Distributionally Robust Multiclass Classification and Applications in Deep CNN Image Classifiers

Ruidi Chen¹, Boran Hao¹, and Ioannis Paschalidis¹,²

¹Department of Electrical and Computer Engineering, Division of Systems Engineering, Boston University
²Department of Biomedical Engineering, and Faculty of Computing & Data Sciences, Boston University

Abstract

We develop a Distributionally Robust Optimization (DRO) formulation for Multiclass Logistic Regression (MLR), which could tolerate data contaminated by outliers. The DRO framework uses a probabilistic ambiguity set defined as a ball of distributions that are close to the empirical distribution of the training set in the sense of the Wasserstein metric. We relax the DRO formulation into a regularized learning problem whose regularizer is a norm of the coefficient matrix. We establish out-of-sample performance guarantees for the solutions to our model, offering insights on the role of the regularizer in controlling the prediction error. We apply the proposed method in rendering deep CNN-based image classifiers robust to random and adversarial attacks. Specifically, using the MNIST and CIFAR-10 datasets, we demonstrate reductions in test error rate by up to 78.8% and loss by up to 90.8%. We also show that with a limited number of perturbed images in the training set, our method can improve the error rate by up to 49.49% and the loss by up to 68.93% compared to Empirical Risk Minimization (ERM), converging faster to an ideal loss/error rate as the number of perturbed images increases.

1 Introduction

We consider the multi-class classification problem under the framework of Distributionally Robust Optimization (DRO), where the ambiguity set is defined via the Wasserstein metric [14, 11]. We focus on developing robust classification algorithms that are immunized against the presence of outliers in the data, motivated by the fact that standard approaches, such as Logistic Regression (LR), are vulnerable to contamination of the dataset by outliers. Robust models are desired in the scenarios where: (i) the training data population differs significantly from the population to which the model shall be applied, e.g., covariate shift [4], or even adversarial contamination of either training or test data; and (ii) we seek a model that works well over the entire data range of interest; or (iii) we value model performance in the less frequently occurring regions.
Robust optimization has been widely used for inducing robustness to classification models [9, 3]. DRO, which minimizes the worst-case loss over a probabilistic ambiguity set, has received an increasing attention in recent years, due to its probabilistic interpretation of the uncertain data, tractability when assembled with certain metrics, and extraordinary performance observed on numerical examples. The ambiguity set in DRO can be defined through moment constraints [27], or as a ball of distributions using some probabilistic distance function such as the Wasserstein distance [11]. The Wasserstein DRO model has been extensively studied in the machine learning community; see, for example, [6, 5] for robustified regression models, [25] for adversarial training in neural networks, and [1] for distributionally robust logistic regression. [24, 13, 7] provided a comprehensive analysis of the Wasserstein-based distributionally robust statistical learning framework.

Most of the works on distributionally robust classification have focused on the binary setting [1]. In this paper, we extend the DRO framework to the multi-class setting by exploring Multiclass Logistic Regression (MLR) and deriving the corresponding robust model which stems from a DRO formulation that minimizes the worst-case expected loss within an ambiguity set defined by the Wasserstein metric. Unlike the binary classification problem where the label/output is a scalar and a coefficient vector defining the classifier is to be learned, in the multi-class setting the label is represented by a one-hot vector, and the classification boundary is described by a coefficient matrix whose columns characterize the class probabilities. We obtain a novel matrix norm regularizer for MLR through reformulating the DRO problem; thus, establishing a connection between robustness and regularization, and enabling a primal-dual interpretation for the data-regularizer relationship. Note that the link between robustness and regularization has been established in the 1-dimensional output setting, see, e.g., [10, 9, 29, 28, 2] for deterministic disturbances, and [1, 6, 5, 24, 13] for disturbances within a Wasserstein set. However, none of these works studied the robust problem with multi-dimensional outputs.

Our problem is closely related to [1, 6] where the Wasserstein DRO problem with a 1-dimensional output was studied. The key differences lie in that: (i) [6] focused on regression problems where the output $y$ is continuous and duality can be applied to the worst-case problem without any difficulty. A classification setting we consider in this work is very different; special considerations need to be made for the discrete label $y$ when applying duality; (ii) [1, 6] only considered a scalar output $y$. We make the non-trivial extension to a multi-class scenario, which is very different and our key and novel contribution. Specifically, in this work we are regularizing a coefficient matrix $B$ and the correlation structure embedded in the responses should be reflected in the regularizer which is derived as the dual norm of the matrix; (iii) the out-of-sample result in Theorem 3.2 is tailored to the classification setting, which is different from the regression setting in [6], and [1] which bounds the out-of-sample risk by the optimal worst-case risk which we discuss in Theorem 3.1, and (iv) we demonstrate a computationally efficient mechanism for applying the DRO model in CNN-based image classifiers, which adds to the accessibility and appeal of this work to practitioners.

