\]

We would like to show equality in the above. To that end, we note that if \( P \) denotes the space of regular conditional probabilities (Markov kernels) from \( Z \) to \( X \), then

\[
\sup_{P,M \in \Pi(P,Q)} \int [f(x) - \gamma c(x,z)] dM(x,z) \geq \sup_{P \in \mathcal{P}} \int [f(x) - \gamma c(x,z)] dP(x \mid z) dQ(z).
\]

Recall that a conditional distribution \( P(\cdot \mid z) \) is regular if \( P(\cdot \mid z) \) is a distribution for each \( z \) and for each measurable \( A \), the function \( z \mapsto P(A \mid z) \) is measurable. Let \( X \) denote the space of all measurable mappings \( z \mapsto x(z) \) from \( Z \) to \( X \). Using the powerful measurability results of [Rockafellar & Wets 1998, Theorem 14.60], we have

\[
\sup_{x \in X} \int [f(x(z)) - \gamma c(x(z),z)] dQ(z) = \int \sup_{x \in X} [f(x) - \gamma c(x,z)] dQ(z)
\]

because \( f - c \) is upper semi-continuous, and the latter function is measurable. Now, let \( x(z) \) be any measurable function that is \( \epsilon \)-close to attaining the supremum above. Define the conditional distribution \( P(\cdot \mid z) \) to be supported on \( x(z) \), which is evidently measurable. Then using the preceding display, we have

\[
\int [f(x) - \gamma c(x,z)] dP(x \mid z) dQ(z) = \int \sup_{x \in X} [f(x(z)) - \gamma c(x(z),z)] dQ(z) - \epsilon.
\]

As \( \epsilon > 0 \) is arbitrary, this gives

\[
\sup_{P,M \in \Pi(P,Q)} \int [f(x) - \gamma c(x,z)] dM(x,z) = \int \sup_{x \in X} |f(x) - \gamma c(x,z)] dQ(z)
\]

as desired, which implies both equality (20) and completes the proof. \( \square \)

C.2 \hspace{1em} PROOF OF LEMMA \( 1 \)

Differentiability is a consequence of one of the many forms of Danskin’s Theorem (e.g. Appendix B in [Başar & Bernhard 2008]). For smoothness, we first argue that \( z^{*}(\theta) \) is continuous in \( \theta \). For any \( \theta \), optimality of \( z^{*}(\theta) \) implies that \( g_1(\theta, z^{*}(\theta))^T (z - z^{*}(\theta)) \leq 0 \). By strong concavity, for any \( \theta_1, \theta_2 \) and \( z^{*}_1 = z^{*}(\theta_1) \) and \( z^{*}_2 = z^{*}(\theta_2) \), we have

\[
\frac{\lambda}{2} \| z^{*}_1 - z^{*}_2 \|^2 \leq f(\theta_2, z^{*}_2) - f(\theta_2, z^{*}_1) \text{ and } f(\theta_2, z^{*}_2) \leq f(\theta_2, z^{*}_1) + g_2(\theta_2, z^{*}_1)^T (z^{*}_2 - z^{*}_1) - \frac{\lambda}{2} \| z^{*}_1 - z^{*}_2 \|^2.
\]
Summing these inequalities gives
\[ \lambda \| z_1^t - z_2^t \|^2 \leq g_{\theta}(\theta_2, z_1^t) - g_{\theta}(\theta_1, z_1^t), \]
where the last inequality follows because \( g_{\theta}(\theta_1, z_1^t) \leq 0 \). Using a cross-Lipschitz condition from above and Holder’s inequality, we obtain
\[ \lambda \| z_1^t - z_2^t \|^2 \leq \| g_{\theta}(\theta_2, z_1^t) - g_{\theta}(\theta_1, z_1^t) \| \| z_1^t - z_2^t \| \leq \| \theta_1 - \theta_2 \| \| z_1^t - z_2^t \|, \]
that is,
\[ \| z_1^t - z_2^t \| \leq \frac{L_{\theta \theta}}{\lambda} \| \theta_1 - \theta_2 \|. \] (21)

Then we have
\[ \| g_{\theta}(\theta_1, z_1^t) - g_{\theta}(\theta_2, z_2^t) \| \leq \| g_{\theta}(\theta_1, z_1^t) - g_{\theta}(\theta_1, z_2^t) \| + \| g_{\theta}(\theta_1, z_2^t) - g_{\theta}(\theta_2, z_2^t) \| \]
\[ \leq L_{\theta z} \| z_1^t - z_2^t \| + \lambda \| \theta_1 - \theta_2 \| \]
\[ \leq \left( L_{\theta \theta} + \frac{L_{\theta \theta} L_{\theta z}}{\lambda} \right) \| \theta_1 - \theta_2 \|, \]
where we have used inequality (21) again. This is the desired result.

