Robust Wasserstein Profile Inference and Applications to Machine Learning

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Abstract. We show that several machine learning estimators, including square-root LASSO (Least Absolute Shrinkage and Selection) and regularized logistic regression can be represented as solutions to distributionally robust optimization (DRO) problems. The associated uncertainty regions are based on suitably defined Wasserstein distances. Hence, our representations allow us to view regularization as a result of introducing an artificial adversary that perturbs the empirical distribution to account for out-of-sample effects in loss estimation. In addition, we introduce RWPI (Robust Wasserstein Profile Inference), a novel inference methodology which extends the use of methods inspired by Empirical Likelihood to the setting of optimal transport costs (of which Wasserstein distances are a particular case). We use RWPI to show how to optimally select the size of uncertainty regions, and as a consequence, we are able to choose regularization parameters for these machine learning estimators without the use of cross validation. Numerical experiments are also given to validate our theoretical findings.

1. Introduction

Regularization has become crucial in machine learning practice and the goal of this paper is to revisit the idea of regularization from an optimal transport perspective. Specifically, we show that the role of regularization in machine learning can often be interpreted as the result of optimally transporting mass from the empirical measure in order to maximize a certain loss under a budget constraint. Thus, our results connect directly optimal transport phenomena (a classical concept in probability reviewed in Section 2.1) to regularization (a key tool in machine learning to be discussed in the sequel).

Moreover, this connection will show that the so-called regularization parameter (i.e. the coefficient of the regularization term) coincides with the size of the budget constraint by which we permit mass transportation to occur. As we shall see, the budget constraint has a natural interpretation based on a Distributionally Robust Optimization (DRO) formulation, which in turn allows us to define a reasonable optimization criterion for the regularization parameter. Thus, our approach uses optimal mass transportation phenomena to explain the nature of regularization and how to select the regularization parameter in several machine learning estimators – including square-root LASSO (Least Absolute Shrinkage and Selection), Regularized Logistic Regression, among others.

The size of the budget constraint is also referred as the radius (or size) of the uncertainty set in the literature of Distributionally Robust Optimization (DRO). The method that we develop for optimally choosing this budget constraint can actually be applied to a wide range
of inference and decision problems, but we have focused our discussion on machine learning applications because of the substantial amount of activity that the area has generated, and as well to demonstrate the utility of the tools that are commonly used in applied probability to this rapidly growing area.

1.1. Regularization in Linear Regression. In order to introduce the proposed method for optimally choosing the radius of the uncertainty set, let us walk through a simple application in a familiar context, namely, that of linear regression. Throughout the paper any vector is understood to be a column vector and the transpose of $x$ is denoted by $x^T$. We use the notation $E_P[\cdot]$ to denote expectation with respect to a probability distribution $P$.

**Example 1** (Square-root Lasso). Consider a training data set $\{(X_1,Y_1), \ldots, (X_n,Y_n)\}$, where the input $X_i \in \mathbb{R}^d$ is a vector of $d$ predictor variables, and $Y_i \in \mathbb{R}$ is the response variable. It is postulated that

$$Y_i = \beta^T X_i + e_i,$$

for some $\beta_0 \in \mathbb{R}^d$ and errors $\{e_1, \ldots, e_n\}$. Under suitable statistical assumptions one may be interested in estimating $\beta_0$. Underlying is a general loss function, $l(x,y;\beta)$, which we shall take for simplicity in this discussion to be the quadratic loss, namely, $l(x,y;\beta) = (y - \beta^T x)^2$. Let $P_n$ denote the empirical distribution:

$$P_n(dx,dy) := \frac{1}{n} \sum_{i=1}^n \delta_{\{(X_i,Y_i)\}}(dx,dy).$$

Over the last two decades, various regularized estimators have been introduced and studied. Many of them have gained substantial popularity because of their good empirical performance and insightful theoretical properties, (see, for example, [50] for an early reference and [21] for a discussion on regularized estimators). One such regularized estimator, implemented, for example in the “flare” package, see [27], is the so-called square-root LASSO estimator; which is obtained by solving the following convex optimization problem in $\beta$

$$\min_{\beta \in \mathbb{R}^d} \left\{ \sqrt{E_{P_n}[l(X,Y;\beta)]} + \lambda \|\beta\|_1 \right\} = \min_{\beta \in \mathbb{R}^d} \left\{ \frac{1}{n} \sum_{i=1}^n l(X_i,Y_i;\beta) + \lambda \|\beta\|_1 \right\}, \quad (1)$$

where $\|\beta\|_p$ denotes the $\ell_p$-norm. The parameter $\lambda$, commonly referred to as the regularization parameter, is crucial for the performance of the algorithm. It is often chosen using cross validation, a procedure that iterates over multitude of choices of $\lambda$ in order to choose the best.

1.1.1. DRO representation of square-root LASSO. One of our contributions in this paper (see Section 2) is a representation of (1) in terms of a Distributionally Robust Optimization formulation. We construct a discrepancy measure, $D_c(P, Q)$, corresponding to a Wasserstein-type distance between two probability measures $P$ and $Q$ which is defined in terms of a suitable transportation cost function $c(\cdot)$. If $c(\cdot)$ is based on the $\ell_q$-distance (for $q > 1$), we show that

$$\min_{\beta \in \mathbb{R}^d} \left\{ \sqrt{E_{P_n}[l(X,Y;\beta)]} + \lambda \|\beta\|_1 \right\}^2 = \min_{\beta \in \mathbb{R}^d} \max_{P: D_c(P,P_n) \leq \delta} \mathbb{E}_P[l(X,Y;\beta)], \quad (2)$$

where $1/p + 1/q = 1$ and $\lambda = \sqrt{\delta}$. We can gain a great deal of insight from (2). For example, note that the regularization parameter, $\lambda = \sqrt{\delta}$, is fully determined by the size (or ‘radius’) of the uncertainty, $\delta$, in the distributionally robust optimization formulation on the right hand side of (2). In addition, we can interpret (2) as a game in which an artificial adversary is introduced in order to explore and quantify out-of-sample effects in our estimates of the expected loss.
1.1.2. Optimal choice of the radius $\delta$. The set $\mathcal{U}_\delta(\mathbb{P}_n) = \{\mathbb{P} : \mathcal{D}_c(\mathbb{P}, \mathbb{P}_n) \leq \delta\}$ is called the uncertainty set in the language of distributionally robust optimization, and it represents the class of models that are, in some sense, plausible variations of $\mathbb{P}_n$. Note that $\mathcal{U}_\delta(\mathbb{P}_n)$ is precisely the feasible region over which the maximization is taken in (2). Then we define the collection,

$$\Lambda_n(\delta) := \bigcup_{\mathbb{P} \in \mathcal{U}_\delta(\mathbb{P}_n)} \arg\min_{\beta \in \mathbb{R}^d} \mathbb{E}_\mathbb{P}[l(X, Y; \beta)],$$

comprising optimal $\beta$ for every $\mathbb{P} \in \mathcal{U}_\delta(\mathbb{P}_n)$ to be the set of plausible selections of the parameter $\beta_*$. For $\delta$ chosen sufficiently large, the set $\Lambda_n(\delta)$ is a natural confidence region for $\beta_*$. Moreover, we shall see that any $\beta$ that solves $\inf_{\beta} \sup_{\mathbb{P} \in \mathcal{U}_\delta(\mathbb{P}_n)} \mathbb{E}[l(X, Y; \beta)]$ is a member of $\Lambda_n(\delta)$.

Given these interpretations, it is natural to select a confidence level, $1 - \alpha$, and then choose $\delta = \delta_n^*$ optimally via,

$$\delta_n^* = \min\{\delta > 0 : \mathbb{P}(\beta_* \in \Lambda_n(\delta)) \geq 1 - \alpha\}. \tag{4}$$

In words, the optimization criterion can be stated as finding the smallest $\delta$ such that $\beta_*$ is, itself, a plausible selection with $1 - \alpha$ confidence. Essentially, given a desired confidence level $1 - \alpha$, we seek to choose a $\delta$ just large enough such that $\Lambda_n(\delta)$ is a $(1 - \alpha)$-confidence region for the parameter $\beta_*$. As we shall see in Section 4 this choice ensures that any $\beta$ that minimizes $\inf_{\beta} \sup_{\mathbb{P} \in \mathcal{U}_\delta(\mathbb{P}_n)} \mathbb{E}[l(X, Y; \beta)]$ is indeed in the confidence region $\Lambda_n(\delta)$. We next explain how to solve the optimization problem in (4) asymptotically as $n \to \infty$.

1.1.3. The associated Wasserstein Profile Function. In order to asymptotically solve (4) we introduce a novel statistical inference methodology, which we call RWPI (Robust Wasserstein-distance Profile-based Inference – pronounced similar to Rupee). RWPI can be understood as an extension of Empirical Likelihood (EL) that uses optimal transport cost rather than the likelihood. The extension is not just a formality, as we shall see, because different phenomena and scalings arise relative to EL.

We next illustrate how $\delta_n^*$ in (4) corresponds to the quantile of a certain object which we call the Robust Wasserstein Profile (RWP) function evaluated at $\beta_*$. This will motivate a systematic study of the RWP function as the sample size, $n$, increases.

Observe by convexity of the loss function that $\beta \in \Lambda_\delta(\mathbb{P}_n)$ if and only if there exists $\mathbb{P} \in \mathcal{U}_\delta(\mathbb{P}_n)$ such that $\beta$ satisfies the first order optimality condition, namely,

$$\mathcal{D}_\beta \mathbb{E}_\mathbb{P}[l(X, Y; \beta)] = \mathbb{E}_\mathbb{P}[\{(Y - \beta^TX)X\} = 0. \tag{5}$$

We then introduce the following object, which is the RWP function associated with the estimating equation (5),

$$R_n(\beta) = \inf \{\mathcal{D}_c(\mathbb{P}, \mathbb{P}_n) : \mathbb{E}_\mathbb{P}[\{(Y - \beta^TX)X\} = 0\}. \tag{6}$$

It turns out that the infimum is achieved in the previous expression, so we can write min instead; this is not crucial for our discussion but it is sometimes helpful to keep in mind. Using this definition of $R_n(\beta)$, we can see immediately that the events,

$$\{R_n(\beta_*) \leq \delta\} = \{\beta_* \in \Lambda_n(\delta)\},$$

which implies that $\delta_n^*$ is precisely the $1 - \alpha$ quantile, $\chi_{1-\alpha}$, of $R_n(\beta_*)$; that is

$$\delta_n^* = \chi_{1-\alpha} = \inf \{z : \mathbb{P}(R_n(\beta_*) \leq z) \geq 1 - \alpha\}. \tag{7}$$

Moreover, note that $R_n(\beta)$ allows to provide an explicit characterization of $\Lambda_n(\chi_{1-\alpha})$, namely,

$$\Lambda_n(\chi_{1-\alpha}) = \{\beta : R_n(\beta) \leq \chi_{1-\alpha}\}.$$
So, $\Lambda_n(\chi_{1-\alpha}) = \{\beta : R_n(\beta) \leq \chi_{1-\alpha}\}$ is a $(1-\alpha)$-confidence region for $\beta^*$.

1.1.4. Further intuition behind the RWP function. In order to further explain the role of $R_n(\beta^*)$, let us define $\mathcal{P}_{opt} := \{P : \mathbb{E}_P[(Y - \beta^T_* X)X] = 0\}$. In words, $\mathcal{P}_{opt}$ is the set of probability measures for which $\beta^*$ is an optimal risk minimization parameter. Naturally, the distribution of $(X, Y)$, from which the samples are generated, is an element of $\mathcal{P}_{opt}$. Since $R_n(\beta^*) = \inf\{D_c(P, P_n) : P \in \mathcal{P}_{opt}\}$, the set $\{P : D_c(P, P_n) \leq R_n(\beta^*)\}$ denotes the smallest uncertainty region around $P_n$ (in terms of $D_c$) for which there exists a distribution $P$ satisfying the optimality condition $\mathbb{E}_P[(Y - \beta^T_* X)X] = 0$. See Figure 1.1.4 for a pictorial representation of $\mathcal{P}_{opt}$ and $R_n(\beta^*)$.