To the best of our knowledge, we are the first to study the robust multi-class classification problem from the standpoint of Wasserstein distributional robustness. The extension from binary to the multi-class case is non-trivial. Our formulations are
completely optimization-based, and are derived by analyzing the fundamental min-max problem, leading to compact and computationally solvable models. Our model is general enough to encompass a class of regularizers that are related to the distance metric in the data space. The significance of our work lies in that it not only establishes a theoretical connection between robustness and regularization in the multi-class setting, but also provides guidance for practitioners on what regularizer to use (dual norm of the metric in the data space), and how to select the regularization coefficient in a much more computationally efficient way without cross-validation. Moreover, we provide a computationally efficient mechanism for inducing robustness in deep neural networks without incurring additional computational burden through incorporating DRO into the final layer of the network.

The rest of the paper is organized as follows. In Section 2, we develop the Wasserstein DRO formulation for MLR. Section 3 establishes the out-of-sample performance guarantees for the DRO solution. Numerical experimental results with deep Convolutional Neural Network (CNN)-based image classifiers are presented in Section 4. In the latter section, we also employ a metric learning approach to learn the appropriate metric in the data space, and how to select the regularization coefficient in a much more computationally efficient way without cross-validation. Moreover, we provide a computational mechanism for inducing robustness in deep neural networks without incurring additional computational burden through incorporating DRO into the final layer of the network.

Notational convention. We use boldfaced lowercase letters to denote vectors, ordinary lowercase letters to denote scalars, boldfaced uppercase letters to denote matrices, and calligraphic capital letters to denote sets. For any integer $n$ we write $[n]$ for the set $\{1, \ldots, n\}$. All vectors are column vectors. For space saving reasons, we write $x = (x_1, \ldots, x_{\dim(x)})$ to denote the column vector $x$, where $\dim(x)$ is the dimension of $x$. We use prime to denote the transpose, $\| \cdot \|_p$ for the $\ell_p$ norm with $p \geq 1$, and $\|x\|_p^W$ for the $W$-weighted $\ell_p$ norm defined as $\|x\|_p^W \equiv \|W^{1/2} x\|_p$, with a positive definite matrix $W$. For a matrix $A \in \mathbb{R}^{m \times n}$, we use $\|A\|_p$ to denote its induced $\ell_p$ norm that is defined as $\|A\|_p \equiv \sup_{x \neq 0} \|Ax\|_p/\|x\|_p$. For a function $h(x)$, we define its convex conjugate as $h^*(\theta) \equiv \sup_{x} \{\theta^T x - h(x)\}$. Finally, $1$ denotes the vector of ones, $0$ the vector of zeros, $e_k$ the $k$-th unit vector, and $\delta_{x_i}(z)$ the Dirac delta function at point $z_i$.

## 2 Problem Formulation

In this section we derive the robust MLR formulation under the DRO framework defined by the Wasserstein metric. Suppose there are $K$ classes, and we are given a predictor vector $x \in \mathbb{R}^p$. Our goal is to predict its class label, denoted by a $K$-dimensional one-hot label vector $y \in \{0, 1\}^K$, where $y = (y_1, \ldots, y_K)$, $\sum_k y_k = 1$, and $y_k = 1$ if and only if $x$ belongs to class $k$, in which case $y = e_k$. The conditional distribution of $y$ given $x$ is modeled as $p(y|x) = \prod_{i=1}^{K} p_i^{y_i}$, where $p_i = e^{w_i^T x}/\sum_{i=1}^{K} e^{w_i^T x}$, and $w_i, i \in \{K\}$, are the coefficient vectors to be estimated that account for the contribution of $x$ in predicting the class labels. The log-likelihood can be expressed as:

$$
\log p(y|x) = \sum_{i=1}^{K} y_i \log(p_i) = y^T B^T x - \log 1^T e^{B^T x},
$$
where $\mathbf{B} \triangleq [w_1 \cdots w_K]$ and the exponential operator is applied element-wise to the exponent vector. The log-loss is defined to be the negative log-likelihood, i.e., $h_{\mathbf{B}}(x, y) \triangleq \log 1^t e^{\mathbf{B}' x} - y' \mathbf{B}' x$. The Wasserstein DRO formulation for MLR minimizes over $\mathbf{B}$ the worst-case expected loss:

$$\inf_{\mathbf{B}} \sup_{\mathcal{Q} \in \Omega} \mathbb{E}_\mathcal{Q} [h_{\mathbf{B}}(x, y)],$$

where $\mathbb{E}_\mathcal{Q}$ denotes expectation under a distribution $\mathcal{Q}$ of the data $(x, y)$, with $\mathcal{Q}$ belonging to a set $\Omega$:

$$\Omega \triangleq \{ \mathcal{Q} \in \mathcal{P}(\mathcal{Z}) : W_1(\mathcal{Q}, \hat{\mathcal{P}}_N) \leq \epsilon \},$$

where $\mathcal{Z}$ is the set of possible values for $(x, y)$, i.e., $\mathcal{Z} = \mathbb{R}^p \times \{ e_1, \ldots, e_K \}$; $\mathcal{P}(\mathcal{Z})$ is the space of all probability distributions supported on $\mathcal{Z}$; $\epsilon$ is a pre-specified positive constant; and $\hat{\mathcal{P}}_N$ is the empirical distribution that assigns equal probability to each observed sample $(x_i, y_i), i \in [N]$. Furthermore in (2), $W_1(\mathcal{Q}, \hat{\mathcal{P}}_N)$ is the order-1 Wasserstein distance between $\mathcal{Q}$ and $\hat{\mathcal{P}}_N$ defined as:

$$W_1(\mathcal{Q}, \hat{\mathcal{P}}_N) \triangleq \min_{\Pi \in \mathcal{P}(\mathcal{Z} \times \mathcal{Z})} \left\{ \int_{\mathcal{Z} \times \mathcal{Z}} l(z_1, z_2) \, \Pi(dz_1, dz_2) \right\},$$

where $z_i = (x_i, y_i), i = 1, 2$, $\Pi$ is the joint distribution of $z_1$ and $z_2$ with marginals $\mathcal{Q}$ and $\hat{\mathcal{P}}_N$, respectively, and $l(\cdot, \cdot)$ is a distance metric on the data space that measures the cost of transporting the probability mass and is defined as:

$$l(z_1, z_2) = \|x_1 - x_2\|_r + M \|y_1 - y_2\|_t,$$

with a positive constant $M$.

Theorem 2.1 derives an equivalent reformulation of (1) by exploiting the dual problem of the inner supremum in (1). The derivation technique is similar to [1], with the difference lying in that we are handling a matrix-indexed loss function that has an additional term $y' \mathbf{B}' x$ because of the multi-class setup, which will contribute an additional factor to the matrix norm regularizer.

**Theorem 2.1.** Suppose we observe $N$ realizations of the data, denoted by $(x_i, y_i), i \in [N]$. When the Wasserstein metric is induced by (4), as $M \to \infty$, the DRO problem (1) can be reformulated as:

$$\inf_{\mathbf{B}} \frac{1}{N} \sum_{i=1}^{N} h_{\mathbf{B}}(x_i, y_i) + \epsilon 2^{1/s} \|\mathbf{B}\|_s,$$

where $r, s \geq 1$, and $1/r + 1/s = 1$. We call (5) the DRO-MLR formulation.

**Proof.** Let us first examine the inner supremum of (1), which can be expressed as:

$$\sup_{\mathcal{Q} \in \Omega} \mathbb{E}_\mathcal{Q} [h_{\mathbf{B}}(x, y)] = \sup_{\mathcal{Q} \in \Omega} \int_{\mathcal{Z}} h_{\mathbf{B}}(z) d\mathcal{Q}(z),$$

4
where \( z = (x, y) \). By definition of the Wasserstein set we can reformulate (6) as:

\[
\sup_{\Pi \in \mathcal{P}(Z \times Z)} \int_Z h_B(z) d\Pi(z, Z)
\]

s.t. \( \int_{Z \times Z} l(z, \tilde{z}) d\Pi(z, \tilde{z}) \leq \epsilon, \)

\[
\int_{Z \times Z} \delta_{z_i}(\tilde{z}) d\Pi(z, \tilde{z}) = \frac{1}{N}, \quad \forall i \in [N],
\]

where \( \Pi \) is the joint distribution of \( z \) and \( \tilde{z} \) with marginals \( Q \) and \( \hat{P}_N \), \( \tilde{z} \) indexes the support of \( \hat{P}_N \), and \( \delta_{z_i}(\cdot) \) is the Dirac delta function at point \( z_i \). Using \( Q_i \) to denote the conditional distribution of \( z \) given \( \tilde{z} = z_i \), we can rewrite (7) as:

\[
\sup_{Q_i} \frac{1}{N} \sum_{i=1}^N \int_Z h_B(z) dQ_i(z)
\]

s.t. \( \frac{1}{N} \sum_{i=1}^N \int_Z l(z, \tilde{z}) dQ_i(z) \leq \epsilon, \)

\[
\int_Z dQ_i(z) = 1, \quad \forall i \in [N].
\]

