Certifiable Distributional Robustness with Principled Adversarial Training

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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. For imperceptible perturbations, our method matches or outperforms heuristic approaches.

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, whether they be from covariate shifts, changes in the underlying domain \[^2\], or adversarial attacks \[^22,28\]. 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 \[^22,28,34,37\]. Subsequently, many researchers have proposed adversarial attack and defense mechanisms \[^44,38,39,40,48,13,31,23\]. 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 \[^26,27,24\] 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 $P_0$ and consider the problem

$$\minimize_{\theta \in \Theta} \sup_{P \in \mathcal{P}} \mathbb{E}_P[\ell(\theta; Z)].$$

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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 $\sup_{P \in \mathcal{P}} E_P[\ell(\theta; Z)]$. On a simple implementation in Tensorflow, our method takes $5\times$ as long as stochastic gradient methods for empirical risk minimization (ERM), matching runtimes for other adversarial training procedures [22, 28, 31]. 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.

We briefly overview our approach. Let $c : Z \times Z \to \mathbb{R}_+ \cup \{\infty\}$, where $c(z, z_0)$ is the “cost” for an adversary to perturb $z_0$ to $z$ (we typically use $c(z, z_0) = \|z - z_0\|_p^2$ with $p \geq 1$). We consider the robustness region $\mathcal{P} = \{P : W_c(P, P_0) \leq \rho\}$, a $\rho$-neighborhood of the distribution $P_0$ under the Wasserstein metric $W_c(\cdot, \cdot)$ (see Section 2 for a formal definition). For deep networks and other complex models, this formulation of problem (1) is intractable with arbitrary $\rho$. Instead, we consider its Lagrangian relaxation for a fixed penalty parameter $\gamma \geq 0$, resulting in the reformulation

$$\minimize_{\theta \in \Theta} \left\{ F(\theta) := \sup_P \{E_P[\ell(\theta; Z)] - \gamma W_c(P, P_0)\} = E_{P_0}[\phi(\gamma; \theta; Z)] \right\} \quad (2a)$$

where $\phi(\gamma; \theta; z_0) := \sup_{z \in Z} \{\ell(\theta; z) - \gamma c(z, z_0)\}$. (See Proposition 1 for a rigorous statement of these equalities.) Here, 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 penalty $\gamma$. We typically solve the penalty problem (2) with $P_0$ replaced by the empirical distribution $P_n$, 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—in particular, defense against imperceptible adversarial perturbations—are achievable at essentially no computational or statistical cost for smooth losses $\ell$. 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 optimize if $\ell(\theta; z)$ is smooth in $z$. Consequently, stochastic gradient methods applied to problem (2) have similar convergence guarantees as for non-robust methods (ERM). In Section 3 we provide a certificate of robustness for any $\rho$; we give an efficiently computable data-dependent upper bound on the worst-case loss $\sup_{P : W_c(P, P_0) \leq \rho} E_P[\ell(\theta; Z)]$. That is, the worst-case performance of the output of our principled adversarial training procedure is guaranteed to be no worse than this certificate. Our bound is tight when $\rho = \hat{\rho}_n$, the achieved robustness for the empirical objective. These results suggest advantages of networks with smooth activations rather than ReLU’s. We experimentally verify our results in Section 4 and show that, even for non-smooth losses, we match or achieve state-of-the-art performance on a variety of adversarial attacks.

Robust optimization and adversarial training The standard robust-optimization approach minimizes losses of the form $\sup_{u \in U} \ell(\theta; z + u)$ for some uncertainty set $U$ [3, 42, 51]. Unfortunately, this approach is intractable except for specially structured losses, such as the composition of a linear and simple convex function [3, 51, 52]. Nevertheless, this robust approach underlies recent advances
in adversarial training \[46, 22, 39, 13, 31\], which heuristically perturb data during a stochastic optimization procedure.

One such heuristic uses a locally linearized loss function \( p = \infty \) as the “fast gradient sign method” \[22\]:

\[
\Delta x_i(\theta) := \arg\max_{\|\eta\|_p \leq \epsilon} \{\nabla_x \ell(\theta; (x_i, y_i))^T \eta\}
\]
and perturb \( x_i \rightarrow x_i + \Delta x_i(\theta) \).

One form of adversarial training simply trains on these perturbed losses \[22, 28\], and many others perform iterated variants \[39, 48, 13, 31\]. Madry et al. \[31\] observe that these procedures attempt to optimize the objective \( E_{P_0}[\sup_{\|u\|_p \leq \epsilon} \ell(\theta; Z + u)] \), 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, it is NP-hard to find worst-case perturbations when deep networks use ReLU activations, 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) \[16\], 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 \( P \) 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 \( P \), such as constraint sets for moments, support, or directional deviations \[14, 17, 21\], as well as non-parametric distances for probability measures such as \( f \)-divergences \[4, 5, 32, 29, 18, 35\], and Wasserstein distances \[8, 19, 45\]. In contrast to \( f \)-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 \( P \) and losses \( \ell \). For example, Ben-Tal et al. \[4\] and Namkoong and Duchi \[34\] use convex optimization approaches for \( f \)-divergence balls. For worst-case regions \( P \) formed by Wasserstein balls, Esfahani and Kuhn \[14\], Shafieezadeh-Abadeh et al. \[45\] and Blanchet et al. \[8\] 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 \( \nabla_z \ell(\theta; \cdot) \) is \( L \)-Lipschitz. Then for any \( c : Z \times Z \rightarrow \mathbb{R}_+ \cup \{\infty\} \) \( 1 \)-strongly convex in its first argument, a Taylor expansion yields

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

For \( \gamma \geq L \) this is the first-order condition for \((\gamma - L)\)-strong 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 (2b) is a strongly-concave optimization problem.

We leverage the insight (1) 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 (2b) 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 ℓ is non-convex) for our relaxed robust problems.

**Wasserstein robustness and duality** Wasserstein distances define a notion of closeness between distributions. Let \( Z \subset \mathbb{R}^m \), and let \( (Z, \mathcal{A}, P_0) \) be a probability space. Let the transportation cost \( c : Z \times Z \to [0, \infty) \) be nonnegative, lower semi-continuous, 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

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

For \( \rho \geq 0 \) and distribution \( P_0 \), we let \( \mathcal{P} = \{ P : W_c(P, P_0) \leq \rho \} \), considering the Wasserstein form of the robust problem (1) and its Lagrangian relaxation (2) with \( \gamma \geq 0 \). The following duality result due to Blanchet and Murthy [7] gives the equality (2) for the relaxation and an analogous result for the problem (1). We give an alternate proof in Appendix C.1 for convex, continuous cost functions.

**Proposition 1.** Let \( \ell : \Theta \times Z \to \mathbb{R} \) and \( c : Z \times Z \to \mathbb{R}_+ \) be continuous. Let \( \phi_{\gamma}(\theta; z_0) = \sup_{z \in Z} \{ \ell(\theta; z) - \gamma c(z, z_0) \} \) be the robust surrogate (2b). For any distribution \( Q \) and any \( \rho > 0 \),

\[
\sup_{P : W_c(P, Q) \leq \rho} \mathbb{E}_P[\ell(\theta; Z)] = \inf_{\gamma \geq 0} \{ \gamma \rho + \mathbb{E}_Q[\phi_{\gamma}(\theta; Z)] \},
\]

and for any \( \gamma \geq 0 \), we have

\[
\sup_P \{ \mathbb{E}_P[\ell(\theta; Z)] - \gamma W_c(P, Q) \} = \mathbb{E}_Q[\phi_{\gamma}(\theta; Z)].
\]

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

\[
\min_{\theta \in \Theta} \left\{ F_n(\theta) := \sup_P \left\{ \mathbb{E}[\ell(\theta; Z)] - \gamma W_c(P, \bar{P}_n) \right\} = \mathbb{E}_{\bar{P}_n}[\phi_{\gamma}(\theta; Z)] \right\}.
\]

**2.1 Optimizing the robust loss by stochastic gradient descent**

We now develop stochastic gradient-type methods for the relaxed robust problem (7), making clear the computational benefits of relaxing the strict robustness requirements of formulation (5). We begin with assumptions we require, which roughly quantify the amount of robustness we can provide.
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 $\bar{z}^t$ of $\ell(\theta^t; z) - \gamma c(z, z^t)$

$\theta^{t+1} \leftarrow \text{Proj}_{\Theta}(\theta^t - \alpha_t \nabla \ell(\theta^t; \bar{z}^t))$

**Assumption A.** The function $c : Z \times Z \rightarrow \mathbb{R}_+$ 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 surrogate (21) is tractably computable, we also require a few smoothness assumptions. Let $\|\cdot\|_*$ 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 $\ell : \Theta \times Z \rightarrow \mathbb{R}$ satisfies the Lipschitzian smoothness conditions

$$\left\| \nabla \theta \ell(\theta; z) - \nabla \theta \ell(\theta'; z) \right\|_* \leq L_{\theta\theta} \|\theta - \theta'\|, \quad \left\| \nabla z \ell(\theta; z) - \nabla z \ell(\theta'; z) \right\|_* \leq L_{zz} \|z - z'\|,$$

$$\left\| \nabla \theta \ell(\theta; z) - \nabla \theta \ell(\theta'; z') \right\|_* \leq L_{\theta z} \|z - z'\|, \quad \left\| \nabla z \ell(\theta; z) - \nabla z \ell(\theta'; z) \right\|_* \leq L_{z\theta} \|\theta - \theta'\|.$$

These properties guarantee both (i) the well-behavedness of the robust surrogate $\phi_\gamma$ and (ii) its efficient computability. Making point (i) precise, Lemma 1 shows that if $\gamma$ is large enough and Assumption 13 holds, the surrogate $\phi_\gamma$ is still smooth. Throughout, we assume $\Theta \subseteq \mathbb{R}^d$.