In summary, $R_n(\beta^*)$ denotes the smallest size of uncertainty that makes $\beta^*$ a plausible choice. If we were to select a radius of uncertainty smaller than $R_n(\beta^*)$, then no probability measure in the neighborhood will satisfy the optimality condition $\mathbb{E}_P[(Y - \beta^T_* X)X] = 0$. On the other hand, if $\delta > R_n(\beta^*)$, the set $\{P : \mathbb{E}_P[(Y - \beta^T_* X)X] = 0, D_c(P, P_n) \leq \delta\}$ is nonempty.

1.2. A broader perspective of our contribution. The previous discussion in the context of linear regression highlights two key ideas: a) the RWP function as a key object of analysis, and b) the role of distributionally robust representation of regularized estimators.

The RWP function can be applied much more broadly than in the context of regularized estimators. We shall study the RWP function for estimating equations generally and systematically but we showcase the use of the RWP function only in the context of optimal regularization. Broadly speaking, RWPI can be seen as a statistical methodology that utilizes a suitably defined RWP function to estimate a parameter of interest. From a philosophical standpoint, RWPI borrows heavily from Empirical Likelihood (EL), introduced in the seminal work of [31, 32]. There are important methodological differences, however, as we shall discuss in the sequel. In the last three decades, there have been a great deal of successful applications of Empirical Likelihood for inference [33, 55, 11, 22, 36]. In principle all of those applications can be revisited using the RWP function and its ramifications.

We now provide a more precise description of our contributions:
A) We explain how, by judiciously choosing $D_c(\cdot)$, we can define a family of regularized regression estimators (see Section 2). In particular, we show how square-root LASSO (see Theorem 1), regularized logistic regression and support vector machines (see Theorem 2) arise as particular cases of suitable DRO formulations.

B) We derive general limit theorems for the asymptotic distribution (as the sample size increases) of the RWP function defined for general estimating equations. These limit theorems, derived in Section 3.3, allow one to employ RWPI to perform inference and choose the radius of uncertainty $\delta$ in settings that are more general than linear/logistic regression.

C) We use our results from B) to obtain prescriptions for regularization parameters in square-root LASSO and regularized logistic regression settings (see Section 4). We also illustrate how coverage results for the optimal risk, that demonstrate $O(n^{-1/2})$ rate of convergence, are obtained immediately as a consequence of choosing $\delta \geq R_n(\beta_*)$.

D) We analyze our regularization selection in the high-dimensional setting for square-root LASSO. Under standard regularity conditions, we show (see Theorem 7) that the regularization parameter $\lambda$ might be chosen as,

$$\lambda = \frac{\pi}{\pi - 2} \Phi^{-1} \left(1 - \frac{\alpha/2d}{\sqrt{n}}\right),$$

where $\Phi(\cdot)$ is the cumulative distribution of the standard normal random variable and $1 - \alpha$ is a user-specified confidence level. The behavior of $\lambda$ as a function of $n$ and $d$ is consistent with regularization selections studied in the literature motivated by different considerations (see Section 4.4 for further details).

E) We analyze the empirical performance of RWPI based selection of regularization parameter in the context of square-root LASSO. In Section 5, we compare the performance of RWPI based optimal regularization with that of cross-validation based approach on both simulated and real data. We conclude that RWPI based approach yields a similar performance, without having to repeat the algorithm over various choices of regularization parameters (as done in cross-validation).

We now provide a discussion on topics which are related to RWPI.

1.3. On related literature in Robust Optimization, Distributionally Robust Optimization and Optimal Transport. Connections between robust optimization and regularization procedures such as LASSO and Support Vector Machines have been studied in the literature, see [53, 54, 3]. The methods proposed here differ subtly: While the papers [53, 54] add deterministic perturbations of a certain size to the predictor vectors $X$ to quantify uncertainty, the Distributionally Robust Representations that we derive measure perturbations in terms of deviations from the empirical distribution. While this change may appear cosmetic, it brings a significant advantage: measuring deviations from the empirical distribution, as we shall see, allows us to derive suitable limit laws (or) probabilistic inequalities that can be used to give a systematic prescription for the radius of uncertainty, $\delta$, in the definition of the uncertainty region $U_\delta(\mathbb{P}_n) = \{\mathbb{P} : D_c(\mathbb{P}, \mathbb{P}_n) \leq \delta\}$.

It is well-understood that as the number of samples $n$ increase, the expected deviation of the empirical distribution from the true distribution decays to zero, as a function of $n$, at a
specific rate. To begin with, as a direct approach towards choosing the size of uncertainty $\delta$, one can perhaps use a suitable concentration inequality that measures such rate of convergence in terms of Wasserstein distances (see, for example, [17], and references therein). Such a simple specification of the size of uncertainty, suitably as a function of $n$, does not arise naturally in the deterministic robust optimization approaches in [53, 54].

For an application of these concentration inequalities to choose the size of uncertainty set in the context of distributionally robust logistic regression and data-driven DRO, refer [42, 28]. The exact representation for regularized logistic regression we derive later in Section 2.4 can be seen as an extension, in which the approximate representation described in [42, Remark 1] is made to coincide exactly with the regularized logistic regression estimator that has been widely used in practice. It is important to note that, despite imposing severe tail assumptions, the concentration inequalities used to choose the radius of uncertainty set in [42, 28] dictate the size of uncertainty to decay at the rate $O(n^{-1/d})$; unfortunately, this prescription scales non-gracefully as the number of dimensions $d$ increase and the resulting coverage guarantees suffer from a poor rate of convergence (see, for example, [42, Theorem 2], [28, Theorem 3.5]). Since most of the modern learning and decision problems have huge number of covariates, application of such concentration inequalities with poor rate of decay with dimensions may not be most suitable for applications.

In contrast to directly using concentration inequalities, as we shall see, the prescription obtained via RWPI typically has a rate of convergence of order $O(n^{-1/2})$ as $n \to \infty$ (for fixed $d$). In particular, as we discuss in the case of LASSO, according to our results corresponding to contribution E), RWPI based prescription of the size of uncertainty actually can be shown (under suitable regularity conditions) to decay at rate $O(\sqrt{\log d/n})$ (uniformly over $d$ and $n$ such that $\log^2 d \ll n$), which is in agreement with the findings of high-dimensional statistics literature (see [12, 29, 2] and references therein). A profile function based approach towards calibrating the radius of uncertainty in the context of empirical likelihood based DRO can be found in [26, 14, 20, 25].

Although we have focused our discussion on the context of regularized estimators, our results are directly applicable to the area of data-driven Distributionally Robust Optimization whenever the uncertainty sets are defined in terms of a Wasserstein distance or, more generally, an optimal transport metric. In particular, consider a distributionally robust formulation of the form

$$
\min_{\theta : G(\theta) \leq 0} \max_{P : D_c(P, P_n) \leq \delta} \mathbb{E}_P [H(W, \theta)],
$$

for a random element $W$ and a convex function $H(W, \cdot)$ defined over a convex region $\{\theta : G(\theta) \leq 0\}$ (assuming $G : \mathbb{R}^d \to \mathbb{R}$ convex). Here $P_n$ is the empirical measure of the sample $\{W_1, ..., W_n\}$. One can then follow a reasoning parallel to what we advocate throughout our LASSO discussion. Argue, by applying the corresponding KKT (Karush-Kuhn-Tucker) conditions, if possible, that an optimal solution $\theta_*$ to the problem

$$
\min_{\theta : G(\theta) \leq 0} \mathbb{E}_{P_{\text{true}}} [H(W, \theta)]
$$

satisfies a system of estimating equations of the form $\mathbb{E}_{P_{\text{true}}} [h(W, \theta_*)] = 0$, for a suitable $h(\cdot)$ (where $P_{\text{true}}$ is the weak limit of the empirical measure $P_n$ as $n \to \infty$). Then, given a confidence level $1 - \alpha$, one should choose $\delta$ as the $(1 - \alpha)$ quantile of the RWP function,

$$
R_n(\theta_*) = \inf \{D_c(P, P_n) : \mathbb{E}_P[h(W, \theta_*)] = 0\}.
$$
The results in Section 2 can then be used directly to approximate the \((1 - \alpha)\)-quantile of \(R_n(\theta^*)\). Just as we explain in our discussion of the square-root LASSO example, the selection of \(\delta\) is the smallest possible choice for which \(\theta^*\) is plausible with \((1 - \alpha)\) confidence.

1.4. Connections to related inference literature. We next discuss the connections between RWPI and EL. In EL one builds a Profile Likelihood for an estimating equation. For instance, in the context of EL applied to estimating \(\beta\) satisfying (5), one would build a Profile Likelihood Function in which the optimization object is defined as the likelihood (or the log-likelihood) between a given distribution \(P\) with respect to \(P_n\). Therefore, the analogue of the uncertainty set \(\{P : D_c(P, P_n) \leq \delta\}\), in the context of EL, will typically contain distributions whose support coincides with that of \(P_n\). In contrast, the definition of the RWP function does not require the likelihood between an alternative plausible model \(P\), and the empirical distribution, \(P_n\), to exist. Owing to this flexibility, for example, we are able to establish the connection between regularization estimators and a suitable profile function.

There are other potential benefits of using a profile function which does not restrict the support of alternative plausible models. For example, it has been observed in the literature that in some settings EL might exhibit low coverage [34, 13, 52]. It is not the goal of this paper to examine the coverage properties of RWPI systematically, but it is conceivable that relaxing the support of alternative plausible models, as RWPI does, can translate into desirable coverage properties.

From a technical standpoint, the definition of the Profile Function in EL gives rise to a finite dimensional optimization problem. Moreover, there is a substantial amount of smoothness in the optimization problems defining the EL Profile Function. This smoothness can be leveraged in order to obtain the asymptotic distribution of the Profile Function as the sample size increases. In contrast, the optimization problem underlying the definition of RWP function in RWPI is an infinite dimensional linear program. Therefore, the mathematical techniques required to analyze the associated RWP function are different (more involved) than the ones which are commonly used in the EL setting.

A significant advantage of EL, however, is that the limiting distribution of the associated Profile Function is typically chi-squared. Moreover, this distribution is self-normalized in the sense that no parameters need to be estimated from the data. Unfortunately, this is typically not the case in using RWPI. In many settings, however, the parameters of the distribution can be easily estimated from the data itself.

Another methodology, strongly related to RWPI, has been studied recently by the name of SOS (Sample-Out-of-Sample) inference [6]. A suitable RWP function is built in this setting as well, but the support of alternative plausible models is assumed to be finite (but not necessarily equal to that of \(P_n\)). Instead, the support of alternative plausible models is assumed to be generated not only by the available data, but additional samples from independent distributions (defined by the user). The limit results obtained for the RWP function in the context of SOS are different from those obtained in this paper. For example, in the SOS setting, the rates of convergence are dimension-dependent, which is not the case in the RWPI. As explained in [6, 7], SOS inference is natural in applications such as semi-supervised learning, in which massive amounts of unlabeled data inform the support of the covariates.

1.5. Organization of the paper. The rest of the paper is organized as follows. Section 2 corresponds to contribution A): we first introduce Wasserstein distances and then discuss distributionally robust representations of popular machine learning algorithms. Section B deals
with contribution $B$); we discuss the RWP function as an inference tool in a way which is parallel to the Profile Likelihood in EL, and derive the asymptotic distribution of the RWP function for general estimating equations. Section 4 discusses contributions $C$, namely the application of the results from $B$ for optimal regularization. Our high-dimensional analysis of the RWP function in the case of square-root LASSO is also presented in Section 4. Numerical experiments using both simulated and real data sets are given in Section 5. Proofs of all the results are presented in the supplementary material [8] made available at the end of this article.

2. Optimal Transport Definitions and DRO Representations of Machine Learning Estimators

We begin with definitions of optimal transport costs and Wasserstein distances.