C.3 PROOF OF THEOREM 2

Our proof is based on that of Ghadimi & Lan [2013].

For shorthand, let \( f(\theta, z; z_0) = \ell(\theta; z) - \gamma c(z, z_0) \), noting that we perform gradient steps with
\[ g^t = \nabla_\theta f(\theta^t, z^t); z^t) \]
for \( z^t \) an \( \epsilon \)-approximate maximizer of \( f(\theta, z; z_0) \) in \( z \), and \( \theta^{t+1} = \theta^t - \alpha_t g^t \). By a Taylor expansion using the \( L \)-smoothness of the objective \( F \), we have
\[ F(\theta^{t+1}) \leq F(\theta^t) + \langle \nabla F(\theta^t), \theta^{t+1} - \theta^t \rangle + \frac{L}{2} \| \theta^{t+1} - \theta^t \|^2 \]
\[ = F(\theta^t) - \alpha_t \| \nabla F(\theta^t) \|^2 + \frac{L_\alpha^2}{2} \| g^t \|^2 + \alpha_t \langle \nabla F(\theta^t), \nabla F(\theta^t) - g^t \rangle \]
\[ = F(\theta^t) - \alpha_t \left( 1 - \frac{L_\alpha}{2} \right) \| \nabla F(\theta^t) \|^2 \]
\[ + \alpha_t \left( 1 + \frac{L_\alpha}{2} \right) \langle \nabla F(\theta^t), \nabla F(\theta^t) - g^t \rangle + \frac{L_\alpha^2}{2} \| g^t - \nabla F(\theta^t) \|^2 \]. (22)

Recalling the definition (21) of \( \phi_\lambda(\theta; z_0) = \sup_{z \in \mathcal{Z}} f(\theta, z; z_0) \), we define the potentially biased errors \( \delta^t = g^t - \nabla_\theta f(\theta^t; z^t) \). Letting \( z^t_* = \text{argmax}_z f(\theta^t, z; z^t) \), these errors evidently satisfy
\[ \| \delta^t \|^2 \leq \| \nabla_\theta f(\theta^t; z^t) - \nabla_\theta f(\theta^t, z^t) \|^2 \leq \| \nabla_\theta f(\theta^t; z^t) - \nabla_\theta f(\theta^t, z^t) \|^2 \]
\[ \leq L_\alpha^2 \| z^t - z^t_* \|^2 \leq \frac{L_\alpha^2}{\lambda}, \]
where the final inequality uses the \( \lambda = \gamma - L_{\alpha z} \) strong-concavity of \( z \mapsto f(\theta, z; z_0) \). For shorthand, let \( \tilde{c} = \frac{2L_\alpha L_{\alpha z}}{\gamma - L_{\alpha z}} \cdot \). Substituting the preceding display into the progress guarantee (21), we have
\[ F(\theta^{t+1}) = F(\theta^t) - \alpha_t \left( 1 - \frac{L_\alpha}{2} \right) \| \nabla F(\theta^t) \|^2 - \alpha_t \left( 1 + \frac{L_\alpha}{2} \right) \langle \nabla F(\theta^t), \delta^t \rangle \]
\[ + \alpha_t \left( 1 + \frac{L_\alpha}{2} \right) \langle \nabla F(\theta^t), \nabla F(\theta^t) - \nabla_\theta f(\theta^t; z_1^t) \rangle + \frac{L_\alpha^2}{2} \| \nabla_\theta f(\theta^t; z_1^t + \delta^t - \nabla F(\theta^t) \|^2 \]
\[ \leq F(\theta^t) - \frac{\alpha_t}{2} \left( 1 - L_\alpha \right) \| \nabla F(\theta^t) \|^2 + \frac{\alpha_t}{2} \left( 1 + \frac{L_\alpha}{2} \right) \| \delta^t \|^2 \]
\[ + \alpha_t \left( 1 + \frac{L_\alpha}{2} \right) \langle \nabla F(\theta^t), \nabla F(\theta^t) - \nabla_\theta f(\theta^t; z^t) \rangle + L_\alpha^2 \langle \nabla_\theta f(\theta^t; z^t) - \nabla F(\theta^t) \|^2 + \| \delta^t \|^2. \]
Noting that $\mathbb{E}[\nabla \phi_\gamma(\theta^t; z^t) \mid \theta^t] = \nabla F(\theta^t)$, we take expectations to find
\[
\mathbb{E}[F(\theta^{t+1}) - F(\theta^t) \mid \theta^t] \leq -\frac{\alpha t}{2} (1 - L\alpha t) \mathbb{E}[\nabla F(\theta^t)]^2 + \left( \frac{\alpha t}{2} + \frac{5L\alpha^2 t}{4} \right) \hat{c} + L\alpha^2 \sigma^2,
\]
where we have used that $\mathbb{E}[\|\nabla \phi_\gamma(\theta; Z) - \nabla F(\theta)\|_2^2] \leq \sigma^2$ by assumption.