**Lemma 1.** Let $f : \Theta \times Z \rightarrow \mathbb{R}$ be differentiable and $\lambda$-strongly concave in $z$ with respect to the norm $\|\cdot\|_2$, and define $\bar{f}(\theta) = \sup_{z \in Z} f(\theta, z)$. Let $g_\theta(\theta, z) = \nabla \theta f(\theta, z)$ and $g_z(\theta, z) = \nabla_z f(\theta, z)$, and assume $g_\theta$ and $g_z$ satisfy Assumption 12 with $f(\theta; z)$ replaced with $f(\theta, z)$. Then $\bar{f}$ is differentiable, and letting $z^*(\theta) = \arg\max_{z \in Z} f(\theta, z)$, we have $\nabla \bar{f}(\theta) = g_\theta(\theta, z^*(\theta))$. Moreover,

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

See Section C.2 for the proof. Fix $z_0 \in Z$ and focus on the $\ell_2$-norm case where $c(z, z_0)$ satisfies Assumption A with $\|\cdot\|_2$. Noting that $f(\theta, z) := \ell(\theta; z) - \gamma c(z, z_0)$ is $\gamma - L_{zz}$-strongly concave from the insight (11) (with $L := L_{zz}$), let us apply Lemma 1. Under Assumptions A and $\phi_\gamma (\cdot; z_0)$ then has $L = L_{\theta\theta} + \frac{L_{zz} L_{z\theta}}{\gamma - L_{zz}}$.Lipschitz gradients, and

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

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 $\ell(\theta^t; z) - \gamma c(z, z^t)$ in $z$ converges linearly and we can compute (approximate) $\bar{z}^t$ efficiently (we initialize our inner gradient ascent iterations with the sampled natural example $z^t$).

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 [15, 25] 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 $\gamma \geq L_{zz}$. Recall that $F(\theta) = \mathbb{E}_{P_0}[\phi_\gamma (\theta; Z)]$ is the robust surrogate objective for the Lagrangian relaxation (2).
Theorem 2 (Convergence of Nonconvex SGD). Let Assumptions A and B hold with the $\ell_2$-norm and let $\Theta = \mathbb{R}^d$. Let $\Delta_F \geq F(\theta^0) - \inf_\theta F(\theta)$. Assume $\mathbb{E}[\|\nabla F(\theta) - \nabla \phi_\gamma(\theta, Z)\|_2^2] \leq \sigma^2$, and take constant stepsize $\alpha = \sqrt{\frac{2c_r L_\phi}{L_\sigma \sqrt{T}}}$ where $L_\phi := L_{\theta\theta} + \frac{L_{\theta X} L_{\theta Z}}{\gamma - L_{zz}}$. Then Algorithm 1 satisfies

$$\frac{1}{T} \sum_{t=1}^{T} \mathbb{E} \left[ \|\nabla F(\theta^t)\|_2^2 \right] - \frac{2L_{\phi z}^2}{\gamma - L_{zz}} \epsilon \leq \sigma \sqrt{\frac{8 L_\phi \Delta_F}{T}}.$$ 

See Section C.3 for the proof. We make a few remarks. First, the condition $\mathbb{E}[\|\nabla F(\theta) - \nabla \phi_\gamma(\theta, Z)\|_2^2] \leq \sigma^2$ holds (to within a constant factor) whenever $\|\nabla \ell(\theta, z)\|_2 \leq \sigma$ for all $\theta$, $z$. Theorem 2 shows that the stochastic gradient method achieves the rates of convergence on the penalty problem (7) achievable in standard smooth non-convex optimization [20]. The accuracy parameter $\epsilon$ has a fixed effect on optimization accuracy, independent of $T$: approximate maximization has limited effects.

Key to the convergence guarantee of Theorem 2 is that the loss $\ell$ is smooth in $z$: the inner supremum [20] is NP-hard to compute for non-smooth deep networks (see Lemma 2 in Section B for a proof of this for ReLU’s). The smoothness of $\ell$ is essential so that a penalized version $\ell(\theta, z) - \gamma c(z, z_0)$ is concave in $z$ (which can be approximately verified by computing Hessians $\nabla^2_{zz} \ell(\theta, z)$ for each training datapoint), allowing computation and our coming certificates of optimality. Replacing ReLU’s with sigmoids or ELU’s [16] allows us to apply Theorem 2 making distributionally robust optimization tractable for deep learning.

In supervised learning scenarios, we are often interested in adversarial perturbations only to feature vectors (and not labels). Letting $Z = (X, Y)$ where $X$ denotes the feature vector (covariates) and $Y$ the label, this is equivalent to defining the Wasserstein cost function $c : \mathcal{Z} \times \mathcal{Z} \to \mathbb{R}_+ \cup \{\infty\}$ by

$$c(z, z') := c_x(x, x') + \infty \cdot 1 \{y \neq y'\} \quad (8)$$

where $c_x : \mathcal{X} \times \mathcal{X} \to \mathbb{R}_+$ is the transportation cost for the feature vector $X$. All of our results suitably generalize to this setting with minor modifications to the robust surrogate (2b) and the above assumptions (see Section D). Similarly, our distributionally robust framework (2) is general enough to consider adversarial perturbations to only an arbitrary subset of coordinates in $Z$. For example, it may be appropriate in certain applications to hedge against adversarial perturbations to a small fixed region of an image [12]. By suitably modifying the cost function $c(z, z')$ to take value $\infty$ outside this small region, our general formulation covers such variants.

### 3 Certificate of robustness 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 $\theta_{\text{WRM}}$, 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 Certificate of robustness

Our main result in this section is a data-dependent upper bound for the worst-case population objective: \( \sup_{P:W_c(P,P_0) \leq \rho} \mathbb{E}_P[\ell(\theta; Z)] \leq \gamma \rho + \mathbb{E}_{\tilde{P}_n}[\phi_\gamma(\theta; Z)] + O(1/\sqrt{n}) \) for all \( \theta \in \Theta \), with high probability. To make this rigorous, fix \( \gamma > 0 \), and consider the worst-case perturbation, typically called the transportation map or Monge map [50],

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

Under our assumptions, \( T_\gamma \) is easily computable when \( \gamma \geq L_{zz} \). Letting \( \delta_z \) denote the point mass at \( z \), Proposition 1 shows the empirical maximizers of the Lagrangian formulation \( \ell(P, \tilde{P}_n; \theta) \) are attained by

\[
P^*_n(\theta) := \arg\max_P \left\{ \mathbb{E}_P[\ell(\theta; Z)] - \gamma W_c(P, \tilde{P}_n) \right\} = \frac{1}{n} \sum_{i=1}^n \delta_{T_\gamma(\theta, Z_i)} \quad \text{and} \quad \rho_n(\theta) := W_c(P^*_n(\theta), \tilde{P}_n) = \mathbb{E}_{\tilde{P}_n}[c(T_\gamma(\theta; Z), Z)].
\]  

Our results imply, in particular, that the empirical worst-case loss \( \mathbb{E}_{P^*_n}[\ell(\theta; Z)] \) gives a certificate of robustness to (population) Wasserstein perturbations up to level \( \rho_n \). \( \mathbb{E}_{P^*_n}[\ell(\theta; Z)] \) is efficiently computable via (10), providing a data-dependent 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. 49], so, despite the infinite-dimensional problem (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 \( \epsilon \)-cover of \( V \) in norm \(|\cdot|\) if for each \( v \in V \), there exists \( v_i \) such that \(|v - v_i| \leq \epsilon\). The covering number of \( V \) with respect to \(|\cdot|\) is

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

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

\[
\epsilon_n(t) := \gamma b_1 \sqrt{\frac{M_t}{n} \int_0^1 \sqrt{\log N(F, M_t \epsilon, |\cdot|_{L^\infty(Z)})} d\epsilon + b_2 M_t \sqrt{\frac{L}{n}}}
\]

where \( b_1, b_2 \) are numerical constants.

We are now ready to state the main result of this section. We first show from the duality result [3] that we can provide an upper bound for the worst-case population performance for any level of robustness \( \rho \). For \( \rho = \rho_n(\theta) \) and \( \theta = \theta_{WRM} \), this certificate is (in a sense) tight as we see below.

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

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

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

\[
\sup_{P:W_c(P,P_0) \leq \rho_n(\theta)} \mathbb{E}_P[\ell(\theta; Z)] \leq \mathbb{E}_{\tilde{P}_n}[\phi_\gamma(\theta; Z)] + \gamma \rho_n(\theta) + \epsilon_n(t)
\]

\[
= \sup_{P:W_c(P,P_0) \leq \rho_n(\theta)} \mathbb{E}_P[\ell(\theta; Z)] + \epsilon_n(t).
\]
See Section C.4 for its proof. We now give a concrete variant of Theorem 3 for Lipschitz functions. When $\Theta$ is finite-dimensional ($\Theta \subset \mathbb{R}^d$), Theorem 3 provides a robustness guarantee scaling linearly with $d$ despite the infinite-dimensional Wasserstein penalty. Assuming there exist $\theta_0 \in \Theta$, $M_\theta < \infty$ such that $|\ell(\theta_0; z)| \leq M_\theta$ for all $z \in Z$, we have the following corollary (see proof in Section C.5).

**Corollary 1.** Let $\ell(\cdot; z)$ be $L$-Lipschitz with respect to some norm $\|\cdot\|$ for all $z \in Z$. Assume that $\Theta \subset \mathbb{R}^d$ satisfies $\text{diam}(\Theta) = \sup_{\theta, \theta' \in \Theta} \|\theta - \theta'\| < \infty$. Then, the bounds (11) and (12) hold with

$$\epsilon_n(t) = b_1 \sqrt{\frac{d(L \text{diam}(\Theta) + M_\theta)}{n}} + b_2(L \text{diam}(\Theta) + M_\theta) \sqrt{\frac{t}{n}},$$

for some numerical constants $b_1, b_2 > 0$.

A key consequence of the bound (11) is that $\gamma \rho + \mathbb{E}_{\tilde{P}_n}[\phi_\gamma(\theta; Z)]$ certifies robustness for the worst-case population objective for any $\rho$ and $\theta$. For a given $\theta$, this certificate is tightest at the achieved level of robustness $\hat{\rho}_n(\theta)$, as noted in the refined bound (12) which follows from the duality result

$$\mathbb{E}_{\tilde{P}_n}[\phi_\gamma(\theta; Z)] + \gamma \hat{\rho}_n(\theta) = \sup_{P: W_c(P, \tilde{P}_n) \leq \hat{\rho}_n(\theta)} \mathbb{E}_P[\ell(\theta; Z)] = \mathbb{E}_{P^*_n(\theta)}[\ell(\theta; Z)]. \tag{13}$$

(See Section C.4 for a proof of these equalities.) We expect $\theta_{\text{WRM}}$, the output of Algorithm 1, to be close to the minimizer of the surrogate loss $\mathbb{E}_{\tilde{P}_n}[\phi_\gamma(\theta; Z)]$ and therefore have the best guarantees. Most importantly, the certificate (13) is easy to compute via expression (10): as noted in Section 2.1, the mappings $T(\theta, Z)$ are efficiently computable for large enough $\gamma$, and $\hat{\rho}_n = \mathbb{E}_{\tilde{P}_n}[c(T(\theta, Z), Z)]$.