2.1. Optimal Transport Costs and Wasserstein Distances. Let $c : \mathbb{R}^m \times \mathbb{R}^m \to [0, \infty]$ be any lower semi-continuous function such that $c(u, u) = 0$ for every $u \in \mathbb{R}^m$. Given two probability distributions $P(\cdot)$ and $Q(\cdot)$ supported on $\mathbb{R}^m$, the optimal transport cost or discrepancy between $P$ and $Q$, denoted by $D_c(P, Q)$, is defined as,

$$D_c(P, Q) = \inf \{ \mathbb{E}_\pi [c(U, W)] : \pi \in \mathcal{P}(\mathbb{R}^m \times \mathbb{R}^m), \pi_U = P, \pi_W = Q \}. \quad (7)$$

Here, $\mathcal{P}(\mathbb{R}^m \times \mathbb{R}^m)$ is the set of joint probability distributions $\pi$ of $(U, W)$ supported on $\mathbb{R}^m \times \mathbb{R}^m$ and $\pi_U, \pi_W$ denote the marginals of $U$ and $W$, respectively, under the joint distribution $\pi$. Intuitively, the quantity $c(u, w)$ can be interpreted as the cost of transporting unit mass from $u$ in $\mathbb{R}^m$ to another element $w$ in $\mathbb{R}^m$. Then the expectation $\mathbb{E}_\pi[c(U, W)]$ corresponds to the expected transport cost associated with the joint distribution $\pi$.

In addition to the stated assumptions on the cost function $c(\cdot)$, if $c^{1/\rho}$ satisfies the properties of a metric for any $\rho > 1$, then $D_{c^{1/\rho}}(P, Q)$ defines a metric between probability distributions (see [21] for a proof and other properties of $D_c$). For example, if $c(u, w) = \|u - w\|_2^2$, then $\rho = 2$ yields that $c(u, w)^{1/2} = \|u - w\|_2$ is symmetric, non-negative, lower semi-continuous and it satisfies the triangle inequality. In that case,

$$D_{c^{1/2}}(P, Q) = \inf \left\{ \sqrt{\mathbb{E}_\pi [\|U - W\|_2^2]} : \pi \in \mathcal{P}(\mathbb{R}^m \times \mathbb{R}^m), \pi_U = P, \pi_W = Q \right\}$$

coincides with the Wasserstein distance of order two. More generally, if we choose $c^{1/\rho}(u, w) = \|u - w\|_q$ for some $\rho, q \geq 1$, then $D_{c^{1/\rho}}(\cdot)$ is the known as the Wasserstein distance of order $\rho$.

Wasserstein distances metrize weak convergence of probability measures under suitable moment assumptions and have received immense attention in probability theory (see [37] [38] [51] for a collection of classical applications). In addition, earth-mover’s distance, a particular example of Wasserstein distances, has been of interest in image processing (see [40] [47]). More recently, optimal transport metrics and Wasserstein distances are being actively investigated for its use in various machine learning applications (see [11] [35] [18] [48] and references therein for a growing list of new applications).

Throughout this paper, we consider optimal transport costs $D_c(\cdot)$ for a judiciously chosen cost function $c(\cdot)$ to result in formulations such as (2). As we shall see in Section 2.1, it is useful to allow $c(\cdot)$ to be lower semi-continuous and potentially be infinite in some region. Thus our setting requires discrepancy choices which are slightly more general than standard Wasserstein distances.
2.2. DRO formulation using optimal transport costs. A common theme in machine learning problems is to find the best fitting parameter in a family of parameterized models that relate a vector of predictor variables $X \in \mathbb{R}^d$ to a response $Y \in \mathbb{R}$. In this section, we shall focus on a useful class of such models, namely, linear and logistic regression models. Associated with these models, we have a loss function $l(X_i, Y_i; \beta)$ which evaluates the fit of regression coefficient $\beta$ for the given data points $\{(X_i, Y_i) : i = 1, \ldots, n\}$. Then, just as we explained in the case of square-root LASSO in the Introduction, our first step will be to show that regularized linear and logistic regression estimators admit a Distributionally Robust Optimization (DRO) formulation of the form,

$$\inf_{\beta \in \mathbb{R}^d} \sup_{P : D_c(P, P_n) \leq \delta} \mathbb{E}_P [l(X, Y; \beta)].$$  \hspace{1cm} (8)

In contrast to the empirical risk minimization that performs well only on the training data, the DRO problem (8) aims to find an optimizer $\beta$ that performs uniformly well over all probability measures in the neighborhood that can be perceived as perturbations to the empirical training data distribution. Hence the solution to (8) is said to be “distributionally robust”, and can be expected to generalize better. See [53, 54] and [42] for earlier works that relate robustness and generalization.

Recasting regularized regression as a DRO problem of form (8) lets us view these regularized estimators under the lens of distributional robustness. The regularized estimators that we consider in this paper include the regularized logistic regression estimators in Example 2 below, the support vector machines (see [21]) and the family of $\ell_p$-norm penalized linear regression estimators of the form,

$$\min_{\beta \in \mathbb{R}^d} \left\{ \sqrt{\mathbb{E}_{P_n}[l(X, Y; \beta)]} + \lambda \|\beta\|_p \right\},$$  \hspace{1cm} (9)

for any $p \in [1, \infty)$. This collection includes the square-root Lasso estimator described in Example 1 as a special case where $p = 1$.

Example 2 (Regularized Logistic Regression). Consider the context of binary classification in which case the training data is of the form $\{(X_1, Y_1), \ldots, (X_n, Y_n)\}$, with $X_i \in \mathbb{R}^d$, response $Y_i \in \{-1, 1\}$ and the model postulates that,

$$\log \frac{\mathbb{P}(Y_i = 1 | X_i = x)}{1 - \mathbb{P}(Y_i = 1 | X_i = x)} = \beta^T x$$

for some $\beta \in \mathbb{R}^d$. In this case, the log-exponential loss function (or negative log-likelihood for binomial distribution) is

$$l(x, y; \beta) = \log \left( 1 + \exp(-y \cdot \beta^T x) \right),$$

and one is interested in estimating $\beta$ by solving

$$\min_{\beta \in \mathbb{R}^d} \left\{ \mathbb{E}_{P_n}[l(X, Y; \beta)] + \lambda \|\beta\|_p \right\},$$  \hspace{1cm} (10)

for $p \in [1, \infty)$. Refer [21] for a more detailed discussion on regularized logistic regression.

2.3. Dual form of the DRO formulation (3). Though the DRO formulation (3) involves optimizing over uncountably many probability measures, recent strong duality results for Wasserstein DRO (see, for example, Theorem 1 in [9]) ensures that the inner supremum in (3) admits a reformulation which is a simple, univariate optimization problem. Before stating the result,
we recall that the definition of discrepancy measure $\mathcal{D}_c$ requires the specification of cost function $c((x, y), (x', y'))$ between any two predictor-response pairs $(x, y), (x', y') \in \mathbb{R}^{d+1}$.

**Proposition 1.** Let $c: \mathbb{R}^{d+1} \times \mathbb{R}^{d+1} \to [0, \infty]$ be a lower semi-continuous cost function satisfying $c((x, y), (x', y')) = 0$ whenever $(x, y) = (x', y')$. For $\gamma \geq 0$ and loss functions $l(x, y; \beta)$ that are upper semi-continuous in $(x, y)$ for each $\beta$, define

$$\phi_{\gamma}(X_i, Y_i; \beta) := \sup_{u, v \in \mathbb{R}^d} \{l(u, v; \beta) - \gamma c((u, v), (X_i, Y_i))\}.$$  \hspace{1cm} (11)

Then

$$\sup_{\mathbb{P} : \mathcal{D}_c(\mathbb{P}, \mathbb{P}_n) \leq \delta} \mathbb{E}_\mathbb{P}[l(X, Y; \beta)] = \min_{\gamma \geq 0} \left\{ \gamma \delta + \frac{1}{n} \sum_{i=1}^{n} \phi_{\gamma}(X_i, Y_i; \beta) \right\}.$$  \hspace{1cm} (12)

Consequently, the DR regression problem \(\text{(5)}\) reduces to

$$\inf_{\beta \in \mathbb{R}^d} \sup_{\mathbb{P} : \mathcal{D}_c(\mathbb{P}, \mathbb{P}_n) \leq \delta} \mathbb{E}_\mathbb{P}[l(X, Y; \beta)] = \inf_{\beta \in \mathbb{R}^d} \min_{\gamma \geq 0} \left\{ \gamma \delta + \frac{1}{n} \sum_{i=1}^{n} \phi_{\gamma}(X_i, Y_i; \beta) \right\}.$$  \hspace{1cm} (13)

Proposition 1 follows as a straightforward application of [9, Theorem 1]. As we shall see in Section 2.4, the function $\phi_{\gamma}(\cdot)$ is explicitly computable for various examples of interest. Of the reformulations in the literature for Wasserstein distance based DRO (see [15, 9, 19]), the general cost structure assumed in [9, Theorem 1] is essential for the exact recovery of machine learning estimators that are presented below in Section 2.4.

2.4. Distributionally Robust Representations.

2.4.1. Example 7 (continued): Recovering regularized estimators for linear regression. We examine the right-hand side of (12) for the square loss function for the linear regression model $Y = \beta^T X + e$, and obtain the following result without any further distributional assumptions on $X, Y$ and the error $e$. For brevity, let $\beta = (-\beta, 1)$, and recall the definition of the discrepancy measure $\mathcal{D}_c$ in (7).

**Proposition 2** (DR linear regression with square loss). Fix $q \in (1, \infty]$. Consider the square loss function and second order discrepancy measure $\mathcal{D}_c$ defined using $\ell_q$-norm. In other words, take $l(x, y; \beta) = (y - \beta^T x)^2$ and $c((x, y), (u, v)) = \|(x, y) - (u, v)\|_q^2$. Then,

$$\inf_{\beta \in \mathbb{R}^d} \sup_{\mathbb{P} : \mathcal{D}_c(\mathbb{P}, \mathbb{P}_n) \leq \delta} \mathbb{E}_\mathbb{P}[l(X, Y; \beta)] = \inf_{\beta \in \mathbb{R}^d} \left( \sqrt{MSE_n(\beta)} + \sqrt{\delta} \|\beta\|_p \right)^2,$$  \hspace{1cm} (13)

where $MSE_n(\beta) = \mathbb{E}_{\mathbb{P}_n}[\|Y - \beta^T X\|^2] = \frac{1}{n} \sum_{i=1}^{n} (Y_i - \beta^T X_i)^2$ is the mean square error for the coefficient choice $\beta$ and $p$ is such that $1/p + 1/q = 1$.

As an important special case, we consider $q = \infty$ and identify the following equivalence for DR regression applying discrepancy measure based on neighborhoods defined using $\ell_\infty$ norm:

$$\arg \min_{\beta \in \mathbb{R}^d} \sup_{\mathbb{P} : \mathcal{D}_c(\mathbb{P}, \mathbb{P}_n) \leq \delta} \mathbb{E}_\mathbb{P}[l(X, Y; \beta)] = \arg \min_{\beta \in \mathbb{R}^d} \left\{ \sqrt{MSE_n(\beta)} + \sqrt{\delta} \|\beta\|_1 \right\}.$$  \hspace{1cm} (14)

The right hand side of (13) resembles $\ell_p$-norm regularized regression (except for the fact that we have $\|\beta\|_p$ instead of $\|\beta\|_p$). In order to obtain the exact equivalence, we introduce a slight...
modification to the norm \( \| \cdot \|_q \) to be used as the cost function, \( c(\cdot) \), in defining \( D_c \). We define
\[
N_q((x, y), (u, v)) = \begin{cases} \|x - u\|_q, & \text{if } y = v, \\ \infty, & \text{otherwise}, \end{cases}
\]
in order to use \( c(\cdot) = N_q(\cdot) \) as the transportation cost instead of the standard \( \ell_q \) norm \( \|(x, y) - (u, v)\|_q \). Subsequently, one can consider modified cost functions of form \( c((x, y), (u, v)) = (N_q((x, y), (u, v)))^p \). As this modified cost function assigns infinite cost when \( y \neq v \), the infimum in (13) is effectively over joint distributions that do not alter the marginal distribution of \( Y \).

As a consequence, the resulting neighborhood set \( \{P : D_c(P, P_n) \leq \delta \} \) admits distributional ambiguities only with respect to the predictor variables \( X \).

The following result is essentially the same as Proposition 2 except for the use of the modified cost \( N_q \) and the resulting norm regularization of form \( \|\beta\|_p \) (instead of \( \|\beta\|_p \)), as in Proposition 2, thus exactly recovering the regularized regression estimators in (9).

