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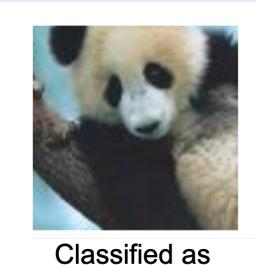
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# **Summary of Contributions**

- Novel adversarial robust training framework integrating distributionally robust optimization and entropic regularization.
- Near-optimal stochastic methods with biased gradient oracles.
- Connections with **regularized** empirical risk minimization training.

# **Motivation and Background**



**Panda** 



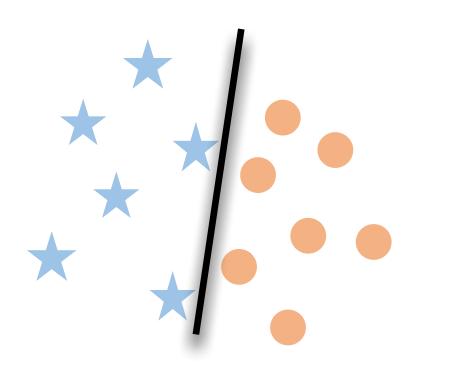


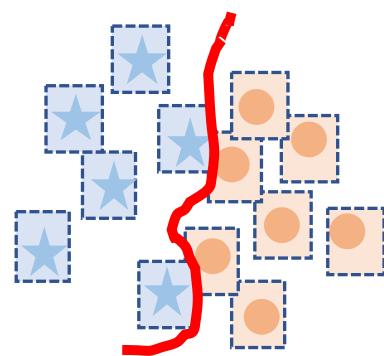
Imperceptible Perturbation

Classified as **Gibbon** 

• Adversarial training (Aleksander et al, 2018):

$$\min_{\theta \in \Theta} \ \Big\{ \mathbb{E}_{x \sim \widehat{\mathbb{P}}} \big[ R_{\rho}(\theta; x) \big] \Big\}, \text{ where } R_{\rho}(\theta; x) \triangleq \sup_{z \in \mathbb{B}_{\rho}(x)} f_{\theta}(z). \tag{AT}$$





**Cons**: Inner supremum of (AT) is generally **nonconcave** in z!**Literature**: Approximately solves  $R_{\rho}(\theta;x)$  by **linear approximation** of  $f_{\theta}(z)$ around x.

• Distributionally robust optimization (DRO) point of view:

$$\begin{split} (\mathsf{AT}) &= \min_{\theta \in \Theta} \ \left\{ \sup_{\mathbb{P}} \ \left\{ \mathbb{E}_{z \sim \mathbb{P}}[f_{\theta}(z)] : \ \mathcal{W}_{\infty}(\mathbb{P}, \widehat{\mathbb{P}}) \leq \rho \right\} \right\} \\ &= \min_{\theta \in \Theta} \ \left\{ \sup_{\mathbb{P}, \gamma} \ \left\{ \mathbb{E}_{z \sim \mathbb{P}}[f_{\theta}(z)] : \ \underset{\mathsf{ess.sup}_{\gamma}}{\mathsf{Proj}_{1 \# \gamma}} = \widehat{\mathbb{P}}, \mathsf{Proj}_{2 \# \gamma} = \mathbb{P} \right\} \right\}. \end{split}$$

where  $\mathcal{W}_{\infty}(\cdot,\cdot)$  is the  $\infty$ -Wasserstein metric:

$$\mathcal{W}_{\infty}(\mathbb{P},\mathbb{Q}) = \inf_{\gamma: \; \operatorname{Proj}_{1\#}\gamma = \mathbb{P}, \operatorname{Proj}_{2\#}\gamma = \mathbb{Q}} \; \Big\{ \operatorname{ess.sup}_{\gamma} \; \|\zeta_1 - \zeta_2\| \Big\}.$$

#### **Proposed Formulation**

• Entropic-regularized formulation:

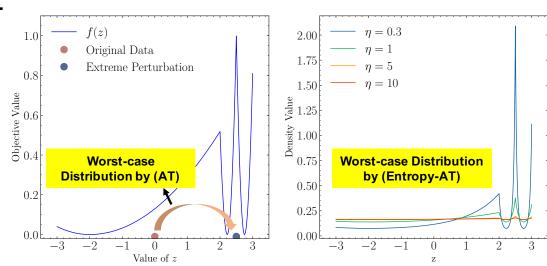
$$\min_{\theta \in \Theta} \ \left\{ \sup_{\mathbb{P}, \gamma} \ \left\{ \mathbb{E}_{z \sim \mathbb{P}} \left[ f_{\theta}(z) \right] - \eta \mathcal{H}(\gamma) : \begin{array}{l} \operatorname{Proj}_{1 \# \gamma} = \widehat{\mathbb{P}}, \operatorname{Proj}_{2 \# \gamma} = \mathbb{P} \\ \operatorname{ess.sup}_{\gamma} \| \zeta_1 - \zeta_2 \| \leq \rho \end{array} \right\} \right\}.$$
 The entropy term  $\mathcal{H}(\gamma) \triangleq \int \log \left( \frac{\mathrm{d} \gamma(x, z)}{\mathrm{d} \widehat{\mathbb{P}}(x) \, \mathrm{d} z} \right) \, \mathrm{d} \gamma(x, z).$  (Entropy-AT)