Notice that the support \( Z \) can be decomposed into \( \mathbb{R}^p \) and a discrete set \( \{e_1, \ldots, e_K\} \). We thus decompose each distribution \( Q_i \) into unnormalized measures \( Q_k^i \) supported on \( \mathbb{R}^p \) such that \( Q_k^i(d\mathbf{x}) \triangleq Q^i(d\mathbf{x}, y = e_k), k \in [K] \). Problem (8) can then be reformulated as:

\[
\sup_{Q_k^i} \frac{1}{N} \sum_{i=1}^N \sum_{k=1}^K \int_{\mathbb{R}^p} h_B(x, e_k) dQ_k^i(x)
\]

s.t. \( \frac{1}{N} \sum_{i=1}^N \sum_{k=1}^K \int_{\mathbb{R}^p} l((x, e_k), (x_i, y_i)) dQ_k^i(x) \leq \epsilon, \)

\[
\sum_{k=1}^K \int_{\mathbb{R}^p} dQ_k^i(x) = 1, \quad \forall i \in [N].
\]

Using the definition of \( l \) in (4), we can write Problem (9) as:

\[
\sup_{Q_k^i} \frac{1}{N} \sum_{i=1}^N \sum_{k=1}^K \int_{\mathbb{R}^p} h_B(x, e_k) dQ_k^i(x)
\]

s.t. \( \frac{1}{N} \sum_{i=1}^N \sum_{k=1}^K \int_{\mathbb{R}^p} \left( ||x - x_i||_r + M||e_k - y_i||_s \right) dQ_k^i(x) \leq \epsilon, \)

\[
\sum_{k=1}^K \int_{\mathbb{R}^p} dQ_k^i(x) = 1, \quad \forall i \in [N].
\]
which can be equivalently written as:

\[
\begin{align*}
\sup_{Q_i^k} & \frac{1}{N} \sum_{i=1}^N \sum_{k=1}^K \int_{\mathbb{R}^p} h_B(x, e_k) dQ_i^k(x) \\
\text{s.t.} & \frac{1}{N} \int_{\mathbb{R}^p} \left( \sum_{i=1}^N \|x - x_i\|_r \left( \sum_{k=1}^K dQ_i^k(x) \right) + 2^{1/t} M \left( \sum_{k} \sum_{i:y_i = e_k} dQ_i^k(x) \right) \right) \leq \epsilon, \\
& \sum_k \int_{\mathbb{R}^p} dQ_i^k(x) = 1, \forall i \in \llbracket N \rrbracket,
\end{align*}
\]

(10)

where \(Q_i^k \triangleq \sum_{j=1}^K Q_j^k - Q_i^k\). In the derivation we used the fact that \(\|e_i - e_j\|_t = 2^{1/t}\), if \(i \neq j\).

Notice that (10) is a linear problem (LP) in \(Q_i^k\). We can apply linear duality with dual variables \(\lambda\) and \(s_i\). (10) is a special LP in that the decision variables \(Q_i^k\) are infinite dimensional. For each \(Q_i^k(x)\), its coefficients in the constraints of (10) are multiplied by the corresponding dual variables to produce the constraints of the dual problem (11) (LP duality). Since \(Q_i^k\) has infinitely many arguments \(x\), the constraints of (11) involve the supremum over \(x\). The dual problem of (10) can be written as:

\[
\begin{align*}
\inf_{\lambda \geq 0, s_i} & \lambda \epsilon + \frac{1}{N} \sum_{i=1}^N s_i \\
\text{s.t.} & \sup_{x \in \mathbb{R}^p} h_B(x, e_k) - \lambda \|x - x_i\|_r - \lambda M \|e_k - y_i\|_t \leq s_i, \forall i \in \llbracket N \rrbracket, k \in \llbracket K \rrbracket.
\end{align*}
\]

(11)

Using Corollary 1.1 in the Supplementary, we can write Problem (11) as:

\[
\begin{align*}
\inf_{\lambda, s_i} & \lambda \epsilon + \frac{1}{N} \sum_{i=1}^N s_i \\
\text{s.t.} & h_B(x_i) - \lambda M \|e_k - y_i\|_t \leq s_i, \forall i \in \llbracket N \rrbracket, k \in \llbracket K \rrbracket, \\
& \lambda \geq \sup \{\|B(\gamma - e_k)\|_s : \gamma \geq 0, 1'\gamma = 1\}, \forall k \in \llbracket K \rrbracket,
\end{align*}
\]