**Theorem 1.** Consider the square loss, \( l(x, y; \beta) = (y - \beta^T x)^2 \), and discrepancy measure \( D_c(P, P_n) \) defined as in (7) using the cost function \( c((x, y), (u, v)) = (N_q((x, y), (u, v)))^p \) with \( p = 2 \). Then,
\[
\inf_{\beta \in \mathbb{R}^d} \sup_{D_c(P, P_n) \leq \delta} \mathbb{E}_P[l(X, Y; \beta)] = \inf_{\beta \in \mathbb{R}^d} \left( \sqrt{\text{MSE}_n(\beta)} + \sqrt{\delta \|\beta\|_p} \right)^2,
\]
where \( \text{MSE}_n(\beta) = \mathbb{E}_{P_n}[(Y - \beta^T X)^2] = n^{-1} \sum_{i=1}^n (Y_i - \beta^T X_i)^2 \) is the mean square error for the coefficient choice \( \beta \) and \( p \) is such that \( 1/p + 1/q = 1 \).

2.4.2. **Example 2 (continued): Recovering regularized estimators for classification.** Apart from exactly recovering norm regularized estimators for linear regression, the discrepancy measure \( D_c \) based on the modified norm \( N_q \) in (14) is natural when our interest is in learning problems where the responses \( Y_i \) take values in a finite set – as in the binary classification problem where the response variable \( Y \) takes values in \{−1, +1\}. The following result allows us to recover the DRO formulation behind the regularized logistic regression estimators discussed in Example 2 and as well for the widely used support vector machines (see [24]).

**Theorem 2** (Regularized regression for Classification). Consider the discrepancy measure \( D_c(\cdot) \) defined using the cost function \( c((x, y), (u, v)) = N_q((x, y), (u, v))^p \) with \( p = 1 \). Then for logistic regression with log-exponential loss function and Support Vector Machine (SVM) with the hinge loss function, we have
\[
\inf_{\beta \in \mathbb{R}^d} \sup_{D_c(P, P_n) \leq \delta} \mathbb{E}_P[\log(1 + e^{-Y \beta^T X})] = \inf_{\beta \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n \log \left( 1 + e^{-Y_i \beta^T X_i} \right) + \delta \|\beta\|_p,
\]
and
\[
\inf_{\beta \in \mathbb{R}^d} \sup_{D_c(P, P_n) \leq \delta} \mathbb{E}_P[(Y \beta^T X)^+] = \frac{1}{n} \sum_{i=1}^n (1 - Y_i \beta^T X_i)^+ + \delta \|\beta\|_p,
\]
where \( p \) is such that \( 1/p + 1/q = 1 \).

The proofs of all of the results in this subsection are provided in Appendix A.1 in the supplementary material [8]. The example of logistic regression with Wasserstein distance based uncertainty sets has been considered in [42]. The representation for regularized logistic regression in Theorem 2 can be seen as an extension in which the approximate representation described in [42, Remark 1] is made to coincide exactly with the regularized logistic regression estimator.
that has been widely used in practice. The approximate representation for regularized logistic regression in [42] is based on the semi-infinite linear programming duality results due to [44]. On the other hand, due to the presence of infinite transportation costs in our DRO formulation that results in the desired exact representation (see Theorem 2), we utilize a different strong duality result, [9, Theorem 1], that is specifically derived for Wasserstein DRO with general cost structures. In addition, other equivalences described for square-root LASSO and Support Vector Machines in terms of Wasserstein DRO, as far as we know, have been reported for the first time in this paper. See [43] for additional examples.

3. The Robust Wasserstein Profile Function

Given an estimating equation $E_{P_n}[h(W, \theta)] = 0$, the objective of this section is to study the asymptotic behavior of the associated RWP function $R_n(\theta)$. As discussed in the Introduction, this analysis is key in our approach towards constructing the confidence region $\Lambda_n(\theta)$ and choosing the radius of the uncertainty set optimally.

3.1. The RWP Function for Estimating Equations and Its Use in Constructing Confidence Regions. The Robust Wasserstein Profile function’s definition is inspired by the notion of the Profile Likelihood function, introduced in the pioneering work of Art Owen in the context of EL (see [34]). We provide the definition of the RWP function for estimating $\theta^* \in \mathbb{R}^l$, which we assume satisfies

$$E[h(W, \theta^*)] = 0, \quad (15)$$

for a given random variable $W$ taking values in $\mathbb{R}^m$ and an integrable function $h: \mathbb{R}^m \times \mathbb{R}^l \to \mathbb{R}^r$. The parameter $\theta^*$ is required to be unique to ensure consistency, but uniqueness is not necessary for the limit theorems that we shall state, unless we explicitly indicate so.

Given a set of samples $\{W_1, ..., W_n\}$, which are assumed to be i.i.d. copies of $W$, we define the Wasserstein Profile function for the estimating equation (15) as,

$$R_n(\theta) := \inf \left\{ D_c(P_n, P_n) : E_P[h(W, \theta)] = 0 \right\}. \quad (16)$$

Here, recall that $P_n$ denotes the empirical distribution associated with the training samples $\{W_1, ..., W_n\}$ and $c(\cdot)$ is a chosen cost function. In this section, we are primarily concerned with cost functions of the form,

$$c(u, w) = \|w - u\|^\rho_q, \quad (17)$$

where $\rho \in [1, \infty)$ and $q \in (1, \infty]$. We remark, however, that the methods presented here can be easily adapted to more general cost functions. For simplicity, we assume that the samples $\{W_1, ..., W_n\}$ are distinct.

Since, as we shall see, the asymptotic behavior of the RWP function $R_n(\theta)$ is dependent on the exponent $\rho$ in (17), we sometimes write $R_n(\theta; \rho)$ to make this dependence explicit; but whenever the context is clear, we drop $\rho$ to avoid notational burden. Also, observe that the profile function defined in [41] for the linear regression example is obtained as a particular case by selecting $W = (X, Y)$, $\beta = \theta$ and defining $h(x, y, \theta) = (y - \theta^T x)x$.

Our goal in this section is to develop an asymptotic analysis of the RWP function which parallels that of the theory of EL. In particular, we shall establish,

$$n^{\rho/2} R_n(\theta^*; \rho) \Rightarrow \bar{R}(\rho), \quad (18)$$

for a suitably defined random variable $\bar{R}(\rho)$. Throughout this paper, the symbol “$\Rightarrow$” is used to denote convergence in distribution.
As the empirical distribution weakly converges to the underlying probability distribution from which the samples are obtained, it follows from the definition of RWP function in [18] that \( R_n(\theta; \rho) \to 0 \), as \( n \to \infty \), if and only if \( \theta \) satisfies \( \mathbb{E}[h(W, \theta)] = 0 \); for every other \( \theta \), we have that \( n^{\rho/2} R_n(\theta; \rho) \to \infty \). Therefore, the result in [18] can be used to provide confidence regions around \( \theta_s \) as follows: Given a confidence level \( 1 - \alpha \) in \((0,1)\), if we denote \( \eta_\alpha \) as the \((1 - \alpha)\)-quantile of \( \bar{R}(\rho) \), that is, \( \mathbb{P}(\bar{R}(\rho) \leq \eta_\alpha) = 1 - \alpha \), then the set,

\[
\bar{\Lambda}_n \left( n^{-\rho/2} \eta_\alpha \right) = \left\{ \theta : R_n(\theta; \rho) \leq n^{-\rho/2} \eta_\alpha \right\}
\]
is an approximate \((1 - \alpha)\)-confidence region for \( \theta_s \). This is because, by definition of \( \bar{\Lambda}_n(\cdot) \),

\[
\mathbb{P} \left( \theta_s \in \bar{\Lambda}_n \left( n^{-\rho/2} \eta_\alpha \right) \right) = \mathbb{P} \left( n^{\rho/2} R_n (\theta_s; \rho) \leq \eta_\alpha \right) \approx \mathbb{P} \left( \bar{R}(\rho) \leq \eta_\alpha \right) = 1 - \alpha.
\]

Throughout the development in this section, the dimension \( m \) of the random vector \( W \) is kept fixed and the sample size \( n \) is sent to infinity; the function \( h(\cdot) \) can be quite general.

### 3.2. The dual formulation of RWP function.

The first step in the analysis of the RWP function \( R_n(\theta) \) is to use the definition of the discrepancy measure \( D_c \) to rewrite \( R_n(\theta) \) as,

\[
R_n(\theta) = \inf_{\pi \in \mathcal{P}(\mathbb{R}^m \times \mathbb{R}^m)} \left\{ \mathbb{E}_\pi[c(U, W)] : \pi \in \mathcal{P}(\mathbb{R}^m \times \mathbb{R}^m), \mathbb{E}_\pi[h(U, \theta)] = 0, \pi_w = \mathbb{P}_n \right\},
\]

which is a problem of moments of the form,

\[
R_n(\theta) = \inf_{\pi \in \mathcal{P}(\mathbb{R}^m \times \mathbb{R}^m)} \left\{ \mathbb{E}_\pi[c(U, W)] : \mathbb{E}_\pi[h(U, \theta)] = 0, \mathbb{E}_\pi[h(W = W_i)] = \frac{1}{n}, i \leq n \right\}. \tag{20}
\]

The problem of moments is a classical linear programming problem for which the respective dual formulation and strong duality have been well-studied (see, for example, [23, 46]). The linear program problem over the variable \( \pi \) in (20) admits a simple dual semi-infinite linear program of form,

\[
\sup_{a_t \in \mathbb{R}, \lambda \in \mathbb{R}} \left\{ a_0 + \frac{1}{n} \sum_{i=1}^{n} a_t : a_0 + \sum_{i=1}^{n} a_t 1_{(u=W_i)}(u, w) + \lambda^T h(u, \theta) \leq c(u, w), \forall u, w \in \mathbb{R}^m \right\}
\]

\[=
\sup_{\lambda \in \mathbb{R}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \inf_{u \in \mathbb{R}^m} \left\{ c(u, W_i) - \lambda^T h(u, \theta) \right\} \right\}
\]

\[=
\sup_{\lambda \in \mathbb{R}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \sup_{u \in \mathbb{R}^m} \left\{ \lambda^T h(u, \theta) - c(u, W_i) \right\} \right\}.
\]

Proposition 3 below states that strong duality holds under mild assumptions, and the dual formulation above indeed equals \( R_n(\theta) \).

**Proposition 3.** Let \( h(\cdot, \theta) \) be Borel measurable, and \( \Omega = \{(u, w) \in \mathbb{R}^m \times \mathbb{R}^m : c(u, w) < \infty\} \) be Borel measurable and non-empty. Further, suppose that \( 0 \) lies in the interior of the convex hull of \( \{h(u, \theta) : u \in \mathbb{R}^m\} \). Then,

\[
R_n(\theta) = \sup_{\lambda \in \mathbb{R}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \sup_{u \in \mathbb{R}^m} \left\{ \lambda^T h(u, \theta) - c(u, W_i) \right\} \right\}.
\]

A proof of Proposition 3 along with an introduction to the problem of moments, is provided in Appendix B in the supplementary material [8].
3.3. Asymptotic Distribution of the RWP Function. In order to gain intuition behind \([18]\), let us first consider the simple example of estimating the expectation \(\theta_* = E[W]\) of a real-valued random variable \(W\), using \(h(w, \theta) = w - \theta\).