Under mild assumptions it holds that  $V_P = V_D$ :

$$\begin{split} V_{\mathsf{P}} &= \sup_{\mathbb{P}, \gamma} \ \left\{ \mathbb{E}_{z \sim \mathbb{P}} \left[ f(z) \right] - \eta \mathcal{H}(\gamma) : \frac{\mathsf{Proj}_{1 \# \gamma} = \widehat{\mathbb{P}}}{\mathsf{ess.sup}_{\gamma} \|\zeta_{1} - \zeta_{2}\| \leq \rho} \right\}, \\ V_{\mathsf{D}} &= \mathbb{E}_{x \sim \widehat{\mathbb{P}}} \left[ \eta \log \mathbb{E}_{z \sim \mathbb{Q}_{x}} \left[ \exp \left( \frac{f(z)}{\eta} \right) \right] \right], \end{split}$$

where  $\mathbb{Q}_x$  is an uniform distribution on  $\mathbb{B}_{\rho}(x)$ .

- Geometry of Worst-Case Distribution:
- For each  $x \in \operatorname{supp}(\widehat{\mathbb{P}})$ , optimal transport maps it to a (conditional) distribution  $\gamma_x$ :  $\frac{\mathrm{d}\gamma_x(z)}{\mathrm{d}z} = \alpha_x \cdot e^{f(z)/\eta}, \quad z \in \mathbb{B}_{\rho}(x).$
- Worst-case distribution  $\widetilde{\mathbb{P}} = \int \gamma_x \, d\widehat{\mathbb{P}}(x)$ .
- ullet When f(z) is a quadratic loss with 1-dimensional input neural network,  $\widehat{\mathbb{P}}=$  $\delta_{x=0}$ , and  $\rho=3$ :



# **Optimization Algorithm**

• Reformulate (Entropy-AT) as a single minimization:

$$\min_{\theta \in \Theta} \left\{ F(\theta) \triangleq \mathbb{E}_{x \sim \widehat{\mathbb{P}}} \left[ \eta \log \mathbb{E}_{z \sim \mathbb{Q}_x} \left[ \exp \left( \frac{f_{\theta}(z)}{\eta} \right) \right] \right] \right\},$$

ullet Biased Stochastic Mirror Descent (BSMD): for  $t=1,\ldots,T$ ,

$$\begin{cases} v(\theta_t) \leftarrow \text{(biased) gradient/subgradient estimate of } F(\theta_t) \\ \theta_{t+1} \leftarrow \mathbf{Prox}_{\theta_t} \big( \tau v(\theta_t) \big) \end{cases}$$

Scenarios	<b>Computation Cost</b>	<b>Memory Cost</b>
Nonsmooth Convex Optimization	$\tilde{O}(\epsilon^{-2})$	$ ilde{O}(1)$
<b>Constrained Smooth Nonconvex Optimization</b>	$\tilde{O}(\epsilon^{-4})$	$\tilde{O}(\epsilon^{-2})$
<b>Unconstrained Nonconvex Optimization</b>	$\tilde{O}(\epsilon^{-4})$	$ ilde{O}(1)$

#### Gradient Estimator using Multi-level Monte-Carlo (MLMC):

• Consider  $O(2^{-\ell})$ -approximation function of  $F(\theta)$ :

$$F^{\ell}(\theta) = \mathbb{E}_{x^{\ell} \sim \widehat{\mathbb{P}}} \mathbb{E}_{\{z_{j}^{\ell}\} \sim \mathbb{Q}_{x^{\ell}}} \left[ \eta \log \left( \frac{1}{2^{\ell}} \sum_{j} \exp \left( \frac{f_{\theta}(z_{j}^{\ell})}{\eta} \right) \right) \right].$$