### 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 $T(\cdot; z)$ is smooth under Assumptions A and B

$$\|T(\theta_1; z) - T(\theta_2; z)\| \leq \frac{L_{zz}}{\gamma - L_{zz}} \|\theta_1 - \theta_2\| \tag{14}$$

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 $\hat{\rho}_n(\theta) = \mathbb{E}_{\tilde{P}_n}[c(T(\theta; Z), Z)]$, the level of robustness achieved for the empirical problem, concentrates uniformly around its population counterpart.

**Theorem 4.** Let $Z \subset \{z \in \mathbb{R}^d : \|z\| \leq M_z\}$ so that $\|Z\| \leq M_z$ almost surely and assume either that (i) $c(\cdot, \cdot)$ is $L_c$-Lipschitz over $\mathcal{Z}$ with respect to the norm $\|\cdot\|$ 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 $1 - e^{-t}$,

$$\sup_{\theta \in \Theta} |\mathbb{E}_{\tilde{P}_n}[c(T(\theta; Z), Z)] - \mathbb{E}_{P_0}[c(T(\theta; Z), Z)]| \leq 4B \sqrt{\frac{1}{n} \left( t + \log N\left(\Theta, \frac{[\gamma - L_{zz}]_+}{4L_c L_{zz}} \|\cdot\|, k\right) \right)}, \tag{15}$$

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

See Section C.6 for the proof. For $\Theta \subset \mathbb{R}^d$, we have $\log N(\Theta, \epsilon, \|\cdot\|) \leq d \log(1 + \frac{\text{diam}(\Theta)}{\epsilon})$ so that the bound (28) gives the usual $\sqrt{d/n}$ generalization rate for the distance between adversarial
perturbations and natural examples. Another consequence of Theorem 4 is that \( \hat{\rho}_n(\theta_{\text{WRM}}) \) in the certificate (12) 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 \( \mathbb{E}_{P_0}[\epsilon T_\gamma(\theta; Z)] = 0 \) iff \( \nabla_x \ell(\theta; z) = 0 \) almost surely, and hence for large enough \( n \), we have \( \hat{\rho}_n(\theta) > 0 \) by the bound (28).

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) (22), its iterated variant (IFGM) (28), and the projected-gradient method (PGM) (31). PGM augments stochastic gradient steps for the parameter \( \theta \) with projected gradient ascent over \( x \mapsto \ell(\theta; x, y) \), iterating (for data point \( x_i, y_i \))

\[
\Delta x_i^{t+1}(\theta) := \arg\max_{\|\eta\|_p \leq \epsilon} \{\nabla_x \ell(\theta; x_i^t, y_i)\}^{T} \eta \quad \text{and} \quad x_i^{t+1} := \Pi_{B_{\epsilon,p}(x_i)}(x_i^t + \alpha_t \Delta x_i^t(\theta))
\]

for \( t = 1, \ldots, T_{\text{adv}} \), where \( \Pi \) denotes projection onto \( B_{\epsilon,p}(x_i) := \{x : \|x - x_i\|_p \leq \epsilon\} \).

The adversarial training literature (e.g. Goodfellow et al. (22)) usually considers \( \|\cdot\|_\infty \)-norm attacks, which allow imperceptible perturbations to all input features. In most scenarios, however, it is reasonable to defend against weaker adversaries that instead perturb influential features more. We consider this setting and train against \( \|\cdot\|_2 \)-norm attacks. Namely, we use the squared Euclidean cost for the feature vectors \( c_\ell(x, x') := \|x - x'\|_2^2 \) and define the overall cost as the covariate-shift adversary (3) for WRM (Algorithm 1), and we use \( p = 2 \) for FGM, IFGM, PGM training in all experiments; we still 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.

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.

WRM enjoys the theoretical guarantees of Sections 2 and 3 for large \( \gamma \), but for small \( \gamma \) (large adversarial budgets), WRM becomes a heuristic like other methods. In Appendix A.4 we compare WRM with other methods on attacks with large adversarial budgets. In Appendix A.5 we further compare WRM—which is trained to defend against \( \|\cdot\|_2 \)-adversaries—with other heuristics trained to defend against \( \|\cdot\|_\infty \)-adversaries. WRM matches or outperforms other heuristics against imperceptible attacks, while it underperforms for attacks with large adversarial budgets.

4.1 Visualizing the benefits of certified robustness

For our first experiment, we generate synthetic data \( Z = (X, Y) \sim P_0 \) by \( X_i \sim \text{iid} \mathcal{N}(0_2, I_2) \) 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 $\gamma = 2$, and to make fair comparisons with FGM we use

$$
\mathcal{e}^2 = \hat{\rho}_n(\theta_{\text{WRM}}) = W_c(P_n(\theta_{\text{WRM}}), \hat{P}_n) = \mathbb{E}_{\hat{P}_n} [c(T(\theta_{\text{WRM}}, Z), Z)],
$$

for the fast-gradient perturbation magnitude $\mathcal{e}$, 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 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. radial asymmetry in the classification surface) due to the lack of robustness guarantees. WRM with ELU’s provides a certified level of robustness, yielding an axisymmetric classification boundary that hedges against adversarial perturbations in all directions.

Recall that our certificates of robustness on the worst-case performance given in Theorem 3 applies for any level of robustness $\rho$. In Figure 2(a), we plot our certificate (11) against the out-of-sample (test) worst-case performance $\sup_{P, \hat{P}_n, c} \mathbb{E}_P [\ell(\theta; Z)]$. Since the worst-case loss is hard to evaluate directly, we solve its Lagrangian relaxation (6) for different values of $\gamma_{\text{adv}}$. For each $\gamma_{\text{adv}}$, we consider the distance to adversarial examples in the test dataset

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

where $\hat{P}_{\text{test}}$ is the test distribution, $c(z, z') := \|x - x'\|^2 + \infty \cdot 1 \{ y \neq y' \}$ as before, 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 verified that for ELU activations with scale parameter 1, this $\gamma$ is large enough for strong concavity of the inner problem (2b). We computed $\nabla_{xx} \ell(\theta, (x, y))$ over the training data. ReLU’s have no guarantees, but we use 15 gradient steps with stepsize decreasing as $1/\sqrt{t}$ for both activations.
The worst-case losses on the test dataset are then given by

\[ E_{P_{\text{test}}} [f_{\gamma_{\text{adv}}} (\theta_{\text{WRM}}; Z)] + \gamma_{\text{adv}} \delta_{\text{test}} (\theta_{\text{WRM}}) = \sup_{P: W_c (P, P_{\text{test}}) \leq \delta_{\text{test}} (\theta_{\text{WRM}})} E_{P} [f(\theta_{\text{WRM}}; Z)]. \]

As anticipated, our certificate is almost tight near the achieved level of robustness \( \hat{\rho}_{n} (\theta_{\text{WRM}}) \) for WRM \( (10) \) and provides a performance guarantee even for other values of \( \rho \).

### 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 WRM with \( \gamma = 0.04 E_{P} [\|X\|_2] \), and for the other methods we choose \( \epsilon \) as the level of robustness achieved by WRM \( (17) \). In the figures, we scale the budgets \( 1/\gamma_{\text{adv}} \) and \( \epsilon_{\text{adv}} \) for the adversary with \( C_p := E_{P} [\|X\|_p] \). \footnote{For this \( \gamma \), \( f_{\gamma} (\theta_{\text{WRM}}; z) \) is strongly concave for 98% of the training data.}

First, in Figure 2(b) we again illustrate the validity of our certificate of robustness \( (11) \) for the worst-case test performance for arbitrary level of robustness \( \rho \). We see that our certificate provides a performance guarantee for out-of-sample worst-case performance.

We now compare adversarial training techniques. 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. It is thus important to distinguish the methods’ abilities to combat attacks. We test performance of the five methods (ERM, FGM, IFGM, PGM, WRM) under PGM attacks \( (16) \) with respect to 2- and \( \infty \)-norms. In Figure 3(a) and (b), all adversarial methods outperform ERM, and WRM offers more robustness even with respect to these PGM attacks. Training with the Euclidean cost still provides robustness to \( \infty \)-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. We note that small values of \( \hat{\rho}_{\text{test}} (\theta) \), the distance to adversarial examples \( (18) \) correspond to small magni-
Figure 3. PGM attacks on the MNIST dataset. (a) and (b) show test misclassification error vs. the adversarial perturbation level $\epsilon_{adv}$ 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 PGM, FGM, and IFGM models as well as the estimated radius $\sqrt{\hat{\rho}_n(\theta_{WRM})}$. For MNIST, $C_2 = 9.21$ and $C_\infty = 1.00$.

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 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 $\sum_t \lambda^t \mathbb{E}[r(s^t)]$ (with discount factor $\lambda$); this is analogous to minimizing $\mathbb{E}_P[\ell(\theta; Z)]$ in supervised learning. Robust MDP’s consider an ambiguity set $P_{sa}$ for state-action transitions. The goal is maximizing the worst-case realization $\inf_{P \in P_{sa}} \sum_t \lambda^t \mathbb{E}_P[r(s^t)]$, analogous to problem (1).

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

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

(19)
such that \( \arg\max_a Q(s,a) \) is (eventually) the optimal action in state \( s \) to maximize cumulative reward. In scenarios where the underlying environment has a continuous state-space and we represent \( Q \) with a differentiable function (e.g. [33]), we can modify the update (19) with an adversarial state perturbation to incorporate distributional robustness. Namely, we draw the nominal state-transition update \( \tilde{s}_{t+1} \sim p_{sa}(s_t, a_t) \), and proceed with the update (19) using the perturbation

\[
\tilde{s}_{t+1} \leftarrow \arg\min_s \left\{ r(s) + \lambda \max_a Q(s,a) + \gamma c(s, \tilde{s}_{t+1}) \right\} . \tag{20}
\]

For large \( \gamma \), we can again solve problem (20) efficiently using gradient descent. This procedure provides robustness to uncertainties in state-action transitions. For tabular Q-learning, where we represent \( Q \) only over a discretized covering of the underlying state-space, we can either neglect the second term in the update (20) and, after performing the update, round \( s_{t+1} \) as usual, or we can perform minimization directly over the discretized covering. In the former case, since the update (20) simply modifies the state-action transitions (independent of \( Q \)), standard results on convergence for tabular Q-learning (e.g. Szepesvári and Littman [47]) apply under these adversarial dynamics.