**Example 3.** Let \(h(w, \theta) = w - \theta\) with \(m = 1 = r\). First, suppose that the choice of cost function is \(c(u, w) = |u - w|^\rho\) for some \(\rho > 1\). As long as \(\theta\) lies in the interior of the convex hull of support of \(W\), Proposition \(3\) implies,

\[
R_n(\theta; \rho) = \sup_{\lambda \in \mathbb{R}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \sup_{u \in \mathbb{R}} \{ \lambda (u - \theta) - |W_i - u|^\rho \} \right\} = \sup_{\lambda \in \mathbb{R}} \left\{ -\frac{\lambda}{n} \sum_{i=1}^{n} (W_i - \theta) - \frac{1}{n} \sum_{i=1}^{n} \sup_{u \in \mathbb{R}} \{ \lambda (u - W_i) - |W_i - u|^\rho \} \right\}.
\]

As \(\max_{\Delta} \{\lambda \Delta - |\Delta|^\rho\} = (\rho - 1)|\lambda/\rho|^{\rho/(\rho - 1)},\) we obtain

\[
R_n(\theta; \rho) = \sup_{\lambda} \left\{ -\frac{\lambda}{n} \sum_{i=1}^{n} (W_i - \theta) - (\rho - 1) \left| \frac{\lambda}{\rho} \right| \right\} = \left| \frac{1}{n} \sum_{i=1}^{n} (W_i - \theta) \right|^\rho.
\]

Then, under the hypothesis that \(E[W] = \theta_*\), and assuming \(\text{Var}[W] = \sigma_w^2 < \infty\), we obtain,

\[n^{\rho/2}R_n(\theta_*; \rho) \Rightarrow \bar{R}(\rho) \sim \sigma_w^\rho \bar{N}(0, 1)\rho^\rho,
\]

where \(\bar{N}(0, 1)\) denotes a standard Gaussian random variable. The limiting distribution for the case \(\rho = 1\) can be formally obtained by setting \(\rho = 1\) in the above expression for \(\bar{R}(\rho)\), but the analysis is slightly different. When \(\rho = 1,\)

\[
R_n(\theta) = \sup_{\lambda \in \mathbb{R}} \left\{ -\frac{\lambda}{n} \sum_{i=1}^{n} (W_i - \theta) - \frac{1}{n} \sum_{i=1}^{n} \sup_{\Delta \in \mathbb{R}} \{ \lambda \Delta - |\Delta| \} \right\}
\]

Following the notion that \(\infty \times 0 = 0\),

\[
R_n(\theta) = \sup_{\lambda} \left\{ \frac{\lambda}{n} \sum_{i=1}^{n} (W_i - \theta) - \infty I(|\lambda| > 1) \right\} = \max_{|\lambda| \leq 1} \frac{\lambda}{n} \sum_{i=1}^{n} (W_i - \theta) = \left| \frac{1}{n} \sum_{i=1}^{n} (W_i - \theta) \right|.
\]

So, indeed if \(E[W] = \theta_*\) and \(\text{Var}[W] = \sigma_w^2 < \infty\), we obtain

\[n^{1/2}R_n(\theta_*) \Rightarrow \sigma_w \bar{N}(0, 1)|\theta_*|\]

We now discuss far reaching extensions to the developments in Example 3 by considering estimating equations that are more general. First, we state a general asymptotic stochastic upper bound, which we believe is the most important result from an applied standpoint as it captures the speed of convergence of \(R_n(\theta_*)\) to zero. Following this, we obtain an asymptotic
stochastic lower bound that matches with the upper bound (and therefore the weak limit) under mild, additional regularity conditions. We discuss the nature of these additional regularity conditions, and also why the lower bound in the case $\rho = 1$ can be obtained basically without additional regularity.

For the asymptotic upper bound we shall impose the following assumptions.

**Assumptions:**

**A1** Assume that $c(u, w) = \|u - w\|_q^p$ for $q \geq 1$ and $\rho \geq 1$. For a chosen $q \geq 1$, let $p$ be such that $1/p + 1/q = 1$.

**A2** Suppose that $\theta_\ast \in \mathbb{R}^p$ satisfies $\mathbb{E}[h(W, \theta_\ast)] = 0$ and $\mathbb{E}\|h(W, \theta_\ast)\|_2^2 < \infty$. (While we do not assume that $\theta_\ast$ is unique, the results are stated for a fixed $\theta_\ast$ satisfying $\mathbb{E}[h(W, \theta_\ast)] = 0$.)

**A3** Suppose that the function $h(\cdot, \theta_\ast)$ is continuously differentiable with derivative $D_w h(\cdot, \theta_\ast)$.

**A4** Suppose that for each $\zeta \neq 0$,

$$\mathbb{P}\left(\|\zeta^T D_w h(W, \theta_\ast)\|_p > 0\right) > 0. \quad (21)$$

Assumptions A1) - A3) make precise the setting considered. Assumption A4) is the only assumption which is technical in nature and it can be equivalently stated as

$$\mathbb{E}[D_w h(W, \theta_\ast)D_w h(W, \theta_\ast)^T] > 0,$$

where $A > 0$ is used to denote that the matrix $A$ is positive definite. Verification of this positive definiteness condition for the linear and logistic regression problems is executed, respectively, in Sections 4.2 and 4.3. In order to state the theorem, let us introduce the notation for asymptotic stochastic upper bound,

$$n^{\rho/2} R_n(\theta_\ast; \rho) \lesssim_D \bar{R}(\rho),$$

which expresses that, for every continuous and bounded non-decreasing function $f(\cdot)$, we have,

$$\lim_{n \to \infty} \mathbb{E}\left[f\left(n^{\rho/2} R_n(\theta_\ast; \rho)\right)\right] \leq \mathbb{E}\left[f\left(\bar{R}(\rho)\right)\right].$$

Similarly, we write $\gtrsim_D$ for an asymptotic stochastic lower bound, namely

$$\lim_{n \to \infty} \mathbb{E}\left[f\left(n^{\rho/2} R_n(\theta_\ast; \rho)\right)\right] \geq \mathbb{E}\left[f\left(\bar{R}(\rho)\right)\right].$$

Therefore, if both stochastic upper and lower bounds hold, then $n^{\rho/2} R_n(\theta_\ast; \rho) \Rightarrow \bar{R}(\rho)$ as $n \to \infty$. (see, for example, [5]). Now we are ready to state our asymptotic upper bound.

**Theorem 3.** Under Assumptions A1) to A4) we have, as $n \to \infty$,

$$n^{\rho/2} R_n(\theta_\ast; \rho) \lesssim_D \bar{R}(\rho),$$

where, for $\rho > 1$,

$$\bar{R}(\rho) := \max_{\zeta \in \mathbb{R}^p} \left\{\rho \zeta^T H - (\rho - 1)\mathbb{E}\|\zeta^T D_w h(W, \theta_\ast)\|_p^{\rho/(\rho - 1)}\right\},$$

and if $\rho = 1$,

$$\bar{R}(1) := \max_{\zeta \in \mathbb{P}(\|\zeta^T D_w h(W, \theta_\ast)\|_p > 1) = 0} \{\zeta^T H\}.$$
We remark that as \( \rho \to 1 \), one can verify that \( \overline{R}(\rho) \Rightarrow \overline{R}(1) \), so formally one can simply keep in mind the expression \( \overline{R}(\rho) \) with \( \rho > 1 \). It is interesting to note that \( \overline{R}(\rho) \) resembles Fenchel transform when viewed as a function of \( H \). Indeed, in the case where \( p = q = \rho = 2 \) and \( \mathbb{E}[D_w h(W, \theta_\ast)] \) is invertible, the expression for \( \overline{R}(\rho) \) simplifies as follows:

\[
\overline{R}(\rho) = \max_{\zeta \in \mathbb{R}} \left\{ 2\zeta^T H - \zeta^T \mathbb{E}[D_w h(W, \theta_\ast)] \zeta \right\} = H^T (\mathbb{E}[D_w h(W, \theta_\ast)])^{-1} H. \tag{22}
\]

We now study some sufficient conditions which guarantee that \( \overline{R}(\rho) \) is also an asymptotic lower bound for \( n^{\rho/2} R_n(\theta_\ast; \rho) \). We consider the case \( \rho = 1 \) first, which will be used in applications to logistic regression discussed later in the paper.

**Proposition 4.** In addition to assuming A1) to A4), suppose that \( W \) has a positive density (almost everywhere) with respect to the Lebesgue measure. Then,

\[
n^{1/2} R_n(\theta_\ast; 1) \Rightarrow \overline{R}(1).
\]

The following set of assumptions can be used to obtain tight asymptotic stochastic lower bounds when \( \rho > 1 \); the corresponding result will be applied to the context of square-root LASSO.

A5) (Growth condition) Assume that there exists \( \kappa \in (0, \infty) \) such that for \( \|w\|_q \geq 1 \),

\[
\|D_w h(w, \theta_\ast)\|_p \leq \kappa \|w\|_q^{\rho - 1}, \tag{23}
\]

and that \( \mathbb{E}\|W_i\|^\rho < \infty \).

A6) (Locally Lipschitz continuity) Assume that there exists \( \bar{\kappa} : \mathbb{R}^m \to [0, \infty) \) such that,

\[
\|D_w h(w + \Delta, \theta_\ast) - D_w h(w, \theta_\ast)\|_p \leq \bar{\kappa}(W_i) \|\Delta\|_q,
\]

for \( \|\Delta\|_q \leq 1 \), and \( \mathbb{E}[\bar{\kappa}(w)'] < \infty \), for \( c \leq \max\{2, \frac{\rho}{\rho - 1}\} \).

We now summarize our last weak convergence result of this section.

**Proposition 5.** If Assumptions A1) to A6) hold and \( \rho > 1 \), then

\[
n^{\rho/2} R_n(\theta_\ast; \rho) \Rightarrow \overline{R}(\rho).
\]

Before we move on with the applications of the previous results, it is worth discussing the nature of the additional assumptions introduced to ensure that an asymptotic lower bound can be obtained which matches the upper bound in Theorem 3.

As we shall see in the technical development in Appendix A.3 (see supplementary material \[3\]) where the proofs of the above results are furnished, the dual formulation of RWP function in Proposition 3 can be re-expressed, assuming only A1) to A4), as,

\[
n^{\rho/2} R_n(\theta_\ast; \rho) = \sup_{\zeta} \left\{ \zeta^T H_n - \frac{1}{n} \sum_{k=1}^n \sup_{\Delta} \left\{ \int_0^1 \zeta^T D_h \left(W_i + \Delta u/n^{1/2}, \theta_\ast\right) \Delta du - \|\Delta\|_q^\rho \right\} \right\}.
\tag{24}
\]

In order to make sure that the lower bound asymptotically matches the upper bound obtained in Theorem 3 we need to make sure that we rule out cases in which the inner supremum is infinite in \[24\] with positive probability in the prelimit.
In Proposition 4 we assume that $W$ has a positive density with respect to the Lebesgue measure because in that case the condition
\[ P \left( \| \zeta^T D_h (W, \theta_*) \|_p \leq 1 \right) = 1, \]
(which appears in the upper bound obtained in Theorem 3) implies that $\| \zeta^T D_h (w, \theta_*) \|_p \leq 1$ almost everywhere with respect to the Lebesgue measure. Due to the appearance of the integral in the inner supremum in (24), an upper bound can be obtained for the inner supremum, which translates into a tight lower bound for $n^{\rho/2} R_n (\theta_*)$.

Moving to the case $\rho > 1$ studied in Proposition 5, condition (23) in A5) guarantees that (for fixed $W_i$ and $n$)
\[ \| D_h (W_i + \Delta u / n^{1/2}, \theta_*) \Delta \| = O \left( \| \Delta \|_q / n^{(\rho-1)/2} \right), \]
as $\| \Delta \|_q \to \infty$. Therefore, the cost term $\left( - \| \Delta \|_q^\rho \right)$ in (24) will ensure a finite optimum in the prelimit for large $n$. The condition that $E \| W \|_\rho^\rho < \infty$ is natural because we are using a optimal transport cost $c(u, w) = \| u - w \|_\rho^\rho$. If this condition is not satisfied, then the underlying nominal distribution is at infinite transport distance from the empirical distribution.

The local Lipschitz assumption A6) is just imposed to simplify the analysis and can be relaxed; we have opted to keep A6) because we consider it mild in view of the applications that we will study in the sequel.

4. Using RWPI for optimal regularization

In this section, we aim to utilize the limit theorems for the RWPI function derived in Section 3.3 to select the radius of uncertainty, $\delta$, in the DRO formulation (8). Then owing to the DRO representations derived in Section 2.4, this would imply an automatic choice of regularization parameter $\lambda = \sqrt{\delta}$ in the square-root LASSO example (following Theorem 1), or $\lambda = \delta$ in the regularized logistic regression (following Theorem 2). In the development below, we follow the logic described in the Introduction for the square-root LASSO setting.