Define samples  $\zeta^{\ell} = (x^{\ell}, \{z_i^{\ell}\}_{i \in [2^{\ell}]})$ , and

$$U_{n_1:n_2}(\theta,\zeta^{\ell}) = \eta \log \left( \frac{1}{n_2 - n_1 + 1} \sum_{j \in [n_1:n_2]} \exp \left( \frac{f_{\theta}(z_j^{\ell})}{\eta} \right) \right),$$

$$G^{\ell}(\theta,\zeta^{\ell}) = \nabla_{\theta} \left[ U_{1:2^{\ell}}(\theta,\zeta^{\ell}) - \frac{1}{2} U_{1:2^{\ell-1}}(\theta,\zeta^{\ell}) - \frac{1}{2} U_{2^{\ell-1}+1:2^{\ell}}(\theta,\zeta^{\ell}) \right].$$

- (a) Sample random level  $\iota \sim \mathbb{Q}_{RT}$  with  $\mathbb{Q}_{RT}(\iota = \ell) = q_\ell \propto 2^{-\ell}, \ell = 0, \dots, L$ .
- (b) Construct  $v^{\text{MLMC}}(\theta) = \frac{1}{a} \cdot G^{\iota}(\theta; \zeta^{\iota})$ .
- MLMC estimator  $v^{\text{MLMC}}(\theta)$  is an unbiased estimator of  $\nabla F^L(\theta)$ :

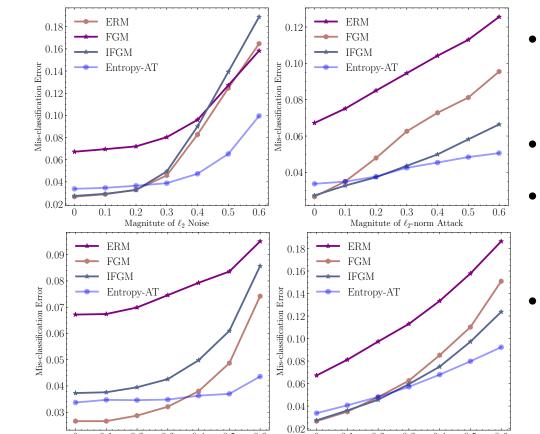
$$\mathbb{E}[v^{\mathsf{RT-MLMC}}(\theta)] = \mathbb{E}_{\iota_1} \left[ \frac{1}{q_{\iota_1}} \mathbb{E}_{\zeta^{\iota_1}}[G^{\iota_1}(\theta,\zeta^{\iota_1})] \right] = \sum_{\ell=0}^L q_\ell \cdot \left[ \frac{1}{q_\ell} \mathbb{E}_{\zeta^\ell}[G^\ell(\theta,\zeta^\ell)] \right]$$

ullet  $U_{1:2^\ell}( heta,\zeta^\ell), U_{1:2^{\ell-1}}( heta,\zeta^\ell),$  and  $U_{2^{\ell-1}+1:2^\ell}( heta,\zeta^\ell)$  are generated using the same  $\zeta^\ell$ , implying  $G^{\bar\ell}(\theta,\zeta^\ell)/v^{
m MLMC}(\theta)$  has small variance (control variate effect).

#### **Regularization Effect:**

$$(\mathsf{Entropy\text{-}AT}) \approx \begin{cases} \min_{\theta \in \Theta} \ \mathbb{E}_{\widehat{\mathbb{P}}}[f_{\theta}(x)] + \rho \mathbb{E}_{x \sim \widehat{\mathbb{P}}}[\|\nabla f_{\theta}(x)\|_{*}], & \text{if } \rho/\eta \to \infty, \\ \min_{\theta \in \Theta} \ \mathbb{E}_{\widehat{\mathbb{P}}}[f_{\theta}(x)] + \frac{\rho^{2}}{\eta} \mathbb{E}_{x \sim \widehat{\mathbb{P}}}\left[\mathsf{Var}_{z \sim \mathbb{Q}_{x}}[\nabla f_{\theta}(x)^{\mathsf{T}}z]\right], & \text{if } \rho/\eta \to 0, \\ \min_{\theta \in \Theta} \ \mathbb{E}_{\widehat{\mathbb{P}}}[f_{\theta}(x)] + \frac{\rho}{C} \mathbb{E}_{x \sim \widehat{\mathbb{P}}}\left[\log \mathbb{E}_{\mathbb{Q}_{x}}\left[\exp\left(C\nabla f_{\theta}(x)^{\mathsf{T}}z\right)\right]\right], & \text{if } \rho/\eta \to C. \end{cases}$$

# **Numerical Study on Supervised Learning**



- Neural network classifier on MNIST dataset;
- Four types of adversarial attack;
- FGM/IFGM are heuristics for solving (AT) based on linear approximation.
- Entropic-AT performs well especially for large adversarial perturbations.