We test our adversarial training procedure 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 from the vertical. Furthermore, we use a tabular representation for \( Q \) with 30 discretized states for \( \beta \) and 15 for its time-derivative \( \dot{\beta} \) (we perform the update (20) without the \( Q \)-dependent term). The action space is binary: push the cart left or right with a fixed force. Due to the nonstationary, policy-dependent 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 both models with perturbations to the physical parameters. Namely, we shrink/magnify the pole’s mass by 2, shrink/magnify the pole’s length by 2, and shrink/magnify the strength of gravity \( g \) by 5. The dynamics of the system are such that the
### Table 1. Episode length over 1000 trials (mean ± standard error)

| Environment | Regular       | Robust        |
|-------------|---------------|---------------|
| Original    | 399.7 ± 0.1   | 400.0 ± 0.0   |
| Easier environments |          |               |
| Light       | 400.0 ± 0.0   | 400.0 ± 0.0   |
| Long        | 400.0 ± 0.0   | 400.0 ± 0.0   |
| Soft g      | 400.0 ± 0.0   | 400.0 ± 0.0   |
| Harder environments |       |               |
| Heavy       | 150.1 ± 4.7   | 334.0 ± 3.7   |
| Short       | 245.2 ± 4.8   | 400.0 ± 0.0   |
| Strong g    | 189.8 ± 2.3   | 398.5 ± 0.3   |

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 preferable 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.
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A Additional Experiments

A.1 MNIST attacks

We repeat Figure 3 using FGM (top row of Figure 6) and IFGM (bottom row of Figure 6) attacks. The same trends are evident as in Figure 3.

![Graphs showing test error vs. adversarial perturbation level for FGM and IFGM attacks.](image)

**Figure 6.** Further attacks on the MNIST dataset. We illustrate test misclassification error vs. the adversarial perturbation level $\epsilon_{\text{adv}}$. Top row: FGM attacks, bottom row: IFGM attacks. Left column: Euclidean-norm attacks, right column: $\infty$-norm attacks. The vertical bar in (a) and (c) indicates the perturbation level that was used for training the PGM, FGM, and IFGM models and the estimated radius $\sqrt{\hat{\rho}_n(\theta_{\text{WRM}})}$.

A.2 MNIST stability of loss surface

In Figure 7 we repeat the illustration in Figure 4(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.
Figure 7. Visualizing stability over inputs. We illustrate the smallest WRM perturbation (largest $\gamma_{adv}$) necessary to make a model misclassify a datapoint.

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 $\gamma$. As the bound (11) 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 $\gamma$, the amount of achieved robustness—measured here by test error on adversarial perturbations with $\gamma_{adv}$—has diminishing gains; this is again consistent with our theory which says that the inner problem (2b) is not efficiently computable for small $\gamma$. 
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 ($\gamma_{adv}$ indicated by the vertical bar).
A.4 MNIST experiments with a larger adversarial budget

Figures 9 and 10 repeat Figures 2(b), 3 and 6 for a larger training adversarial budget ($\gamma = 0.02C_2$) as well as larger test adversarial budgets. The distinctions in performance between various methods are less apparent now. For our method, the inner supremum is no longer strongly concave for over 10% of the data, indicating that we no longer have guarantees of performance. For large adversaries (i.e. large desired robustness values) our approach becomes a heuristic just like the other approaches.

**Figure 9.** Empirical comparison between certificate of robustness (blue) and out-of-sample (test) worst-case performance (red) for the experiments on MNIST with a larger training adversary. The statistical error term $\epsilon_n(t)$ is omitted from the certificate. The vertical bar indicates the achieved level of robustness on the training set $\hat{\rho}_n(\theta_{\text{WRM}})$. 

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Figure 10. Attacks on the MNIST dataset with larger (training and test) adversarial budgets. We illustrate test misclassification error vs. the adversarial perturbation level $\epsilon_{adv}$. Top row: PGM attacks, middle row: FGM attacks, bottom row: IFGM attacks. Left column: Euclidean-norm attacks, right column: $\infty$-norm attacks. The vertical bar in (a), (c), and (e) indicates the perturbation level that was used for training the PGM, FGM, and IFGM models and the estimated radius $\sqrt{\hat{\rho}_n(\theta_{WRM})}$. 

(a) Test error vs. $\epsilon_{adv}$ for $\| \cdot \|_2$-PGM attack 
(b) Test error vs. $\epsilon_{adv}$ for $\| \cdot \|_\infty$-PGM attack 
(c) Test error vs. $\epsilon_{adv}$ for $\| \cdot \|_2$-FGM attack 
(d) Test error vs. $\epsilon_{adv}$ for $\| \cdot \|_\infty$-FGM attack 
(e) Test error vs. $\epsilon_{adv}$ for $\| \cdot \|_2$-IFGM attack 
(f) Test error vs. $\epsilon_{adv}$ for $\| \cdot \|_\infty$-IFGM attack
A.5 MNIST ∞-norm experiments

We consider training FGM, IFGM, and PGM with \( p = \infty \). We first compare with WRM trained in the same manner as before—with the squared Euclidean cost. Then, we consider a heuristic Lagrangian approach for training WRM with the squared ∞-norm cost.

A.5.1 Comparison with standard WRM

Our method (WRM) is trained to defend against \( \| \cdot \|_2 \)-norm attacks by using the cost function

\[
c((x, y), (x_0, y_0)) = \|x - x_0\|_2^2 + \infty \cdot 1 \{y \neq y_0\}
\]

with the convention that \( 0 \cdot \infty = 0 \). Standard adversarial training methods often train to defend against \( \| \cdot \|_\infty \)-norm attacks, which we compare our method against in this subsection. Direct comparison between these approaches is not immediate, as we need to determine a suitable \( \epsilon \) to train FGM, IFGM, and PGM in the ∞-norm that corresponds to the penalty parameter \( \gamma \) for the \( \| \cdot \|_2 \)-norm that we use. Similar to the expression (17), we use

\[
\epsilon := \mathbb{E} \hat{P}_n \left[ \| T(\theta_{WRM}, Z) - Z \|_\infty \right]
\]

as the adversarial training budget for FGM, IFGM and PGM with \( \| \cdot \|_\infty \)-norms. Because 2-norm adversaries tend to focus budgets on a subset of features, the resulting ∞-norm perturbations are relatively large. In Figure 11 we show the results trained with a small training adversarial budget. In this regime, \( (\text{large } \gamma, \text{small } \epsilon) \), WRM matches the performance of other techniques.

In Figure 12 we show the results trained with a large training adversarial budget. In this regime \( (\text{small } \gamma, \text{large } \epsilon) \), performance between WRM and other methods diverge. WRM, which provably defends against small perturbations, outperforms other heuristics against imperceptible attacks for both Euclidean and ∞ norms. Further, it outperforms other heuristics on natural images, showing that it consistently achieves a smaller price of robustness. On attacks with large adversarial budgets \( (\text{large } \epsilon_{\text{adv}}) \), however, the performance of WRM is worse than that of the other methods (especially in the case of ∞-norm attacks). These findings verify that WRM is a practical alternative over existing heuristics for the moderate levels of robustness where our guarantees hold.

A.5.2 Comparison with \( \| \cdot \|_\infty \)-WRM

Our computational guarantees given in Theorem 2 does not hold anymore when we consider ∞-norm adversaries:

\[
c((x, y), (x_0, y_0)) = \|x - x_0\|_\infty^2 + \infty \cdot 1 \{y \neq y_0\}.
\]

Optimizing the Lagrangian formulation (2b) with the ∞-norm is difficult since subtracting a multiple of the ∞-norm does not add (negative) curvature in all directions. In Appendix E, we propose a heuristic algorithm for solving the inner supremum problem (2b) with the above cost function (22). Our approach is based on a variant of proximal algorithms.

We compare our proximal heuristic introduced in Appendix E with other adversarial training procedures that were trained against ∞-norm adversaries. Results are shown in Figure 13 for a small training adversary and Figure 14 for a large training adversary. We observe that similar trends as in Section A.5.1 hold again.
Figure 11. Attacks on the MNIST dataset. We compare standard WRM with $\infty$-norm PGM, FGM, IFGM. We illustrate test misclassification error vs. the adversarial perturbation level $\epsilon_{\text{adv}}$. Top row: PGM attacks, middle row: FGM attacks, bottom row: IFGM attacks. Left column: Euclidean-norm attacks, right column: $\infty$-norm attacks. The vertical bar in (a), (c), and (e) indicates the estimated radius $\sqrt{\hat{\rho}_n(\theta_{\text{WRM}})}$. The vertical bar in (b), (d), and (f) indicates the perturbation level that was used for training the PGM, FGM, and IFGM models via \cite{21}.
Figure 12. Attacks on the MNIST dataset with larger (training and test) adversarial budgets. We compare standard WRM with $\infty$-norm PGM, FGM, IFGM models. We illustrate test misclassification error vs. the adversarial perturbation level $\epsilon_{adv}$. Top row: PGM attacks, middle row: FGM attacks, bottom row: IFGM attacks. Left column: Euclidean-norm attacks, right column: $\infty$-norm attacks. The vertical bar in (a), (c), and (e) indicates the estimated radius $\sqrt{\hat{\rho}_n(\theta_{WRM})}$. The vertical bar in (b), (d), and (f) indicates the perturbation level that was used for training the PGM, FGM, and IFGM models via (21).
Figure 13. Attacks on the MNIST dataset. All models are trained in the $\infty$-norm. We illustrate test misclassification error vs. the adversarial perturbation level $\epsilon_{adv}$. Top row: PGM attacks, middle row: FGM attacks, bottom row: IFGM attacks. Left column: Euclidean-norm attacks, right column: $\infty$-norm attacks. The vertical bar in (b), (d), and (f) indicates the perturbation level that was used for training the PGM, FGM, and IFGM models and the estimated radius $\sqrt{\hat{\rho}_n(\theta_{WRM})}$. 