4.1. Selection of $\delta$ and coverage properties. Throughout this section, let $\beta_*$ denote the underlying linear or logistic regression model parameter from which the training samples $\{ (X_i, Y_i) : i = 1, \ldots, n \}$ are obtained. Lemma 1 below establishes that the infimum and the supremum in the DRO formulation (8) can be exchanged. See Appendix C for a proof of Lemma 1.

Lemma 1. In the settings of Theorems 1 and 2 if $E \| X \|_2^2 < \infty$, we have that
\[ \inf_{\beta \in \mathbb{R}^d} \sup_{P \in \Upsilon (\mathbb{P}_n)} \mathbb{E}_P \left[ l(X, Y; \beta) \right] = \sup_{P \in \Upsilon (\mathbb{P}_n)} \inf_{\beta \in \mathbb{R}^d} \mathbb{E}_P \left[ l(X, Y; \beta) \right]. \]
Due to the optimality of $\beta_*$, the convexity of the loss $\ell(x, y; \cdot)$ in Examples 1, 2 and finiteness of $\mathbb{E}\|X\|_2^2$, we have that $\mathbb{E}[D_\beta l(X, Y; \beta_*)] = 0$. Consider the RWP function with estimating equation $D_\delta(x, y; \beta) = 0$ given by,

$$R_n(\delta) = \inf \left\{ \mathcal{D}_c(P, P_n) : D_\beta \mathbb{E}_P [l(X, Y; \beta)] = 0 \right\}.$$  

Then, as explained in Section 1.1.3 the events $\{R_n(\beta_*) \leq \delta\}$ and $\{\beta_* \in \Lambda_n(\delta)\}$ coincide. If $\delta$ is selected so that $\delta \geq R_n(\beta_*)$, then the worst-case loss estimated by the DRO formulation (8) can be shown to form an upper bound to the empirical risk evaluated at $\beta_*$, thus controlling the bias portion of the generalization error. This is the content of Proposition 6 below.

**Proposition 6.** In the settings of Theorems 1 and 2, if $\delta \geq R_n(\beta_*)$, we have,

$$\left| \mathbb{E}_{P_n} [l(X, Y; \beta_*)] - \inf_{\beta \in \mathcal{U}(P_n)} \sup_{\mathbb{P} \in \mathcal{U}_n(P_n)} \mathbb{E}_{\mathbb{P}} [l(X, Y; \beta)] \right| \leq C_1 \delta + C_2(n) \mathbf{1}_{(\rho=2)} \sqrt{\delta},$$

where $C_1 := (2\rho - 1)\|\beta_*\|^\rho$ and $C_2(n) := 2\|\beta_*\|_p \mathbb{E}_{P_n} [l(X, Y; \beta_*)]$.

Now, in order to guarantee that $\delta \geq R_n(\beta_*)$ (or equivalently, $\beta^* \in \Lambda_n(\delta)$) with a desired confidence $1 - \alpha$, it is sufficient to proceed as in Section 3.1. Let $\eta_0$ be the $(1 - \alpha)$-quantile of the weak limit, $\bar{R}$, resulting from $n^{\rho/2}R_n(\beta_*) \Rightarrow \bar{R}$, derived in Section 3.3. In light of Theorems 1 and 2, we have $\rho = 2$ for Example 1 and $\rho = 1$ for Example 2. If we take $n \geq \eta_0$,

$$\delta = n^{-\rho/2} \eta^* \quad \text{and} \quad \Lambda_n(\delta) = \{ \beta : R_n(\beta) \leq n^{-\rho/2} \eta^* \},$$

then $\lim_{n \to \infty} \mathbb{P}(R_n(\beta_*) > n^{-\rho/2} \eta^*) \leq \alpha$. Then, as demonstrated in (19), we have $\lim_{n \to \infty} \mathbb{P}(\beta_* \in \Lambda_n(\delta)) \geq 1 - \alpha$. In Sections 4.2 - 4.3 below, we illustrate the application of this prescription by deriving upper bounds for $\bar{R}$ that are not dependent on the knowledge of $\beta_*$. 

**Theorem 4.** In the settings of Theorems 1 and 2, suppose that the samples $\{(X_i, Y_i) : i \leq n\}$ are obtained from the distribution $P_*$ and $\mathbb{E}_{P_*} \|X\|_2^2 < \infty$. For any $1 - \alpha < 1/2$, if $\delta$ is chosen to be $n^{-\rho/2} \eta^*$ for some $\eta^* \geq \eta_0$, then we have that,

$$\lim_{n \to \infty} \mathbb{P} \left( \inf_{\beta \in \mathbb{R}^d} \mathbb{E}_{P_*} [l(X, Y; \beta)] - \inf_{\beta \in \mathbb{R}^d} \sup_{\mathbb{P} \in \mathcal{U}_n(P_n)} \mathbb{E}_{\mathbb{P}} [l(X, Y; \beta)] \right) \leq \frac{C}{\sqrt{n}} \geq 1 - 2\alpha,$$

for some positive constant $C$ depending on $\rho$, $\mathbb{E}_{P_*} [l(X, Y; \beta_*)]$ and $\mathbb{V}_{P_*} [l(X, Y; \beta_*)]$.

Proofs of Proposition 6 and Theorem 4 are furnished in Appendix A.2 in the supplementary material. Explicit prescriptions for the selection of $\delta$ satisfying conditions of Theorem 4 for the case of linear and logistic regression examples are provided in Sections 4.2 and 4.3.

In contrast to the $O(n^{-1/d})$ rate of convergence for the prescription of $\delta$ resulting from concentration inequalities for $D_c(P_n, P_*)$ (see, for example, [12 Theorem 2], [28 Theorem 3.5]), Theorem 4 asserts that the DRO formulation with RWPI based prescription for $\delta$ enjoys the optimal $O(n^{-1/2})$—rate of convergence for the optimal risk. Roughly speaking, this is because the objective of RWPI is to choose the radius $\delta$ resulting in good coverage properties for the optimal parameter $\beta_*$, which has $d-$degrees of freedom; on the other hand, the objective behind concentration inequalities is to choose $\delta$ with good coverage properties for the data-generating probability distribution itself, which is an infinite dimensional object. It is well-known that the distance between a probability distribution and an empirical version of itself constituting $n-$independent samples is $\Omega(n^{-1/d})$ as $n \to \infty$ (see, for example, [49]).
Coverage for the optimal risk, for the particular example of LASSO estimator, can also be derived, for example, from the limit theorems in [24]. Once $\delta$ is chosen using RWP function, as it can be seen from the proofs of Proposition 6 and Theorem 4, the deduction of the rate of convergence and coverage turns out to be fairly intuitive and simple. This serves to illustrate the fundamental role played by the RWP function in determining the radius of the uncertainty set. A unified profile function based method to deduce coverage of optimal risk for regularized estimators is entirely novel. We believe that the approach described here could serve as a template for deducing similar coverage guarantees for more general DRO formulations that are not necessarily amenable to be recast as regularized estimators.

4.2. Linear regression models with squared loss function. In this section, we derive the asymptotic limiting distribution of suitably scaled profile function corresponding to the estimating equation, $E[(Y - \beta^T X)X] = 0$. The chosen estimating equation describes the optimality condition for the expected loss $E[(Y - \beta^T X)^2]$, and therefore, the corresponding $R_n(\beta_*)$ is suitable for choosing $\delta$ as in (26), and the regularization parameter $\lambda = \sqrt{\delta}$ in Example 1.

4.2.1. A stochastic upper bound for the RWP limit. Let $H_0$ denote the null hypothesis that the training samples $\{(X_1,Y_1), \ldots, (X_n,Y_n)\}$ are obtained independently from the linear model $Y = \beta^T X + e$, where the error term $e$ has zero mean, variance $\sigma^2$, and is independent of $X$. Let $\Sigma = E[XX^T]$.

**Theorem 5.** Consider the discrepancy measure $D_c(\cdot)$ defined as in (7) using the cost function $c((x,y),(u,v)) = \left(N_q((x,y),(u,v))\right)^2$ (the function $N_q$ is defined in (14)). For $\beta \in \mathbb{R}^d$, let

$$R_n(\beta) = \inf \{ D_c(\mathbb{P}, \mathbb{P}_n) : E\mathbb{P}\left[(Y - \beta^T X)X\right] = 0 \}.$$ 

Then, under the null hypothesis $H_0$,

$$nR_n(\beta_*) \Rightarrow L_1 := \max_{\zeta \in \mathbb{R}^d} \left\{ 2\sigma \zeta^T Z - E \| \epsilon \zeta - (\zeta^T X)\beta_* \|_p^2 \right\},$$

as $n \to \infty$. In the above limiting relationship, $Z \sim \mathcal{N}(0, \Sigma)$. Further,

$$L_1 \overset{D}{\leq} L_2 := \frac{E|\epsilon|^2}{E|\epsilon|^2 - (E|\epsilon|)^2} \| Z \|_q^2.$$

Specifically, if the additive error term $e$ follows a centered normal distribution, then

$$L_1 \overset{D}{\leq} L_2 := \frac{\pi}{\pi - 2} \| Z \|_q^2.$$ 

In the above theorem, the relationship $L_1 \overset{D}{\leq} L_2$ denotes that $L_1$ is stochastically dominated by $L_2$, in the sense that, $\mathbb{P}(L_1 \geq x) \leq \mathbb{P}(L_2 \geq x)$ for all $x \in \mathbb{R}$. Note that this notation for stochastic upper bound is different from the notation $\preceq_D$ introduced in Section 3.3 to denote asymptotic stochastic upper bound. A proof of Theorem 5 as an application of Theorem 3 and Proposition 5 is presented in Appendix Section A.4 (see supplementary material [5]).

4.2.2. Using Theorem 5 to obtain regularization parameter for (9). Let $\eta_{1-\alpha}$ denote the $(1 - \alpha)$ quantile of the limiting random variable $L_1$ in Theorem 5 or its stochastic upper bound $L_2$. Then following the prescription in (26) and the DRO equivalence in Theorem 4, regularization parameter for the $\ell_p$-penalized linear regression in (9) can be chosen as follows:
1) Draw samples $Z$ from $\mathcal{N}(0, \Sigma)$ to estimate the $1 - \alpha$ quantile of one of the random variables $L_1$ or $L_2$ in Theorem 5. Let us use $\hat{\eta}_{1-\alpha}$ to denote the estimated quantile. While $L_2$ is simply the norm of $Z$, obtaining realizations of limit law $L_1$ involves solving an optimization problem for each realization of $Z$. If $\Sigma = E[XX^T]$ is not known, one can use a simple plug-in estimator for $E[XX^T]$ in place of $\Sigma$.

2) Choose the regularization parameter $\lambda$ to be,

$$\lambda = \sqrt{\delta} = \sqrt{\hat{\eta}_{1-\alpha}}/n.$$ 

It is interesting to note that the prescription of regularization parameter obtained by using $L_2$ does not depend on the variance of $e$, thus removing the need for estimating the variance of $e$. This property is a key advantage of the use of square-root LASSO estimator over the traditional LASSO (see [2]).

4.2.3. On the approximation ratio $L_2/L_1$ when $p = q = 2$. In the case where $q$ is taken to be $p = q = 2$ in Theorem 1 (corresponding to $\ell_2$-penalization as in ridge regression), it is possible to obtain an explicit expression for the limit law $L_1$ as follows: Under the assumptions stated in Theorem 5 we have $E[(c^* - X\beta^*_1)(c^* - X\beta^*_2)^T] = \sigma^2 I_d + \|\beta^*_s\|^2 \Sigma$. Then, as in (22), we obtain, $L_1 = \sigma^2 Z^T (\sigma^2 I_d + \|\beta^*_s\|^2 \Sigma)^{-1} Z$. Suppose that $X$ is centered so that $E[X] = 0$ and $\Sigma$ is invertible. Then, if $\Sigma = U\Lambda U^T$ is the eigen decomposition of $\Sigma$, we have that $N = \Lambda^{-1/2} U^T Z$ has normal distribution with mean 0 and covariance $I_d$. As a result,

$$L_1 = \sigma^2 Z^T (\sigma^2 I_d + \|\beta^*_s\|^2 \Sigma)^{-1} Z = \sum_{i=1}^d \frac{\Lambda_{ii}}{1 + \Lambda_{ii}\|\beta^*_s\|^2/\sigma^2} N_i^2,$$

and

$$\frac{E[e^2] - (E[e])^2}{E[e^2]} L_2 = \|Z\|^2_2 = \sum_{i=1}^d \Lambda_{ii} N_i^2.$$

If we let $c_1 = 1 + \sigma^{-2}\|\beta^*_s\|^2 \max_{i=1,\ldots,d} \Lambda_{ii}$ and $c_2 = \text{Var}[e]/\text{Var}[e]$, we arrive at the relationship that, $L_1 \leq L_2 \leq c_1 c_2 L_1$.