The bound (23) gives the theorem essentially immediately for fixed stepsizes $\alpha$, as we have
\[
\frac{\alpha}{2} (1 - L\alpha) \mathbb{E}\left[ \sum_{t=1}^{T} \|\nabla F(\theta^t)\|_2^2 \right] \leq F(\theta^0) - \mathbb{E}[F(\theta^{T+1})] + \frac{T\alpha}{2} \left( 1 + \frac{5L\alpha^2}{4} \right) \hat{c} + TL\alpha^2 \sigma^2.
\]

Noting that $\inf_\theta F(\theta) \leq F(\theta^{T+1})$ gives the final result.

C.4 Proof of Theorem[3]

We first show the bound (10). From the duality result [5], we have the deterministic result that
\[
\sup_{P: W_\rho(P, Q) \leq \rho} \mathbb{E}_Q[\ell(\theta; Z)] \leq \gamma \rho + \mathbb{E}_Q[\phi_\gamma(\theta; Z)]
\]
for all $\rho > 0$, distributions $Q$, and $\gamma \geq 0$. Next, we show that $\mathbb{E}_{\hat{P}_n}[\phi_\gamma(\theta; Z)]$ concentrates around its population counterpart at the usual rate (Boucheron et al., 2005). First, we have that
\[
\phi_\gamma(Z; z) \in [-M_\ell, M_\ell],
\]
because $-M_\ell \leq \ell(t; z) \leq \phi_\gamma(\theta; z) \leq \sup_{\ell(t; z)} \leq M_\ell$. Thus, the functional $\theta \mapsto F_n(\theta)$ satisfies bounded differences (Boucheron et al., 2013, Thm. 6.2), and applying standard results on Rademacher complexity (Bartlett & Mendelson, 2002) and entropy integrals (van der Vaart & Wellner, 1996, Ch. 2.2) gives the result.

To see the second result (11), we substitute $\rho = \hat{\rho}_n$ in the bound (10). Then, with probability at least $1 - e^{-t}$, we have
\[
\sup_{P: W_\rho(P, P_0) \leq \hat{\rho}_n(\theta)} \mathbb{E}_P[\ell(\theta; Z)] \leq \gamma \hat{\rho}_n(\theta) + \mathbb{E}_\hat{P}_n[\phi_\gamma(\theta; Z)] + \epsilon_{n,1}(t).
\]

Since we have
\[
\sup_{P: W_\rho(P, P_0) \leq \hat{\rho}_n(\theta)} \mathbb{E}_P[\ell(\theta; Z)] = \mathbb{E}_\hat{P}_n[\phi_\gamma(\theta; Z)] + \gamma \hat{\rho}_n(\theta),
\]
from the strong duality in Proposition[1] our second result follows.

C.5 Proof of Theorem[4]

Define
\[
P_n^*(\theta) := \arg\max_P \left\{ \mathbb{E}_P[\ell(\theta; Z)] - \gamma W_\rho(P, \hat{P}_n) \right\},
\]
\[
P^*(\theta) := \arg\max_P \left\{ \mathbb{E}_P[\ell(\theta; Z)] - \gamma W_\rho(P, P_0) \right\}.
\]

First, we show that $P^*(\theta)$ and $P_n^*(\theta)$ are attained for all $\theta \in \Theta$. We omit the dependency on $\theta$ for notational simplicity and only show the result for $P^*(\theta)$ as the case for $P_n^*(\theta)$ is symmetric. Let $P^*$ be an $\epsilon$-maximizer, so that
\[
\mathbb{E}_P[\ell(\theta; Z)] - \gamma W_\rho(P^*, P_0) \geq \sup_P \left\{ \mathbb{E}_P[\ell(\theta; Z)] - \gamma W_\rho(P, P_0) \right\} - \epsilon.
\]