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Figure 14. Attacks on the MNIST dataset with larger (training and test) adversarial budgets. All models are trained in the $\infty$-norm. We illustrate test misclassification error vs. the adversarial perturbation level $\epsilon_{\text{adv}}$. Top row: PGM attacks, middle row: FGM attacks, bottom row: IFGM attacks. Left column: Euclidean-norm attacks, right column: $\infty$-norm attacks. The vertical bar in (b), (d), and (f) indicates the perturbation level that was used for training the PGM, FGM, and IFGM models and the estimated radius $\sqrt{\hat{\rho}_n(\theta_{WRM})}$. 
B Finding worst-case perturbations with ReLU’s is NP-hard

We show that computing worst-case perturbations \( \sup_{u \in U} \ell(\theta; z + u) \) is NP-hard for a large class of feedforward neural networks with ReLU activations. This result is essentially due to Katz et al.\cite{26}. 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 \( \{ u \in U \} \) can be recognized in polynomial time (i.e. a deterministic algorithm can decide in polynomial time whether \( u \in U \)), 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.\footnote{Note that \( z, u \in \mathbb{R}^m \), so trivially the dimensionality of the solution grows polynomially.}

Furthermore, we impose separable structure on \( U \), that is, \( U := \{ v \leq u \leq w \} \) for some \( v < w \in \mathbb{R}^m \).

**Lemma 2.** Consider feedforward neural networks with ReLU’s and let \( U := \{ v \leq u \leq w \} \), where \( v < w \) such that the optimization problem \( \max_{u \in U} \ell(\theta; z + u) \) 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.\cite{26} 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

For completeness, we provide an alternative proof to that given in Blanchet and Murthy\cite{7} using convex analysis. Our proof is less general, requiring the cost function \( c \) to be continuous and convex in its first argument. The below general duality result gives Proposition 1 as an immediate special case. Recalling Rockafellar and Wets\cite{43, 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\cite{43, Cor. 14.34}; therefore, \( g(x, z) = \gamma c(x, z) - \ell(\theta; x) \) is a normal integrand. We have the following theorem.

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

**Proof** First, the mapping \( P \mapsto W_c(P, Q) \) is convex in the space of probability measures. As taking \( P = Q \) yields \( W_c(Q, Q) = 0 \), Slater’s condition holds and we may apply standard (infinite dimensional) duality results [30, Thm. 8.7.1] to obtain
\[
\sup_{P: W_c(P, Q)} \int f(x) dP(x) = \sup_{P: W_c(P, Q)} \inf_{\gamma \geq 0} \left\{ \int f(x) dP(x) - \gamma W_c(P, Q) + \gamma \rho \right\}
= \inf_{\gamma \geq 0} \sup_{P: W_c(P, Q)} \left\{ \int f(x) dP(x) - \gamma W_c(P, Q) + \gamma \rho \right\}.
\]

Now, noting that for any \( M \in \Pi(P, Q) \) we have \( \int f dP = \int \int f(x) dM(x, z) \), 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
\[
\sup_{P: W_c(P, Q)} \int f(x) dP(x) = \inf_{\gamma \geq 0} \sup_{M \in \Pi(P, Q)} \left\{ \int [f(x) - \gamma c(x, z)] dM(x, z) + \gamma \rho \right\}. \tag{23}
\]

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 (23), we have that
\[
\sup_{P, M \in \Pi(P, Q)} \int [f(x) - \gamma c(x, z)] dM(x, z) \leq \int \sup_{x \in X} [f(x) - \gamma c(x, z)] dQ(z).
\]
We would like to show equality in the above. To that end, we note that if \( \mathcal{P} \) denotes the space of regular conditional probabilities (Markov kernels) from \( Z \) to \( X \), then
\[
\sup_{P, M \in \Pi(P, Q)} \int [f(x) - \gamma c(x, z)] dM(x, z) \geq \sup_{P \in \mathcal{P}} \int [f(x) - \gamma c(x, z)] dP(x | z) dQ(z).
\]
Recall that a conditional distribution \( P(\cdot | z) \) is regular if \( P(\cdot | z) \) is a distribution for each \( z \) and for each measurable \( A \), the function \( z \mapsto P(A | z) \) is measurable. Let \( \mathcal{X} \) denote the space of all measurable mappings \( z \mapsto x(z) \) from \( Z \) to \( X \). Using the powerful measurability results of Rockafellar and Wets [43, Theorem 14.60], we have
\[
\sup_{x \in \mathcal{X}} \int [f(x(z)) - \gamma c(x(z), z)] dQ(z) = \int \sup_{x \in \mathcal{X}} [f(x) - \gamma c(x, z)] dQ(z)
\]
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 \( P(\cdot | z) \) to be supported on \( x(z) \), which is evidently measurable. Then using the
Lemma 3. the following result.

\[ \Theta \times Z \]

for all \( \theta \) such that \( C \subset \Theta \) from above and Holder's inequality, we obtain

\[ g \]

using a variant of the envelope (or Danskin’s) theorem, we first show directional differentiability

\[ \bar{\Theta} \]

Summing these inequalities gives

\[ \lambda \| z^*_1 - z^*_2 \|^2 \leq f(\theta_2, z^*_2) - f(\theta_2, z^*_1) \] and \( f(\theta_2, z^*_2) \leq f(\theta_2, z^*_1) + g_z(\theta_2, z^*_1) + g_z(\theta_2, z^*_1)^T (z^*_2 - z^*_1) - \frac{\lambda}{2} \| z^*_1 - z^*_2 \|^2. \]

Summing these inequalities gives

\[ \lambda \| z^*_1 - z^*_2 \|^2 \leq g_z(\theta_2, z^*_1) + g_z(\theta_1, z^*_1)^T (z^*_2 - z^*_1), \]

where the last inequality follows because \( g_z(\theta_1, z^*_1)^T (z^*_2 - z^*_1) \leq 0. \) Using a cross-Lipschitz condition from above and Holder’s inequality, we obtain

\[ \lambda \| z^*_1 - z^*_2 \|^2 \leq \| g_z(\theta_2, z^*_1) - g_z(\theta_1, z^*_1) \| \| z^*_1 - z^*_2 \| \leq \frac{L_{x\theta}}{\lambda} \| \theta_1 - \theta_2 \| \| z^*_1 - z^*_2 \|, \]

that is,

\[ \| z^*_1 - z^*_2 \| \leq \frac{L_{x\theta}}{\lambda} \| \theta_1 - \theta_2 \|. \] (24)

To see the second inequality, we show that \( \bar{f} \) is differentiable with \( \nabla \bar{f}(\theta) = g_\theta(\theta, z^*(\theta)). \) By using a variant of the envelope (or Danskin’s) theorem, we first show directional differentiability of \( \bar{f} \). Recall that we say \( f \) is inf-compact if for all \( \theta_0 \in \Theta \), there exists \( \alpha > 0 \) and a compact set \( C \subset \Theta \) such that

\[ \theta \neq \{ z \in Z : f(\theta, z) \leq \alpha \} \subset C \]

for all \( \theta \) in some neighborhood of \( \theta_0 \). See Bonnans and Shapiro [8, Theorem 4.13] for a proof of the following result.

Lemma 3. Suppose that \( f(\cdot, z) \) is differentiable in \( \theta \) for all \( z \in Z \), and \( f, \nabla_z f \) are continuous on \( \Theta \times Z \). If \( f \) is inf-compact, then \( f \) is directionally differentiable with

\[ \bar{f}'(\theta, d) = \sup_{z \in S(\theta)} \nabla_z f(\theta, z)^T d \]

where \( S(\theta) = \arg\min_z f(\theta, z) \).
Now, note that from Assumption B, we have

\[ |f(\theta, z) - f(\theta_0, z) - \nabla_{\theta} f(\theta_0, z)^\top (\theta - \theta_0)| \leq L_{\theta\theta} \|\theta - \theta_0\| \]

from which it is easy to see that \( f \) is inf-compact. Applying Lemma 3 to \( \bar{f} \) and noting that \( S(\theta) \) is unique by strong convexity of \( f(\theta, \cdot) \), we have that \( \bar{f} \) is directionally differentiable with \( \nabla \bar{f}(\theta) = g_\theta(\theta, z^*(\theta)) \). Since \( g_\theta \) is continuous by Assumption B and \( z^*(\theta) \) is Lipschitz (24), we conclude that \( \bar{f} \) is differentiable.

Finally, we have

\[
\|g_\theta(\theta_1, z_1^*) - g_\theta(\theta_2, z_2^*)\|_* \leq \|g_\theta(\theta_1, z_1^*) - g_\theta(\theta_1, z_2^*)\|_* + \|g_\theta(\theta_1, z_2^*) - g_\theta(\theta_2, z_2^*)\|_* \\
\leq L_{\theta\theta} \|z_1^* - z_2^*\| + L_{\theta\theta} \|\theta_1 - \theta_2\| \\
\leq \left( L_{\theta\theta} + \frac{L_{\theta^2} L_{\theta\theta}}{\lambda} \right) \|\theta_1 - \theta_2\|, 
\]

where we have used inequality (24) again. This is the desired result.

### C.3 Proof of Theorem 2

Our proof is based on that of Ghadimi and Lan [20].