One could aim to achieve lower bias in estimation by working with the $(1 - \alpha)$-quantile of the limit law $L_1$ (see Proposition 4), instead of that of the stochastic upper bound $L_2$. In order to do so, we propose to use any consistent estimator for $\beta^*_s$ to be plugged in the expression for $L_1$ to result in asymptotically optimal prescription for $\delta$. The argument goes as follows: Let us write the limit law $L_1$ as $L_1(\beta^*_s)$ in order to make the dependence of the limit law $L_1$ on $\beta^*_s$ explicit. As $L_1(\cdot)$ is a continuous function, if $\beta_n \rightarrow \beta^*_s$ in probability, we have

$$n R_n(\beta^*_s) - L_1(\beta^*_s) = (n R_n(\beta^*_s) - L_1(\beta^*_s)) + (L_1(\beta^*_s) - L_1(\beta_n)) \Rightarrow 0.$$ 

One could use, for example, sample average approximations (without regularization) to compute $\beta_n$. We seek to verify in future research that the estimator obtained via this plug-in approach indeed enjoys better generalization guarantees.

4.3. Logistic Regression with log-exponential loss function. In this section, we apply results in Section 4.3.3 to prescribe regularization parameter for $\ell_p$-penalized logistic regression in Example 2.
4.3.1. A stochastic upper bound for the RWP function. Let $H_0$ denote the null hypothesis that the training samples $(X_1, Y_1), \ldots, (X_n, Y_n)$ are obtained independently from a logistic regression model satisfying

$$
\log \left( \frac{P(Y = 1 | X = x)}{1 - P(Y = 1 | X = x)} \right) = \beta^T x,
$$

for predictors $X \in \mathbb{R}^d$ and corresponding responses $Y \in \{-1, 1\}$; further, under null hypothesis $H_0$, the predictor $X$ has positive density almost everywhere with respect to the Lebesgue measure on $\mathbb{R}^d$. The log-exponential loss (or negative log-likelihood) that evaluates the fit of a logistic regression model with coefficient $\beta$ is given by

$$
l(x, y; \beta) = -\log p(y|x; \beta) = \log \left( \frac{1 + \exp(-y\beta^T x)}{1 + \exp(y\beta^T x)} \right).
$$

If we let

$$
h(x, y; \beta) = D_\beta l(x, y; \beta) = \frac{-yx}{1 + \exp(y\beta^T x)},
$$

then the optimal $\beta^*$ satisfies the first order condition that $E[h(x, y; \beta^*)] = 0$.

**Theorem 6.** Consider the discrepancy measure $D_c(\cdot)$ defined as in (27) using the cost function $c((x, y), (u, v)) = N_q((x, y), (u, v))$ (the function $N_q$ is defined in (14)). For $\beta \in \mathbb{R}^d$, let

$$R_n(\beta) = \inf \left\{ D_c(\mathbb{P}, \mathbb{P}_n) : E_\mathbb{P} [h(x, y; \beta)] = 0 \right\},$$

where $h(\cdot)$ is defined in (27). Then, under the null hypothesis $H_0$,

$$\sqrt{n}R_n(\beta_0) \Rightarrow L_3 := \sup_{\xi \in A} \xi^T Z
$$
as $n \to \infty$. In the above limiting relationship,

$$Z \sim \mathcal{N} \left( 0, E \left[ \frac{XX^T}{1 + \exp(Y\beta_0^T X)} \right] \right) \text{ and } A = \left\{ \xi \in \mathbb{R}^d : \text{ess sup}_{x,y} ||\xi^T D_x h(x, y; \beta_0)||_p \leq 1 \right\}.$$

Moreover, the limit law $L_3$ admits the following simpler stochastic bound:

$$L_3 \overset{D}{=} L_4 := \|\tilde{Z}\|_q,$$

where $\tilde{Z} \sim \mathcal{N}(0, E[XX^T])$.

A proof of Theorem 6 as an application of Theorem 3 and Proposition 4 is presented in Appendix A.4 (see supplementary material [8]).

4.3.2. Using Theorem 6 to obtain regularization parameter for (10). Similar to linear regression, the regularization parameter for Regularized Logistic Regression discussed in Example 2 can be chosen by the following procedure:

1) Estimate the $(1 - \alpha)$-quantile of $L_4 := \|\tilde{Z}\|_q$, where $\tilde{Z} \sim \mathcal{N}(0, E[XX^T])$. Let us use $\hat{\eta}_{1-\alpha}$ to denote the estimate of the quantile.

2) Choose the regularization parameter $\lambda$ in the norm regularized logistic regression estimator (10) in Example 2 to be,

$$\lambda = \delta = \hat{\eta}_{1-\alpha}/\sqrt{n}.$$
4.4. Optimal regularization in high-dimensional square-root LASSO. In this section, let us restrict our attention to the square-loss function \( l(x, y; \beta) = (y - \beta^T x)^2 \) for the linear regression model and the discrepancy measure \( D_\beta \) defined using the cost function \( c = N_q \) with \( q = \infty \) in \([4, 29, 2, 1]\). Then, due to Theorem 4, this corresponds to the interesting case of square-root LASSO or \( \ell_2 \)-LASSO that was rather a particular example in the class of \( \ell_p \) norm penalized linear regression estimators considered in Section 4.2.

As an interesting byproduct of the RWP function analysis, the following theorem presents a prescription for regularization parameter even in high dimensional settings where the ambient dimension \( d \) is larger than the number of samples \( n \). Given observations \( \{(X_i, Y_i) : i = 1, \ldots, n\} \) from the linear model \( Y = \beta^T X + e \), let \( \hat{e}_i := (Y_i - \beta^T X_i)/\sigma \), for \( i = 1, \ldots, n \). We have that the variance of the normalized error terms \( \hat{e}_i \) do not depend on \( \sigma \).

**Theorem 7.** Suppose that the assumptions imposed in Theorem 3 hold. Then,

\[
nR_n(\beta_*) \leq \frac{D}{\sqrt{n}} \frac{\|Z_n\|_\infty}{\text{Var}_n[\hat{e}]},
\]

where, \( Z_n := \frac{1}{\sqrt{n}} \sum_{i=1}^n \hat{e}_i X_i \) and \( \text{Var}_n[\hat{e}] := \sum_{i=1}^n (|\hat{e}_i| - n^{-1} \sum_{k=1}^n |\hat{e}_k|)^2 \).

**Remark 1.** Suppose that the additive error \( e \) is normally distributed and the observations \( X_i = (X_{i1}, \ldots, X_{id}) \) are normalized so that \( n^{-1} \sum_{i=1}^n X_{ij}^2 = 1 \) for \( j = 1, \ldots, d \). Then, for any \( \alpha < 1/8 \), \( C > 0, \varepsilon > 0 \), due to Lemma 1(iii) of \([2]\), the stochastic bound in Theorem 4 simplifies as follows: Conditional on the observations \( \{X_i : i = 1, \ldots, n\} \), we have,

\[
\sqrt{R_n(\beta_*)} \leq \frac{\pi}{\pi - 2} \frac{\Phi^{-1}(1 - \alpha/2d)}{\sqrt{n}},
\]

with probability asymptotically larger than \( 1 - \alpha \), as \( n \to \infty \), uniformly in \( d \) such that \( \log d \leq Cn^{1/2 - \varepsilon} \). Here, \( \Phi^{-1}(1 - \alpha) \) denotes the quantile \( x \) satisfying \( \Phi(x) = 1 - \alpha \) and \( \Phi(\cdot) \) is the cumulative distribution function of the standard normal distribution defined on \( \mathbb{R} \). Moreover, if the additive error \( e \) is not normally distributed, then under additional assumption that \( \sup_{n \geq 1} \sup_{1 \leq j \leq d} \mathbb{E} [\beta_{n|j}]^a < \infty \) for some \( a > 2 \), we obtain from Lemma 2(iii) of \([2]\) that,

\[
\sqrt{R_n(\beta_*)} \leq \frac{\mathbb{E}[\hat{e}^2]}{\mathbb{E}[\hat{e}^2] - (\mathbb{E}[\hat{e}])^2} \frac{\Phi^{-1}(1 - \alpha/2d)}{\sqrt{n}},
\]

with probability asymptotically larger than \( 1 - \alpha \), as \( n \to \infty \), uniformly in \( d \) such that \( d \leq 0.5\alpha n^{(a - 2 - \varepsilon)/2} \).

A proof of Theorem 7 is presented in Appendix A.4 (see supplementary material \([8]\)). A commonly adopted approach in the high dimensional regression literature (see, for example, \([4, 29, 2, 1]\) and references therein) is to start with any choice \( \lambda > \|\hat{S}\|_q \), where \( \hat{S} \) is the score function \( D_{\beta_0} \mathbb{E}_n [l(X, Y; \beta_0)] \). This choice, in the context of square-root Lasso, results in the regularization parameter to be chosen larger than the \( (1 - \alpha) \)-quantile of \( n^{-1/2} \|Z\|_\infty / \sqrt{\text{Var}_n[\hat{e}]} \) (see (10) in \([2]\)). As observed in Theorem 7 working with an upper bound of the RWP function results in choosing the \( (1 - \alpha) \)-quantile of \( n^{-1/2} \|Z\|_\infty / \sqrt{\text{Var}_n[\hat{e}]} \). Indeed, this agreement of the regularization parameter with the high dimensional linear regression literature strengthens the RWPI based approach for selecting the radius of uncertainty. Since the RWPI based approach results in a prescription of regularization parameter that is larger (by a factor \( \text{Var}_n[\hat{e}] / \sqrt{\text{Var}_n[\hat{e}]} \)), the generalization error bounds derived in the literature for high dimensional regularized regression (see, for example, \([2] \) Corollary 1) hold.
The approach in Theorem 1 is to identify an upper bound that does not depend on $\beta_*$. Instead, one could choose $\delta \geq R_n(\hat{\beta}_n)$, by plugging in any consistent estimator $\hat{\beta}_n$. We identify investigating the possibility of obtaining tighter error bounds via this plug-in approach as a subject of future research.

5. Numerical Examples

In this section, we consider two examples that compare the numerical performances of the square-root LASSO algorithm (see Example 1) when the regularization parameter $\lambda$ is selected in the following two ways: 1) as described in Section 4.2 using a suitable quantile of the RWPI limiting distribution, and 2) using cross-validation. For comparison purposes, we also list the performance of the respective ordinary least squares estimator. As such, in both the examples, cross-validation based approach iterates over multitude of choices of $\lambda$, whereas the optimal regularization via RWPI utilizes the respective square-root LASSO algorithm only once for the prescribed value of $\lambda$. This naturally suggests potentially huge savings in computation that could be valuable in large scale settings.