As $Z$ is compact, the collection $\{P_{1/k}\}_{k \in \mathbb{N}}$ is a uniformly tight collection of measures. By Prohorov’s theorem (Billingsley, 1999, Ch 1.1, p. 57), (restricting to a subsequence if necessary), there exists some distribution $P^*$ on $Z$ such that $P_{1/k} \overset{d}{\to} P^*$ as $k \to \infty$. Continuity properties of Wasserstein distances (Villani, 2009, Corollary 6.11) then imply that
\[
\lim_{k \to \infty} W_\rho(P_{1/k}, P_0) = W_\rho(P^*, P_0).
\]
Combining (24) and the monotone convergence theorem, we obtain
\[
\mathbb{E}_{P^*}[\ell(\theta; Z)] - \gamma W_c(P^*, P_0) = \lim_{k \to \infty} \left\{ \mathbb{E}_{P_1/k}[\ell(\theta; Z)] - \gamma W_c(P_1/k, P_0) \right\} \\
\geq \sup_{P} \{ \mathbb{E}_P[\ell(\theta; Z)] - \gamma W_c(P, P_0) \}
\]
We conclude that $P^*$ is attained for all $P_0$.

Next, we show the concentration result (14). Recall the definition (9) of the transportation mapping
\[
T(\theta, z) := \arg\max_{z^*} \{ \ell(\theta; z^*) - \gamma c(z^*, z) \},
\]
which is unique and well-defined under our strong concavity assumption that $\gamma > L_{zz}$, and smooth (recall Eq. (13)) in $\theta$. Then by Proposition 1 (or by using a variant of Kantorovich duality [Villani 2009 Chs. 9-10]), we have
\[
\mathbb{E}_{P_n}[\ell(\theta; Z)] = \mathbb{E}_{\hat{P}_n}[\ell(\theta; T(\theta; Z))] \quad \text{and} \quad \mathbb{E}_{P_n}[\ell(\theta; Z)] = \mathbb{E}_{\hat{P}_0}[\ell(\theta; T(\theta; Z))]
\]
\[
W_c(P_n(\theta), \hat{P}_n) = \mathbb{E}_{\hat{P}_n}[c(T(\theta; Z), Z)] \quad \text{and} \quad W_c(P_n(\theta), \hat{P}_0) = \mathbb{E}_{\hat{P}_0}[c(T(\theta; Z), Z)].
\]

We now proceed by showing the uniform convergence of
\[
\mathbb{E}_{\hat{P}_n}[c(T(\theta; Z), Z)] \quad \text{to} \quad \mathbb{E}_{\hat{P}_0}[c(T(\theta; Z), Z)]
\]
under both cases (i), that $c$ is Lipschitz, and (ii), that $\ell$ is Lipschitz in $z$, using a covering argument on $\Theta$. Recall inequality (13) (i.e. Lemma 1), which is that
\[
\|T(\theta_1; z) - T(\theta_2; z)\| \leq \frac{L_{z\theta}}{\gamma - L_{zz}} \| \theta_1 - \theta_2 \|.
\]
We have the following lemma.

**Lemma 3.** Assume the conditions of Theorem 2. Then for any $\theta_1, \theta_2 \in \Theta$,
\[
|c(T(\theta_1; z), z) - c(T(\theta_2; z), z)| \leq \frac{L_{c} L_{z\theta}}{\gamma - L_{zz}} \| \theta_1 - \theta_2 \|.
\]

**Proof.** In the first case, that $c$ is $L_{c}$-Lipschitz in its first argument, this is trivial: we have
\[
|c(T(\theta_1; z), z) - c(T(\theta_2; z), z)| \leq L_{c} \|T(\theta_1; z) - T(\theta_2; z)\| \leq \frac{L_{c} L_{z\theta}}{\gamma - L_{zz}} \| \theta_1 - \theta_2 \|
\]
by the smoothness inequality (13) for $T$.