(12)

where \(1/r + 1/s = 1\). As \(M \to \infty\), i.e., we assign a very large weight on the labels, implying that samples from different classes are infinitely far away (see Eq. (4)), the first set of constraints in Problem (12) reduces to: \(h_B(x_i, y_i) \leq s_i, \forall i \in \llbracket N \rrbracket\). Therefore, the optimal value of (12) is:

\[
\begin{align*}
\frac{1}{N} \sum_{i=1}^N h_B(x_i, y_i) + \lambda \epsilon,
\end{align*}
\]

(13)

where \(\lambda = \max_k \sup \{\|B(\gamma - e_k)\|_s : \gamma \geq 0, 1'\gamma = 1\}\). To compute \(\lambda\), notice that

\[
\|B(\gamma - e_k)\|_s \leq \|B\|_s \|\gamma - e_k\|_s,
\]

where \(\|B\|_s\) is the induced \(\ell_s\) norm of the matrix \(B\). The maximum of \(\|\gamma - e_k\|_s\) can
be obtained as:
\[
\|\gamma - e_k\|_s^s = \sum_{i=1}^{k-1} \gamma_i^s + (1 - \gamma_k)^s + \sum_{j=k+1}^{K} \gamma_j^s
\leq \sum_{i=1}^{k-1} \gamma_i + (1 - \gamma_k) + \sum_{j=k+1}^{K} \gamma_j
= 1 - 2\gamma_k + 1
\leq 2,
\]
where \(\gamma = (\gamma_1, \ldots, \gamma_K)\). Therefore, (13) can be reformulated into (5) by setting \(\lambda = 2^{1/s}\|B\|_s\).

Remark 1: selection of the radius \(\epsilon\). To guarantee that the Wasserstein set includes the true measure with high confidence, the measure concentration results [12] suggest that \(\epsilon\) should be set as:
\[
\epsilon_N(\alpha) = \begin{cases} \left(\frac{\log(c_1\alpha^{-1})}{c_2 N}\right)^{1/\max(p+K,2)}, & \text{if } N \geq \frac{\log(c_1\alpha^{-1})}{c_2} \\ \left(\frac{\log(c_1\alpha^{-1})}{c_2 N}\right)^{1/a}, & \text{if } N < \frac{\log(c_1\alpha^{-1})}{c_2} \end{cases},
\]
where \(\alpha\) is the confidence level, \(a > 1\) is an exponent such that \(\mathbb{E}[\exp(\|x, y\|^a)] < \infty\), with \(P^*\) the true measure of the data, and \(c_1, c_2\) positive constants; see [11]. The dependency on unknown constants makes (14) hard to implement. [17, 30] proposed ways of getting rid of the exogenous constants when the true distribution is discrete. In practice, cross-validation can also be used to select \(\epsilon\) if the data size is not too large.

Remark 2: a weighted norm space. When the feature space is equipped with a weighted norm, e.g.,
\[
l(z_1, z_2) = \|x_1 - x_2\|_W^r + M\|y_1 - y_2\|_t,
\]
where \(\|x\|_W^r \triangleq \|W^{1/2}x\|_r\), with \(W\) a positive definite matrix, the corresponding DRO-MLR formulation can be written as:
\[
\inf_B \frac{1}{N} \sum_{i=1}^{N} h_B(x_i, y_i) + \epsilon 2^{1/s}\|W^{-1/2}B\|_s,
\]
where \(r, s \geq 1, 1/r + 1/s = 1\). This is due to the fact that the dual norm of \(\|\cdot\|_r^W\) is simply \(\|\cdot\|_W^{-1}\).

3 Out-of-Sample Performance

In this section we establish out-of-sample performance guarantees for the DRO-MLR solution, i.e., given a new test sample, we bound the expected log-loss of our prediction. The resulting bounds shed light on the role of the regularizer in inducing a low prediction error.

Following from the measure concentration result, we know that if the radius \(\epsilon\) is set according to (14), the Wasserstein set \(\Omega\) will include the true measure \(P^*\) with
probability at least $1 - \alpha$, and thus the expected log-loss can be bounded by the optimal value of the DRO formulation (1).