For shorthand, let \( f(\theta, z; z_0) = \ell(\theta; z) - \gamma c(\theta, z_0) \), noting that we perform gradient steps with

\[ g^t = \nabla \theta f(\theta^t, z(\theta^t; z^t); z^t) \]

for \( \bar{z}^t \) an \( \epsilon \)-approximate maximizer of \( f(\theta, z; z^t) \) in \( z \), and \( \theta^{t+1} = \theta^t - \alpha_t g^t \). By a Taylor expansion using the \( L_{\phi}\)-smoothness of the objective \( F \), we have

\[
F(\theta^{t+1}) \leq F(\theta^t) + \langle \nabla F(\theta^t), \theta^{t+1} - \theta^t \rangle + \frac{L_{\phi}}{2} \|\theta^{t+1} - \theta^t\|^2_2 \\
= F(\theta^t) - \alpha_t \|\nabla F(\theta^t)\|^2_2 + \frac{L_{\phi} \alpha_t^2}{2} \|g^t\|^2_2 + \alpha_t \langle \nabla F(\theta^t), \nabla F(\theta^t) - g^t \rangle \\
= F(\theta^t) - \alpha_t \left( 1 - \frac{L_{\phi} \alpha_t}{2} \right) \|\nabla F(\theta^t)\|^2_2 \\
+ \alpha_t \left( 1 + \frac{L_{\phi} \alpha_t}{2} \right) \langle \nabla F(\theta^t), \nabla F(\theta^t) - g^t \rangle + \frac{L_{\phi} \alpha_t^2}{2} \|g^t - \nabla F(\theta^t)\|^2_2. \tag{25} \]

Recalling the definition (23) of \( \phi_\gamma(\theta; z_0) = \sup_{z \in \mathcal{Z}} f(\theta, z; z_0) \), we define the potentially biased errors \( \delta^t = g^t - \nabla_{\theta} \phi_\gamma(\theta^t; z^t) \). Letting \( z^*_t = \text{argmax}_z f(\theta^t, z; z^t) \), these errors evidently satisfy

\[
\|\delta^t\|^2_2 = \|\nabla_{\theta} \phi_\gamma(\theta^t; z^t) - \nabla_{\theta} f(\theta, z^*_t; z^t)\|^2_2 = \|\nabla_{\theta} \ell(\theta, z^*_t) - \nabla_{\theta} \ell(\theta, \hat{z}^*_t)\|^2_2 \\
\leq L_{\theta z}^2 \|\hat{z}^t - z^*_t\|^2_2 \leq \frac{L_{\theta z}^2}{\lambda} \epsilon, 
\]

where the final inequality uses the \( \lambda = \gamma - L_{zz} \) strong-concavity of \( z \mapsto f(\theta, z; z_0) \). For shorthand,
let \( \hat{\epsilon} = \frac{2L_t^2}{\gamma - L_t^2} \epsilon \). Substituting the preceding display into the progress guarantee (25), we have
\[
F(\theta^{t+1}) = F(\theta^t) - \alpha_t \left( 1 - \frac{L_\theta \alpha_t}{2} \right) \| \nabla F(\theta^t) \|^2 - \alpha_t \left( 1 + \frac{L_\theta \alpha_t}{2} \right) \langle \nabla F(\theta^t), \delta^t \rangle \\
+ \alpha_t \left( 1 + \frac{L_\theta \alpha_t}{2} \right) \langle \nabla F(\theta^t), \nabla F(\theta^t) - \nabla \phi_{\gamma}(\theta; z^t) \rangle + \frac{L_\theta \alpha_t^2}{2} \| \nabla \phi_{\gamma}(\theta; z^t) + \delta^t - \nabla F(\theta^t) \|^2_2 \\
\leq F(\theta^t) - \frac{\alpha_t}{2} (1 - L_\theta \alpha_t) \| \nabla F(\theta^t) \|^2_2 + \frac{\alpha_t}{2} \left( 1 + \frac{L_\theta \alpha_t}{2} \right) \| \delta^t \|^2_2 \\
\alpha_t \left( 1 + \frac{L_\theta \alpha_t}{2} \right) \langle \nabla F(\theta^t), \nabla F(\theta^t) - \nabla \phi_{\gamma}(\theta; z^t) \rangle + L_\theta \alpha_t^2 \| \nabla \phi_{\gamma}(\theta; z^t) - \nabla F(\theta^t) \|^2_2 + \| \delta^t \|^2_2.
\]
Noting that \( \mathbb{E}[\nabla \phi_{\gamma}(\theta^t; z^t) | \theta^t] = \nabla F(\theta^t) \), we take expectations to find
\[
\mathbb{E}[F(\theta^{t+1}) - F(\theta^t) | \theta^t] \leq -\frac{\alpha_t}{2} (1 - L_\theta \alpha_t) \| \nabla F(\theta^t) \|^2_2 + \left( \frac{\alpha_t}{2} + \frac{5L_\theta \alpha_t^2}{4} \right) \hat{\epsilon} + L_\theta \alpha_t^2 \sigma^2,
\]
where we have used that \( \mathbb{E}[\| \nabla \phi_{\gamma}(\theta; Z) - \nabla F(\theta) \|^2_2] \leq \sigma^2 \) by assumption.

The bound (26) gives the theorem essentially immediately for fixed stepsizes \( \alpha \), as we have
\[
\frac{\alpha_t}{2} \left( 1 - L_\theta \alpha_t \right) \mathbb{E} \left[ \sum_{t=1}^{T} \| \nabla F(\theta^t) \|^2_2 \right] \leq F(\theta^0) - \mathbb{E}[F(\theta^{T+1})]+ \frac{T \alpha}{2} \left( 1 + \frac{5L_\theta \alpha_t}{4} \right) \hat{\epsilon} + TL_\theta \alpha_t^2 \sigma^2.
\]
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 (11). From the duality result (5), we have the deterministic result that
\[
\sup_{P : W_c(P,Q) \leq \rho} \mathbb{E}_Q[\ell(\theta; Z)] \leq \gamma \rho + \mathbb{E}_Q[\phi_{\gamma}(\theta; Z)]
\]
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 [10].

First, we have that
\[
\phi_{\gamma}(\theta; z) \in [-M_\ell, M_\ell],
\]
because \( -M_\ell \leq \ell(\theta; z) \leq \phi_{\gamma}(\theta; z) \leq \sup_z \ell(\theta; z) \leq M_\ell \). Thus, the functional \( \theta \mapsto F_n(\theta) \) satisfies bounded differences [11, Thm. 6.2], and applying standard results on Rademacher complexity [1] and entropy integrals [49, Ch. 2.2] gives the result.

To see the second result (12), we substitute \( \rho = \hat{\rho}_n \) in the bound (11). Then, with probability at least \( 1 - e^{-t} \), we have
\[
\sup_{P : W_c(P,P_0) \leq \hat{\rho}_n(\theta)} \mathbb{E}_P[\ell(\theta; Z)] \leq \gamma \hat{\rho}_n(\theta) + \mathbb{E}_{\hat{P}_n}[\phi_{\gamma}(\theta; Z)] + \epsilon_n(t).
\]
Since we have
\[
\sup_{P : W_c(P,P_0) \leq \hat{\rho}_n(\theta)} \mathbb{E}_P[\ell(\theta; Z)] = \mathbb{E}_{\hat{P}_n}[\phi_{\gamma}(\theta; Z)] + \gamma \hat{\rho}_n(\theta).
\]
from the strong duality in Proposition [11] our second result follows.
C.5  Proof of Corollary 6.11

The result is essentially standard [49], 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 \(\min \|\ell(\theta; z) - \ell(\theta_i; z)\| \leq L\epsilon\) 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 \(\text{diam}(\Theta) = \sup_{\theta, \theta' \in \Theta} \|\theta - \theta'\|\). Noting that \(|\ell(\theta; Z)| \leq L \text{diam}(\Theta) + M_0 =: M_\ell\), we have the result.

C.6  Proof of Theorem 4.11

Define

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

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

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 \(P^\epsilon\) be an \(\epsilon\)-maximizer, so that

\[
\mathbb{E}_{P^\epsilon}[\ell(\theta; Z)] - \gamma W_\epsilon(P^\epsilon, P_0) \geq \sup_P \{\mathbb{E}_P[\ell(\theta; Z)] - \gamma W_\epsilon(P_n, P_0)\} - \epsilon.
\]

As \(Z\) is compact, the collection \(\{P^{1/k}\}_{k \in \mathbb{N}}\) is a uniformly tight collection of measures. By Prohorov’s theorem [3, 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 [50, Corollary 6.11] then imply that

\[
\lim_{k \to \infty} W_\epsilon(P^{1/k}, P_0) = W_\epsilon(P^*, P_0).
\]

Combining (27) and the monotone convergence theorem, we obtain

\[
\mathbb{E}_{P^*}[\ell(\theta; Z)] - \gamma W_\epsilon(P^*, P_0) = \lim_{k \to \infty} \left\{ \mathbb{E}_{P^{1/k}}[\ell(\theta; Z)] - \gamma W_\epsilon(P^{1/k}, P_0) \right\}
\]

\[
\geq \sup_P \{\mathbb{E}_P[\ell(\theta; Z)] - \gamma W_\epsilon(P, P_0)\}.
\]

We conclude that \(P^*\) is attained for all \(P_0\).

Next, we show the concentration result (28). Recall the definition (9) of the transportation mapping

\[
T(\theta, z) := \arg\max_{z' \in Z} \left\{ \ell(\theta; z') - \gamma c(z', z) \right\},
\]

which is unique and well-defined under our strong concavity assumption that \(\gamma > L z z\), and smooth (recall Eq. (13)) in \(\theta\). Then by Proposition 11 (or by using a variant of Kantorovich duality [50, Chs. 9–10]), we have

\[
\mathbb{E}_{P_n^*}[\ell(\theta; Z)] = \mathbb{E}_{P_n^*}[\ell(\theta; T(\theta; Z))]
\]

\[
W_\epsilon(P_n^*(\theta), \hat{P}_n) = \mathbb{E}_{P_n^*}[c(T(\theta; Z), Z)]
\]

\[
W_\epsilon(P^*(\theta), P_0) = \mathbb{E}_{P_0}[c(T(\theta; Z), Z)].
\]
We now proceed by showing the uniform convergence of
\[ \mathbb{E}_{P_n}[c(T(\theta; Z), Z)] \to \mathbb{E}_{P_0}[c(T(\theta; Z), Z)] \]
under both cases (i), that \( c \) is Lipschitz, and (ii), that \( \ell \) is Lipschitz in \( z \), using a covering argument on \( \Theta \). Recall inequality (14) (i.e. Lemma 1), which is that
\[ \|T(\theta_1; z) - T(\theta_2; z)\| \leq \frac{L_{2\theta}}{[\gamma - L_{zz}]_+} \|\theta_1 - \theta_2\|. \]
We have the following lemma.

**Lemma 4.** Assume the conditions of Theorem 4. Then for any \( \theta_1, \theta_2 \in \Theta \),
\[ |c(T(\theta_1; z), z) - c(T(\theta_2; z), z)| \leq \frac{L_c L_{2\theta}}{[\gamma - L_{zz}]_+} \|\theta_1 - \theta_2\|. \]

**Proof.** In the first case, that \( c \) is \( L_c \)-Lipschitz in its first argument, this is trivial: we have
\[ |c(T(\theta_1; z), z) - c(T(\theta_2; z), z)| \leq L_c \|T(\theta_1; z) - T(\theta_2; z)\| \leq \frac{L_c L_{2\theta}}{[\gamma - L_{zz}]_+} \|\theta_1 - \theta_2\| \]
by the smoothness inequality (14) for \( T \).