In the second case, that $z \mapsto \ell(\theta, z)$ is $L_{\ell}$-Lipschitz, let $z_i = T(\theta_i; z)$ for shorthand. Then we have
\[
\gamma c(z_2, z) - \gamma c(z_1, z) = \gamma c(z_2, z) - \ell(\theta_2, z_2) + \ell(\theta_2, z_2) - \gamma c(z_1, z) \\
\leq \gamma c(z_2, z) - \ell(\theta_2, z_1) + \ell(\theta_2, z_2) - \gamma c(z_1, z) \leq \ell(\theta_2, z_2) - \ell(\theta_2, z_1),
\]
and similarly,
\[
\gamma c(z_2, z) - \gamma c(z_1, z) = \gamma c(z_2, z) - \ell(\theta_1, z_2) + \ell(\theta_1, z_1) - \gamma c(z_1, z) \\
\geq \gamma c(z_2, z) - \ell(\theta_1, z_1) + \ell(\theta_1, z_2) - \gamma c(z_2, z) \leq \ell(\theta_2, z_1) - \ell(\theta_1, z_1).
\]
Combining these two inequalities and using that
\[
|\ell(\theta, z_2) - \ell(\theta, z_1)| \leq \gamma L_{\ell} \| z_2 - z_1 \|
\]
for any $\theta$ gives the result.

Using Lemma 3 we obtain that $\theta \mapsto |\mathbb{E}_{\hat{P}_n}[c(T(\theta; Z), \theta)] - \mathbb{E}_{\hat{P}_0}[c(T(\theta; Z), \theta)]|$ is $2L_{c} L_{z\theta}/[\gamma - L_{zz}]_+ -$Lipschitz. Let $\Theta_{\text{cover}} = \{ \theta_1, \ldots, \theta_N \}$ be a $\frac{[\gamma - L_{z\theta}]_+}{4L_{c} L_{z\theta}}$-cover of $\Theta$ with respect
to $\|\cdot\|$. From Lipschitzness of $|E_{\bar{P}_n}[c(T(\theta; Z), Z)] - E_{P_0}[c(T(\theta; Z), Z)]|$, we have that if for all $\theta \in \{\Theta_{\text{cover}}\}$,

$$|E_{\bar{P}_n}[c(T(\theta; Z), Z)] - E_{P_0}[c(T(\theta; Z), \theta)]| \leq \frac{t}{2},$$

then it follows that

$$\sup_{\theta \in \Theta} |E_{\bar{P}_n}[c(T(\theta; Z), Z)] - E_{P_0}[c(T(\theta; Z), Z)]| \leq t.$$

Under the first assumption $(i)$, we have $|c(T(\theta; Z), Z)| \leq 2L_cM_z$. Applying Hoeffding’s inequality, for any fixed $\theta \in \Theta$

$$P\left(\sup_{\theta \in \Theta} |E_{\bar{P}_n}[c(T(\theta; Z), Z)] - E_{P_0}[c(T(\theta; Z), Z)]| \geq \frac{t}{2}\right) \leq 2 \exp\left(-\frac{nt^2}{32L_c^2M_z^2}\right).$$

Taking a union bound over $\theta_1, \ldots, \theta_N$, we conclude that

$$P\left(\sup_{\theta \in \Theta} |E_{\bar{P}_n}[c(T(\theta; Z), Z)] - E_{P_0}[c(T(\theta; Z), Z)]| \geq t\right) \leq \sum_{i=1}^{N} N\left(\Theta, \frac{\gamma - L_{z\theta}}{4L_cL_{z\theta}}, \|\cdot\|\right) \exp\left(-\frac{nt^2}{32L^2M_z^2}\right)$$

which was our desired result (14).

Under the second assumption $(ii)$, we have from the definition of the transport map $T$

$$\gamma c(T(\theta; z), z) \leq \ell(\theta; z) \leq M_\ell$$

and hence $|c(T(\theta; Z), Z)| \leq M_\ell/\gamma$. The result for the second case follows from an identical reasoning.

### C.6 Proof of Corollary [1]

The result is essentially standard (van der Vaart & Wellner 1996), which we now give for completeness.

Note that for $\mathcal{F} = \{\ell(\theta; \cdot) : \theta \in \Theta\}$, any $(\epsilon, \|\cdot\|)$-covering $\{\theta_1, \ldots, \theta_N\}$ of $\Theta$ guarantees that

$$min_{i} |\ell(\theta; z) - \ell(\theta_i; z)| \leq \epsilon$$

for all $\theta, z$, or

$$N(\mathcal{F}, \epsilon, \|\cdot\|_{L_{\infty}(Z)}) \leq N(\Theta, \epsilon/L, \|\cdot\|) \leq \left(1 + \frac{\text{diam}(\Theta)L}{\epsilon}\right)^d,$$

where diam$(\Theta) = \sup_{\theta, \theta' \in \Theta} \|\theta - \theta'\|$. Noting that $|\ell(\theta; Z)| \leq L \text{diam}(\Theta) + M_0 =: M_\ell$, we have the result.