**Theorem 3.1** ([11], Theorem 3.5). Suppose $\hat{J}_N$ and $\hat{B}_N$ are respectively the optimal value and optimal solution to the DRO problem (1) with the ambiguity set radius specified in (14), where $\alpha \in (0, 1)$. Then we have, with probability at least $1 - \alpha$ with respect to the sampling,

$$E^* [h_{\hat{B}_N}(x, y)] \leq \hat{J}_N,$$

where $E^*$ denotes the true measure of the data $(x, y)$.

Note that $\hat{J}_N$ is the maximum expected loss evaluated at $\hat{B}_N$ over all distributions $Q \in \Omega$:

$$\hat{J}_N \triangleq \inf_{\hat{B}} \sup_{Q \in \Omega} E^Q [h_{\hat{B}}(x, y)] = \sup_{Q \in \Omega} E^Q [h_{\hat{B}_N}(x, y)].$$

The upper bound stated in Theorem 3.1 is thus too conservative. We want to measure the out-of-sample performance in terms of the empirical loss, which is typically used in Empirical Risk Minimization (ERM), so that we can illustrate the advantage of DRO-MLR compared to ERM. By bounding the Rademacher complexity of the class of loss functions, Theorem 3.2 bounds the expected log-loss by the empirical loss plus additional terms that are inversely proportional to $\sqrt{N}$.

**Assumption A.** For any $x$: $\|x\|_s \leq R$ almost surely, for some scalar $R$.

**Assumption B.** For any feasible solution $B$ to (5): $\|B\|_s \leq \bar{C}$, for some scalar $\bar{C}$.

With standardized predictors, $R$ in Assumption A can be assumed to be small. The form of the constraint in Assumptions B is consistent with the form of the regularizers in DRO-MLR. We will see later that the bound $\bar{C}$ controls the out-of-sample log-loss of the solution to DRO-MLR, which validates the role of the regularizer in improving the out-of-sample performance.

**Theorem 3.2.** Suppose the solution to the DRO-MLR formulation (5) is $\hat{B}_N$. Under Assumptions A and B, for any $0 < \alpha < 1$, with probability at least $1 - \alpha$ with respect to the sampling,

$$E^* [h_{\hat{B}_N}(x, y)] \leq E^* [h_{\hat{B}_N}(x, y)] + \frac{2(\log K + \bar{C}R(1 + K^{1/r}))}{\sqrt{N}} + \left(\log K + \bar{C}R(1 + K^{1/r})\right) \sqrt{\frac{8 \log \left(\frac{K}{\alpha}\right)}{N}}.

The bound derived in Theorem 3.2 depends on $R$ and $\bar{C}$, which implicitly depend on the problem dimension $p + K$. Theorem 3.2 says that, if we make the empirical risk arbitrarily small through overfitting (as done in ERM), the regularization strength will be very large, so is the generalization error. This trade-off essentially validates the effectiveness of our model (5) (since it controls both the empirical risk and the regularization strength) compared to a simple ERM model. The out-of-sample generalization (test) error is bounded by the average training error plus a bias term of order $1/\sqrt{N}$, which is controlled by the magnitude of the regularizer in (5). The form of the bound in Theorem 3.2 demonstrates the validity of DRO-MLR in leading to a good out-of-sample performance.
4 DRO-MLR in Deep CNN Image Classifiers

In this section, we apply the DRO-MLR formulation to deep CNN-based image classifiers, and show that our model improves the out-of-sample loss and accuracy by a significant margin under random and adversarial attacks on images. We provide a computationally efficient mechanism for inducing robustness to random and adversarial attacks in deep neural networks without incurring additional computational burden through interfering with only the final layer of the network. This is the key advantage compared to several past works [8, 23] which are computationally much more expensive. We adopt a metric learning based approach to approximate the transformation on the features resulted from the previous CNN layers. We compare our model with ERM (the final layer trained by ERM) to demonstrate the effectiveness of our model in inducing a smaller generalization error and test error rate, showing the power of the regularization scheme which is fundamentally rooted in DRO.

4.1 Experimental Setup

To evaluate the robustness of DRO-MLR to perturbed images and demonstrate its generalization performance on noisy data, we design two settings: (i) the training set is contaminated with noise, and we want to learn a model that is immunized against the noise whose performance will be measured on a clean test set, and (ii) the training data is pure, but the test set is contaminated with outliers. In the image classification task, the perturbed samples are produced through either random or adversarial attacks. The random attack, injects White Gaussian Noise (WGN) by perturbing each pixel of the image by a normally distributed random variable with zero mean and standard deviation $\sigma$. Adversarial attacks, such as the Iterative Fast Gradient Sign Method (I-FGSM) [19] and the Projected Gradient Descent (PGD) [21] generate small perturbations using the gradient of the loss. We adopt an image-agnostic Universal Adversarial Perturbation (UAP) [22], which seeks a universal perturbation for a set of training points and is obtained by aggregating atomic perturbation vectors derived from a small subset of training points. UAP has been shown to fool new images with high probability irrespective of the CNN architecture.