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

Using Lemma 4 we obtain that \( \theta \mapsto |\mathbb{E}_{P_n}[c(T(\theta; Z), \theta)] - \mathbb{E}_{P_0}[c(T(\theta; Z), Z)]| \) is \( 2L_c L_{2\theta}/[\gamma - L_{zz}]_+ \)-Lipschitz. Let \( \Theta_{\text{cover}} = \{\theta_1, \cdots, \theta_N\} \) be a \( \frac{t}{2L_c L_{2\theta}} \)-cover of \( \Theta \) with respect to \( \|\cdot\| \). From Lipschitzness of \( |\mathbb{E}_{P_n}[c(T(\theta; Z), Z)] - \mathbb{E}_{P_0}[c(T(\theta; Z), Z)]| \), we have that if for all \( \theta \in \{\Theta_{\text{cover}}\} \),
\[ |\mathbb{E}_{P_n}[c(T(\theta; Z), Z)] - \mathbb{E}_{P_0}[c(T(\theta; Z), \theta)]| \leq \frac{t}{2}, \]
then it follows that
\[ \sup_{\theta \in \Theta} |\mathbb{E}_{P_n}[c(T(\theta; Z), Z)] - \mathbb{E}_{P_0}[c(T(\theta; Z), Z)]| \leq t. \]

Under the first assumption (i), we have \( |c(T(\theta; Z), Z)| \leq 2L_c M_2 \). Applying Hoeffding’s inequality, for any fixed \( \theta \in \Theta \)
\[ \mathbb{P} \left( |\mathbb{E}_{P_n}[c(T(\theta; Z), Z)] - \mathbb{E}_{P_0}[c(T(\theta; Z), Z)]| \geq \frac{t}{2} \right) \leq 2 \exp \left( -\frac{nt^2}{32L_c^2 M_2^2} \right). \]

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Taking a union bound over \(\theta_1, \ldots, \theta_N\), we conclude that
\[
P \left( \sup_{\theta \in \Theta} \left| \mathbb{E}_{F_n}[c(T(\theta; Z), Z)] - \mathbb{E}_{F_0}[c(T(\theta; Z), Z)] \right| \geq t \right) \leq 2N \left( \Theta, \frac{[\gamma - L_{z\theta}]^+ + 1}{8L_{z\theta}}, \|\cdot\| \right) \exp \left( -\frac{nt^2}{32L_{z\theta}^2M_z^2} \right)
\]
which was our desired result (28).

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.

\section{Supervised Learning}

In supervised learning settings, it is often natural—for example, in classification—to only consider adversarial perturbations to the feature vectors (covariates). In this section, we give an adaptation of the results in Sections 2 and 3 (Theorems 2 and 4) to such scenarios. Let \(Z = (X, Y) \in \mathcal{X} \times \mathbb{R}\) where \(X \in \mathcal{X}\) is a feature vector and \(Y \in \mathbb{R}\) is a label. In classification settings, we have \(Y \in \{1, \ldots, K\}\). We consider an adversary that can only perturb the feature vector \(X\), which can be easily represented in our robust formulation (2) by defining the cost function \(c: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}_+ \cup \{\infty\}\) as follows: for \(z = (x, y)\) and \(z' = (x', y')\), recall the covariate shift cost function (8)
\[
c(z, z') := c_x(x, x') + \infty \cdot 1 \{y \neq y'\},
\]
where \(c_x: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}_+\) is the transportation cost for the feature vector \(X\). As before, we assume that \(c_x\) is nonnegative, continuous, convex in its first argument and satisfies \(c_x(x, x) = 0\).

Under the cost function (8), the robust surrogate loss in the penalty problem (2) and its empirical counterpart (7) becomes
\[
\phi_{\gamma}(\theta; (x_0, y_0)) = \sup_{x \in \mathcal{X}} \{\ell(\theta; (x, y_0)) - \gamma c_x(x, x_0)\}.
\]

Similarly as in Section 2.1, we require the following two assumptions that guarantee efficient computability of the robust surrogate \(\phi_{\gamma}\).

\textbf{Assumption C.} The function \(c_x: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}_+\) is continuous. For each \(x_0 \in \mathcal{X}\), \(c_x(\cdot; x_0)\) is 1-strongly convex with respect to the norm \(\|\cdot\|\).

Let \(\|\cdot\|_\ast\) be the dual norm to \(\|\cdot\|\); we again abuse notation by using the same norm \(\|\cdot\|\) on \(\Theta\) and \(\mathcal{X}\), though the specific norm is clear from context.

\textbf{Assumption D.} The loss \(\ell: \Theta \times \mathcal{X} \rightarrow \mathbb{R}\) satisfies the Lipschitzian smoothness conditions
\[
\|\nabla_{\theta}\ell(\theta; (x, y)) - \nabla_{\theta}\ell(\theta'; (x, y))\|_\ast \leq L_{\theta\theta} \|\theta - \theta'\|, \quad \|\nabla_{x}\ell(\theta; (x, y)) - \nabla_{x}\ell(\theta; (x', y))\|_\ast \leq L_{x\theta} \|x - x'\|,
\]
\[
\|\nabla_{\theta}\ell(\theta; (x, y)) - \nabla_{\theta}\ell(\theta; (x', y))\|_\ast \leq L_{\theta\theta} \|\theta - \theta'\|, \quad \|\nabla_{x}\ell(\theta; (x, y)) - \nabla_{x}\ell(\theta; (x, y))\|_\ast \leq L_{x\theta} \|\theta - \theta'\|.
\]

Under Assumptions C and D an analogue of Lemma 4 still holds. The proof of the following result is nearly identical to that of Lemma 4, we state the full result for completeness.

\footnote{We assume that \(\mathcal{X}\) is a subset of normed vector space.}
Lemma 5. Let $f : \Theta \times \mathcal{X} \to \mathbb{R}$ be differentiable and $\lambda$-strongly concave in $x$ with respect to the norm $\|\cdot\|$, and define $\hat{f}(\theta) = \sup_{x \in \mathcal{X}} f(\theta, x)$. Let $g_\theta(\theta, x) = \nabla_\theta f(\theta, x)$ and $g_x(\theta, x) = \nabla_x f(\theta, x)$, and assume $g_\theta$ and $g_x$ satisfy the Lipschitz conditions of Assumption B. Then $\hat{f}$ is differentiable, and letting $x^*(\theta) = \arg\max_{x \in \mathcal{X}} f(\theta, x)$, we have $\nabla \hat{f}(\theta) = g_\theta(\theta, x^*(\theta))$. Moreover,

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

From Lemma 5, our previous results (Theorems 2 and 4) follow. The following is an analogue of Theorem 2 for the cost function (8).

Theorem 6 (Convergence of Nonconvex SGD). Let Assumptions C and D hold with the $\ell_2$-norm and let $\Theta = \mathbb{R}^d$. Let $\Delta_F \geq F(0^0) - \inf_{\theta} F(\theta)$. Assume $\mathbb{E}[\|\nabla F(\theta) - \nabla \phi_{\gamma}(\theta, Z)\|_2^2] \leq \sigma^2$, and take constant stepsizes $\alpha = \sqrt{\frac{2\Delta_F}{L_{\sigma_\theta}^2}}$, where $L = L_{\phi_\theta} + \frac{L_{\phi_\theta} L_{\phi_\theta}}{\gamma - L_{\sigma_\theta}}$. Then Algorithm 1 satisfies

$$\frac{1}{T} \sum_{t=1}^T \mathbb{E} \left[ \|\nabla F(\theta^t)\|_2^2 \right] - \frac{2L_{\phi_\theta}^2}{\gamma - L_{\sigma_\theta}} \epsilon \leq \sigma \sqrt{\frac{8L_{\Delta_F}}{T}}.$$ 

Similarly, an analogous result to Theorem 4 holds. Define the transport map for the covariate shift

$$T_{\gamma}(\theta; (x_0, y_0)) := \arg\max_{x \in \mathcal{X}} \left\{ \ell(\theta; (x, y_0)) - \gamma c_x(x, x_0) \right\}.$$ 

Theorem 7. Let $\mathcal{Z} \subset \{ z \in \mathbb{R}^m : \|z\| \leq M_z \}$ so that $\|z\| \leq M_z$ almost surely and assume either that (i) $c_x(\cdot, \cdot)$ is $L_c$-Lipschitz over $\mathcal{X}$ with respect to the norm $\|\cdot\|$ in each argument, or (ii) that $\ell(\theta, z) \in [0, M_{\ell}]$ and $x \mapsto \ell(\theta, (x, y))$ is $\gamma L_c$-Lipschitz for all $\theta \in \Theta$. If Assumptions C and D hold, then with probability at least $1 - e^{-t}$,

$$\sup_{\theta \in \Theta} \|\mathbb{E}_{P_n}[c(T_{\gamma}(\theta; Z), Z)] - \mathbb{E}_{P_0}[c(T_{\gamma}(\theta; Z), Z)]\| \leq 4D \sqrt{\frac{1}{n} \left( t + \log N \left( \Theta, \frac{[\gamma - L_{\sigma_\theta}]_+ t}{4L_c L_{\sigma_\theta}}, \|\cdot\| \right) \right)}.$$ 

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

For both results, the proofs are essentially identical as before, but with an application of Lemma 5 instead of Lemma 1.