4.2 Method

We use deep CNNs to train the underlying classifier on an input image $x$. The final layer estimates an MLR model on the transformed features, denoted by $\phi(x)$, produced by the second to last layer. We apply DRO-MLR only to the training process of the last layer, while freezing all previous layers (represented by the $\phi$ function) which are pre-trained using a standard CNN. This has a similar flavor to the fine-tuning strategy of [15] which modifies the parameters of an existing network to train for a new task while preserving representations learned from the original task. The pre-trained CNN extracts representative features from the original images, which are fed into the DRO-MLR model that improves the robustness of the final classifier. Moreover, interfering with only the training of the last layer is more computationally efficient and stable, and could be implemented without access to the original training data.
We split the dataset into a training set $D$, a validation set $V$, and a test set $T$, and train a standard CNN model on $D$ to estimate $\phi(x)$ which is the input to the final layer. A perturbed image $\tilde{x}$ is generated as $\tilde{x} = x + \delta$, where the perturbation $\delta$ is generated by either a random attack (WGN) or an adversarial attack (UAP). The regularization coefficient $\epsilon$ is cross-validated on the set $V$. We compare DRO-MLR to Empirical Risk Minimization (ERM), which simply minimizes the empirical log-loss in the final layer without adding any regularizer, in terms of the log-loss and classification error on the test set $T$.

We use $r = 2$ to define the distance metric (4). It is worth noting that the DRO-MLR model is applied to a transformed feature space $\phi(x)$, and thus we need to estimate a proper distance metric in the transformed space to account for the distributional shift resulted from $\phi$. We adopt a weighted norm metric as defined in (15) to approximate the effect of $\phi$, and estimate the weight matrix $W$ by solving the following metric learning problem on the validation set $V$:

$$
\min_{W \succeq 0} \sum_{x_i \in V} \| W^{1/2}(\phi(\tilde{x}_i) - \phi(x_i)) \|_2^2 \\
\text{s.t.} \frac{1}{|S|} \sum_{(i,j) \in S} \| W^{1/2}(\phi(\tilde{x}_i) - \phi(\tilde{x}_j)) \|_2^2 \geq c \\
\frac{1}{|S|} \sum_{(i,j) \in S} \| W^{1/2}(\phi(x_i) - \phi(x_j)) \|_2^2 \geq c,
$$

where $\tilde{x}_i$ is the perturbed version of $x_i$, $S \triangleq \{(i,j) \mid x_i, x_j \in V, y_i \neq y_j\}$, $|S|$ denotes the cardinality of the set $S$, and $c$ is a fixed parameter. Problem (17) enforces that the distances between similar samples (evaluated in the transformed space $\phi(x)$) are being minimized while the distances between dissimilar samples are sufficiently far away. (17) is a semidefinite programming problem (SDP). We solve it using the solver SDPT3 v4.0 [26].

### 4.3 Results

We demonstrate the results on the MNIST [20] and CIFAR-10 [18] datasets. MNIST and CIFAR-10 contain 50k/10k/10k and 40k/10k/10k training/validation/test samples, respectively. We apply a 4-layer CNN on MNIST to estimate $\phi(x)$, while for CIFAR-10, we use the 110-layer residual network (ResNet-110) [16] architecture. A dropout rate of 0.1 was applied in the training process. We run the experiments on two local GPU workstations with 4 NVIDIA RTX 2080ti (11GB VRAM) and 2 NVIDIA Titan RTX (24GB VRAM) GPUs, respectively. The experiment on MNIST took about 5 GPU days while CIFAR-10 took about 85 GPU days.

In scenario (i) described in Section 4.1, we apply the WGN and UAP attacks to the training set respectively, and measure the performance on a clean test set, to illustrate the immunity of DRO-MLR to training data perturbations. The WGN attack perturbs each pixel by a Gaussian noise with zero mean and standard deviation $\sigma$, while the UAP attack is generated using 10,000 images from the validation set $V$, with $\|\delta\|_\infty \leq k$, where $\|\cdot\|_\infty$ is evaluated on the vectorized $\delta$. The results are shown in the first column of Fig. 1, where we plot the average log-loss $h_T$ and classification error $e_T$ on the test set $T$ for DRO-MLR and ERM, as the perturbation strength $\sigma$ or $k$ varies. We
Table 1: Percentage improvement of DRO-MLR over ERM at maximum attack strength under WGN and UAP attacks (first 2 rows), and maximum improvement with limited number of perturbed training images (last row).

|                      | MNIST   | CIFAR-10 |
|----------------------|---------|----------|
|                      | WGN     | UAP      | WGN     | UAP      |
| Attacking $\mathcal{D}$ |         |          |         |          |
| Loss                 | 75.10%  | 53.95%   | 13.08%  | 19.54%   |
| Error rate           | 50.58%  | 22.91%   | 9.19%   | 12.30%   |
| Attacking $\mathcal{T}$ |        |          |         |          |
| Loss                 | 90.75%  | 83.15%   | 83.12%  | 83.02%   |
| Error rate           | 78.81%  | 64.69%   | 21.42%  | 24.22%   |
| Adversarial training |         |          |         |          |
| Loss                 | 59.76%  | 68.93%   | 49.73%  | 45.19%   |
| Error rate           | 42.36%  | 49.49%   | 10.01%  | 7.22%    |

see that DRO-MLR achieves a significantly better performance than ERM under both random and adversarial attacks. The performance gap becomes more prominent as the perturbation strength increases.

In scenario (ii), we train the classifier on a clean dataset $\mathcal{D}$, and test its performance on a noisy test set $\mathcal{T}$ which is perturbed by the WGN or UAP attack. The purpose is to demonstrate the generalization ability of DRO-MLR to perturbed data. The results are shown in the second column of Fig. 1. To better visualize the results, Table 1 summarizes the reduction in the loss and error rate at maximum $\sigma$ and $k$. DRO-MLR reduces the test error rate by up to 79% and log-loss by up to 91% on MNIST, and on CIFAR-10 the reduction is up to 24% for error rate, and 83% for log-loss. The improvement under the adversarial UAP attack is in general smaller than that under the random WGN attack. On the other hand, Fig. 1 shows that DRO-MLR has a comparable performance to ERM under very small perturbations, indicating that DRO-MLR is able to induce robustness to perturbations without compromising the accuracy on unperturbed data.

Compared to MNIST, we see a less significant improvement of DRO-MLR on the CIFAR-10 dataset. The reason might be that, the 110-layer ResNet which was used on CIFAR-10 has a delicate structure which transforms the original image $x$ into a different space that cannot be well approximated by a simple linear transformation indexed by $W$. With a more complex network structure, the improvement that DRO-MLR can achieve by retraining only the final layer is limited. Nevertheless, DRO-MLR is still able to achieve a 12% improvement in the error rate on CIFAR-10 under the adversarial attack by modifying only the training process of the last layer.

Lastly, we want to investigate the sample efficiency of the two models by gradually increasing the number of perturbed training samples. The average error rate and loss on a noisy test set are shown in the last column of Fig. 1. With a limited number of perturbed images in the training set, our method achieves a significantly lower error rate and loss compared to ERM. The maximum improvement in the error rate (loss) is 49.49% (68.93%), see the last row of Table 1. Moreover, DRO-MLR converges faster to an ideal loss/error rate as the number of perturbed images increases, showing that
it is a more efficient way to introduce robustness without sacrificing performance. On the CIFAR-10 dataset where the improvement is less significant (Fig. 1), there is a 45% (27%) improvement in loss and 7.2% (3.2%) improvement in error rate when there are only 100 (200) perturbed images. With more than 600 perturbed images, the error rates converge, but the improvement in loss stays at 15%.

5 Conclusion

We proposed a novel distributionally robust framework for *Multiclass Logistic Regression (MLR)*, where the worst-case loss over a probabilistic ambiguity set defined by the Wasserstein metric is being minimized. By exploiting duality of the worst-case loss, we reformulate the min-max formulation to a regularized empirical loss minimization problem. The regularizer is the induced dual norm of the coefficient matrix, establishing a connection between robustness and regularization in the multivariate setting. We provide both theoretical results on the out-of-sample performance to our estimator, and empirical evidence on deep CNN-based image classifiers showing that our DRO-MLR model reduces the test error by up to 78.8% and loss by up to 90.8% under random and adversarial attacks. We also show that with a limited number of perturbed images in the training set, our method can improve the error rate by up to 49.49% and the loss by up to 68.93% compared to Empirical Risk Minimization (ERM), converging faster to an ideal loss/error rate as the number of perturbed images increases.

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Figure 1: Out-of-sample classification error and log-loss of DRO-MLR and ERM under WGN and UAP attacks.