E Proximal algorithm for $\|\cdot\|_\infty$-norm robustness

In this section, we give an efficient training algorithm that learns to defend against $\|\cdot\|_\infty$-norm perturbations. For simplicity, we assume $\mathcal{Z} = \mathbb{R}^m$ for the rest of this section. Let $\theta \in \Theta$ be some fixed model, $z^0 \in \mathcal{Z}$ a natural example, and define $f(z) := \ell(\theta; z)$ to ease notation. Concretely, we are interested in solving the optimization problem

$$\max_{z} f(z) - \frac{\alpha}{2} \|z - z^0\|_\infty^2$$

Note that this is equivalent to computing the surrogate loss $\phi_{\gamma}(\theta; z^0) = \sup_{z \in \mathcal{Z}} \{ \ell(\theta; z) - \gamma c(z, z^0) \}$ for $c(z, z^0) = \|z - z^0\|_\infty^2$ and $\alpha = 2\gamma$. Our following treatment can easily be modified for the

Footnote: We depart from our convention of denoting original datapoints as $z_0$ to ease forthcoming notation.
supervised learning scenario \( c((x, y), (x^0, y^0)) = \|x - x^0\|_\infty^2 + \infty \cdot 1 \{ y = y^0 \} \) with the convention that \( \infty \cdot 0 = 0 \). To make our notation consistent with the optimization literature, we consider the minimization problem

\[
\min_{z} -f(z) + \frac{\alpha}{2} \|z - z^0\|_\infty^2. \tag{29}
\]

A simple gradient descent algorithm applied to the problem \((29)\) may be slow to converge in practice. Intuitively, this is because the subgradient of \( z \mapsto \frac{1}{2} \|z - z^0\|_\infty^2 \) is given by \( \|z - z^0\|_\infty \cdot s \) where \( s \) is a \( m \)-dimensional vector taking values in \([-1, 1]\) whose coordinates are non-zero only when \( |z_j - z_{0,j}| = \|z - z^0\|_\infty \). Hence, at any given iteration of gradient descent, the \( \|\cdot\|_\infty \) norm penalty term only gets accounted for by at most a few coordinates.

To remedy this issue, we consider a proximal algorithm for solving the problem \((29)\) (see, for example, Parikh and Boyd \[41\] for an comprehensive review of proximal algorithms). For a function \( g : \mathbb{R} \to \mathbb{R} \) and a positive number \( \lambda > 0 \), the proximal operator for \( \lambda g \) is defined by

\[
\text{prox}_{\lambda g}(v) := \arg\min_{z} \left\{ g(z) + \frac{1}{2\lambda} \|z - v\|_2^2 \right\}.
\]

Then, the proximal algorithm on the problem \((29)\) consists of two steps at each iteration \( t \): (i) for the smooth function \(-f(z)\), take a gradient descent step at the current iterate \( z^t \) \((z^{t+\frac{1}{2}}\) below) and (ii) for the non-smooth function \( \|z - z^0\|_\infty^2 \), take a proximal step for the function \( \frac{\lambda}{2} \|\cdot - z^0\|_\infty^2 \) at \( z^{t+\frac{1}{2}} \) \((z^{t+1}\) below):

\[
z^{t+\frac{1}{2}} = z^t + \lambda \nabla f(z^t), \quad z^{t+1} = \text{prox}_{\frac{\lambda}{2} \|\cdot - z^0\|_\infty^2} \left( z^{t+\frac{1}{2}} \right). \tag{30}
\]

The following proposition shows that we can compute the proximal step \( z^{t+1} \) efficiently, simply by sorting the vector \( |z^{t+\frac{1}{2}} - z^0| \). We denote by \( v^t \), the sorted vector of \( |z^{t+\frac{1}{2}} - z^0| \) in decreasing order. In the proposition, we use the notation \( [.]_+ = \max(\cdot, 0) \).

**Proposition 8.** Define the scale parameter \( \beta^t > 0 \) by

\[
\beta^t := \frac{1}{1 + \alpha \lambda^t} \sum_{i=1}^{j^t} v_i \quad \text{where} \quad j^t := \max \left\{ j \in [m] : \sum_{i=1}^{j-1} v_i - \left( \frac{1}{\alpha \lambda^t} + (j - 1) \right) v_j < 0 \right\}. \tag{31}
\]

Then, \( z^{t+1} \) in the proximal update \((30)\) is given by

\[
z^{t+1} = z^{t+\frac{1}{2}} - \left[ |z^{t+\frac{1}{2}} - z^0| - \beta^t \right]_+ \text{sign} \left( z^{t+\frac{1}{2}} - z^0 \right). \tag{32}
\]

See Section \[E.1\] for the proof of the proposition. From the proposition, we obtain the proximal procedure in Algorithm \[2\] that can be used to solve for the approximate maximizer of \( \ell(\theta; z) - \gamma c(z, z^0) \) in Algorithm \[1\] Heuristically, ignoring the truncation term in the proximal update \((32)\), we have

\[
z^{t+1} \approx z^0 + \beta^t \text{sign}(z^t + \lambda \nabla f(z^t) - z^0).
\]

Here, we move towards the sign of \( z^t + \lambda \nabla f(z^t) - z^0 \) modulated by the term \( \beta^t \), as opposed to just the sign of \( \nabla f(z^t) \) for the iterated fast sign gradient method \[22, 28\].

**E.1 Proof of Proposition 8**

In this proof, we drop the subscript on the iteration \( t \) to ease notation. We assume without loss of generality that \( z^{t+\frac{1}{2}} - z^0 \neq 0 \). For some convex, lower semi-continuous function \( g : \mathbb{R}^m \to \mathbb{R} \),
Algorithm 2  Proximal Algorithm for Maximizing $f(z) - \frac{q}{2} \| z - z^0 \|_\infty^2$

\begin{algorithm}
\textbf{INPUT:} Stepsizes $\lambda^t$
\textbf{for} $t = 0, \ldots, T-1$ \textbf{do}
\hspace{1em} $z^{t+\frac{1}{2}} \leftarrow z^t + \lambda^t \nabla f(z^t)$
\hspace{1em} $v^t \leftarrow \text{sort}([|z^{t+\frac{1}{2}} - z^0|, \text{dec})}$
\hspace{1em} Compute $\beta^t$ as in (31)
\hspace{1em} $z^{t+1} \leftarrow z^{t+\frac{1}{2}} - \left[ |z^{t+\frac{1}{2}} - z^0| - \beta^t \right] \cdot \text{sign} (z^{t+\frac{1}{2}} - z^0)$
\end{algorithm}

let $g^*(s) = \sup_s \{ s^\top t - g(t) \}$ be the Fenchel conjugate of $g$. From the Moreau decomposition \cite{41}, Section 2.5, we have

$$\text{prox}_g(w) + \text{prox}_{g^*}(w) = w$$

for any $w \in \mathbb{R}^m$. Noting that the conjugate of $z \mapsto \frac{\alpha}{2} \| z - z_0 \|_\infty^2$ is given by $z \mapsto z^\top z_0 + \frac{1}{2\alpha} \| z \|_1^2$, we have

$$\text{prox}_{\frac{1}{2\alpha} \| z - z_0 \|_\infty^2}(w) = w - \text{prox}_{\alpha\|\cdot\|_1 + \frac{1}{\alpha\lambda} \| \cdot \|_1^2}(w) = w - \text{prox}_{\frac{1}{2\alpha\lambda} \| \cdot \|_1^2}(w - z_0)$$

Let us denote the sorted vector (in decreasing order) of $|w - z^0|$ by $v$. Then, in light of the preceding display, it suffices to show that

$$\text{prox}_{\frac{1}{2\alpha\lambda} \| \cdot \|_1^2}(w - z_0) = \| w - z - \beta^* \|_1 \cdot \text{sign} (w - z_0)$$

where $\beta^*$ is defined as in (31). To show that equality (33) holds, note that the first order optimality conditions for

$$\text{prox}_{\frac{1}{2\alpha\lambda} \| \cdot \|_1^2}(w - z_0) = \arg\min_z \left\{ \frac{1}{2} \| z \|_1^2 + \frac{\alpha\lambda}{2} \| z - (w - z_0) \|_2^2 \right\}$$

is given by

$$\| z \|_1 \text{sign}(z_i) + \alpha\lambda(z_i - w_i + z^0_i) = 0 \quad \text{if} \quad \| z_i \|_1 \neq 0$$

$$\| z \|_1 [ -1, 1] - \alpha\lambda(w_i - z^0_i) \geq 0 \quad \text{if} \quad \| z_i \|_1 = 0.$$ (34a)

Now, we use the following elementary lemma.

**Lemma 6.** For $0 \neq v \geq 0$ with decreasing coordinates, the solution to the equation

$$\sum_{i:v_i \beta} (v_i - \beta) = \alpha\lambda\beta$$

exists and is given by

$$\beta^* := \frac{1}{1 + \alpha\lambda j^*} \sum_{i=1}^j v_i \quad \text{where} \quad j^* := \max \left\{ j \in [m]: \sum_{i=1}^{j-1} v_i - \frac{1}{\alpha\lambda} (j - 1) v_j < 0 \right\}.$$ (34b)

**Proof of Lemma** First, note that $\beta \mapsto \sum_{i:v_i \beta} (v_i - \beta) - \alpha\lambda\beta =: h(\beta)$ is decreasing. Noting that $\| v \|_1 > 0$ and $-\alpha\lambda \| v \|_\infty < 0$, there exists $\beta'$ such that $h(\beta') = 0$ and $\beta' \in (0, \| v \|_\infty)$. Since $v_i$’s are decreasing and nonnegative, there exists $j'$ such that $v_{j'} > \beta' \geq v_{j'+1}$ (we abuse notation and let $v_{m+1} := 0$). Then, we have

$$\sum_{i=1}^{j'-1} (v_i - v_{j'}) - \alpha\lambda v_{j'} < 0 \leq \sum_{i=1}^{j'} (v_i - v_{j'+1}) - \alpha\lambda v_{j'+1}.$$
That is, $j' = j^*$. Solving for $\beta'$ in

$$0 = h(\beta') = \sum_{i=1}^{j^*} v_i - (\alpha \lambda + j^*) \beta',$$

we obtain $\beta' = \beta^*$ as claimed.

Now, define

$$z^* = \left[ |w - z^0| - \beta^* \right] + \text{sign} \left( w - z^0 \right).$$

Then, we have from Lemma 6 that

$$\|z^*\|_1 = \sum_{i:|w_i - z_i^0| > \beta^*} (|w_i - z_i^0| - \beta^*) = \sum_{i=1}^{j^*} (v_i - \beta^*) = \alpha \lambda \beta^*.$$

If $z_i^* > 0$, then $\text{sign}(z_i^*) = \text{sign}(w_i - z_i^0)$ so that

$$\|z^*\|_1 \text{sign}(z_i) + \alpha \lambda (z_i^* - w_i + z_i^0) = 0.$$

If $z_i^* = 0$, then $|w_i - z_i^0| \leq \beta^*$ and

$$\|z^*\|_1 [-1, 1] - \alpha \lambda (w_i - z_i^0) = \alpha \lambda \beta^*[1, 1] - \alpha \lambda (w_i - z_i^0) \geq 0.$$

Hence, $z^*$ satisfies the optimality condition (34) as desired.