Example 4. Consider the linear model $Y = 3X_1 + 2X_2 + 1.5X_4 + \varepsilon$ where the vector of predictor variables $X = (X_1, \ldots, X_d)$ is distributed according to the multivariate normal distribution $\mathcal{N}(0, \Sigma)$ with $\Sigma_{k,j} = 0.5^{|k-j|}$ and additive error $\varepsilon$ is normally distributed with mean 0 and standard deviation $\sigma = 10$. Letting $n$ denote the number of training samples, we illustrate the effectiveness of the RWPI based square-root LASSO procedure for various values of $d$ and $n$ by computing the mean square loss / error (MSE) over a simulated test data set of size $N = 10000$. Specifically, we take the number of predictors to be $d = 300$ and 600, the number of standardized i.i.d. training samples to range from $n = 350, 700, 3500, 10000$, and the desired confidence level to be 95%, that is, $1 - \alpha = 0.95$. In each instance, we run the square-root LASSO algorithm using the ‘flare’ package proposed in [27] (available as a library in R) with regularization parameter $\lambda$ chosen as prescribed in Section 4.2. Repeating each experiment 100 times, we report the average training and test MSE in Tables 1 and 2, along with the respective results for ordinary least squares regression (OLS) and square-root LASSO algorithm with regularization parameter chosen as prescribed by cross-validation (denoted as SQ-LASSO CV in the tables.) We also report the average $\ell_1$ and $\ell_2$ error of the regression coefficients in Tables 1 and 2. In addition, we report the empirical coverage probability that the optimal error $E[(Y - \beta_0^T X)^2] = \sigma^2 = 100$ is smaller than the worst case expected loss computed by the DRO formulation [5]. As this empirical coverage probability reported in Table 4 is closer to the desired confidence $1 - \alpha = 0.95$, the worst case expected loss computed by [5] can be seen as a tight upper bound of the optimal loss $E[l((X, Y; \beta_*))$ (thus controlling generalization) with probability at least $1 - \alpha = 0.95$.

Example 5. Consider the diabetes data set from the ‘lars’ package in R (see [15]), where there are 64 predictors (including 10 baseline variables and other 54 possible interactions) and 1 response. After standardizing the variables, we split the entire data set of 442 observations into $n = 142$ training samples (chosen uniformly at random) and the remaining $N = 300$ samples as test data for each experiment, in order to compute training and test mean square errors using the square-root LASSO algorithm with regularization parameter picked as in Section 4.2. After repeating the experiment 100 times, we report the average training and test errors in Table 4 and compare the performance of RWPI based regularization parameter selection with other standard procedures such as OLS and square-root LASSO algorithm with regularization parameter chosen according to cross-validation.
### Table 1. Sparse linear regression for $d = 300$ predictor variables in Example [4]

The training and test mean square errors of RWPI based square-root LASSO regularization parameter selection is compared with ordinary least squares estimator (written as OLS) and cross-validation based square-root LASSO estimator (written as SQ-LASSO CV)

| Training data size, $n$ | Method        | Training Error | Test Error | $\ell_1$ loss | $\ell_2$ loss |
|------------------------|---------------|----------------|------------|---------------|---------------|
| 350                    | RWPI          | 101.16±8.11    | 122.59±6.64| 4.08±0.69     | 5.23±0.76     |
|                        | SQ-LASSO CV   | 92.23±7.91     | 117.25±6.07| 3.91±0.42     | 5.02±1.28     |
|                        | OLS           | 13.95±2.63     | 702.73±188.05| 31.59±3.64 | 436.19±50.55 |
| 700                    | RWPI          | 101.81±3.01    | 117.96±4.80| 3.31±0.40     | 4.38±0.48     |
|                        | SQ-LASSO CV   | 99.66±4.64     | 115.46±4.36| 2.96±0.37     | 3.98±0.66     |
|                        | OLS           | 56.82±3.94     | 178.44±21.74| 10.99±0.57  | 152.04±8.25  |
| 3500                   | RWPI          | 102.55±2.39    | 108.44±2.54| 2.18±0.16     | 3.28±1.66     |
|                        | SQ-LASSO CV   | 100.74±2.35    | 113.83±2.33| 2.66±0.14     | 3.91±2.18     |
|                        | OLS           | 90.37±2.17     | 114.78±5.50| 3.96±0.20     | 54.67±3.09    |
| 10000                  | RWPI          | 102.12±8.11    | 105.97±0.88| 1.13±0.08     | 1.63±0.11     |
|                        | SQ-LASSO CV   | 100.69±7.91    | 112.82±0.71| 1.15±0.07     | 1.94±0.12     |
|                        | OLS           | 95.91±11.11    | 107.74±2.96| 2.23±0.10     | 30.91±1.43    |

### Table 2. Sparse linear regression for $d = 600$ predictor variables in Example [4]

The training and test mean square errors of RWPI based square-root LASSO regularization parameter selection is compared with ordinary least squares estimator (written as OLS) and cross-validation based square-root LASSO estimator (written as SQ-LASSO CV). As $n < d$ when $n = 350$, OLS estimation is not applicable in that case (denoted by a blank)

| Training data size, $n$ | Method        | Training Error | Test Error | $\ell_1$ loss | $\ell_2$ loss |
|------------------------|---------------|----------------|------------|---------------|---------------|
| 350                    | RWPI          | 108.05±8.38    | 109.46±4.68| 4.02±0.71     | 4.08±0.70     |
|                        | SQ-LASSO CV   | 93.17±10.83    | 104.51±4.76| 2.23±0.38     | 6.89±2.35     |
|                        | OLS           | --             | --         | --            | --            |
| 700                    | RWPI          | 104.33±5.03    | 103.18±2.14| 2.91±0.42     | 2.99±0.43     |
|                        | SQ-LASSO CV   | 100.50±4.70    | 99.92±2.18 | 1.45±0.28     | 2.82±0.64     |
|                        | OLS           | 14.27±2.02     | 699.06±137.45| 31.66±2.21 | 518.02±44.87 |
| 3500                   | RWPI          | 101.52±2.52    | 96.38±0.80 | 1.23±0.24     | 1.32±0.24     |
|                        | SQ-LASSO CV   | 102.58±2.49    | 98.55±0.94 | 1.18±0.15     | 1.94±0.24     |
|                        | OLS           | 82.22±2.31     | 102.01±6.14| 6.76±0.23     | 114.05±5.73  |
| 10000                  | RWPI          | 101.36±1.11    | 94.86±0.36 | 0.75±0.13     | 0.81±0.14     |
|                        | SQ-LASSO CV   | 103.00±1.11    | 98.55±0.49 | 1.16±0.08     | 1.94±0.13     |
|                        | OLS           | 95.11±1.10     | 99.53±4.83 | 3.26±0.11     | 63.67±2.16    |

### 6. Conclusions

We showed that popular machine learning estimators such as square-root LASSO, regularized logistic regression, support vector machines, etc. can be recast as particular examples of optimal transport based DRO formulation in [5]. We introduced Robust Wasserstein Profile function...
| No. of predictors | Training sample size | $d$ |
|------------------|----------------------|-----|
|                  | 350                  | 0.974 |
|                  | 700                  | 0.977 |
|                  | 3500                 | 0.975 |
|                  | 10000                | 0.969 |
|
|                  | 600                  | 0.963 |
|                  | 0.966                |
|                  | 0.970                |
|                  | 0.968                |

Table 3. Coverage Probability of empirical worst case expected loss in Example 1

|                  | Training Error | Testing Error |
|------------------|----------------|---------------|
| RWPI             | 0.58(±0.05)    | 0.60(±0.04)   |
| SQ-LASSO CV      | 0.44(±0.06)    | 0.57(±0.03)   |
| OLS              | 0.26(±0.05)    | 1.38(±0.68)   |

Table 4. Linear Regression for Diabetes data in Example 2 with 142 training samples and 300 test samples. The training and test mean square errors of RWPI based square-root LASSO regularization parameter selection is compared with ordinary least squares estimator (written as OLS) and cross-validation based square-root LASSO estimator (written as SQ-LASSO CV).

and utilized its behaviour at the optimal parameter $\beta^*$ to present a criterion for choosing the radius, $\delta$, in the DRO formulation. We illustrated how this translates to choosing regularization parameters and coverage guarantees for optimal risk in the settings of $\ell_p$-norm regularized linear and logistic regression. We observe that the proposed prescriptions of the radius $\delta$ for the DRO formulation result in similar prescriptions that arise from independent considerations in Statistics literature. This indeed strengthens the Wasserstein Profile function based approach towards choosing the radius, $\delta$, for the DRO formulation.

Following the results presented in this paper, we investigate the behaviour of the profile function $R_m(\theta)$ in the vicinity of the optimal parameter $\theta^*$ in and establish a limiting relationship of the form, $u^{\rho/2}R_m(\theta^* + \Delta/\sqrt{n}) \Rightarrow L(\Delta)$, for a continuous $L(\cdot)$. Such a relationship can be used to accomplish the following tasks: 1) construct confidence intervals for the optimal parameter $\theta^*$, 2) establish error bounds for the solution to the DRO formulation, and 3) systematically establish the validity of plugging-in any consistent estimator for $\theta^*$ in order to obtain an asymptotically optimal prescription of the radius $\delta$. Such a plug-in approach would obviate the need to derive stochastic upper bounds, on a case-by-case basis, as is presently required in Section 4.

SUPPLEMENTARY MATERIAL

Proofs of the all the results in this article are furnished in the supplementary material available after the References section below.

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Supplementary material to the paper

Robust Wasserstein Profile Inference and Applications to Machine Learning

This supplementary material to the paper “Robust Wasserstein Profile Inference and Applications to Machine Learning” is organized as follows: Proofs of all the main results in the paper are furnished in Section A. As some of the main results in our paper utilize strong duality for problems of moments, a quick introduction to problem of moments along with a well-known strong duality result that is useful in our context is provided in Section B. A technical result on exchange of sup and inf in the DRO formulation is presented in Section C. Relevant bibliography utilized in this supplementary material is available at the end of this supplementary material.

Appendix A. Proofs of main results

This section, comprising the proofs of the main results, is organized as follows: Subsection A.1 is devoted to derive the results on distributionally robust representations presented in Section 2.4. The proofs of results on coverage properties are presented in Section A.2. Subsection A.3 contains the proofs of stochastic upper and lower bounds (and hence weak limits) presented in Section 3.3. Subsection A.4 contains the proofs of Theorems 5 and 6 as applications of the stochastic upper and lower bounds presented in Section 3.3. Some of the useful technical results that are not central to the argument are presented in Sections B and C.

A.1. Proofs of the distributionally robust representations in Section 2.4.

Here we provide proofs for results in Sections 2.3 and 2.4 that recover various norm regularized regressions as a special cases of distributionally robust regression (Propositions 1 and 2).

Proof of Proposition 2. We utilize the duality result in Proposition 1 to prove Proposition 2. For brevity, let $\tilde{X}_i = (X_i, Y_i)$ and $\tilde{\beta} = (-\beta, 1)$. Then the loss function becomes $l(X_i, Y_i; \beta) = (\tilde{\beta}^T \tilde{X}_i)^2$. We first decipher the function $\phi_\gamma(X_i, Y_i; \beta)$ defined in Proposition 1:

$$\phi_\gamma(X_i, Y_i; \beta) = \sup_{\tilde{u} \in \mathbb{R}^{d+1}} \left\{ (\tilde{\beta}^T \tilde{u})^2 - \gamma \| \tilde{X}_i - \tilde{u} \|_q^2 \right\}$$

To proceed further, we change the variable to $\Delta = \tilde{u} - \tilde{X}_i$, and apply Hölder’s inequality to see that $|\tilde{\beta}^T \Delta| \leq \|\tilde{\beta}\|_p \|\Delta\|_q$, where the equality holds for some $\Delta \in \mathbb{R}^{d+1}$. Therefore,

$$\phi_\gamma(\tilde{X}_i; \beta) = \sup_{\Delta \in \mathbb{R}^{d+1}} \left\{ (\tilde{\beta}^T \tilde{X}_i + \tilde{\beta}^T \Delta)^2 - \gamma \|\Delta\|_q^2 \right\}$$

$$= \sup_{\Delta \in \mathbb{R}^{d+1}} \left\{ (\tilde{\beta}^T \tilde{X}_i + \text{sign}(\tilde{\beta}^T \tilde{X}_i) |\tilde{\beta}^T \Delta|)^2 - \gamma \|\Delta\|_q^2 \right\}$$

$$= \sup_{\Delta \in \mathbb{R}^{d+1}} \left\{ (\tilde{\beta}^T \tilde{X}_i + \text{sign}(\tilde{\beta}^T \tilde{X}_i) \|\Delta\|_q \|\tilde{\beta}\|_p)^2 - \gamma \|\Delta\|_q^2 \right\}.$$
On expanding the squares, the above expression simplifies as below:
\[
\phi_\gamma(X_i; \beta) = (\beta^T \bar{X}_i)^2 + \sup_{\Delta \in \mathbb{R}^{d+1}} \left\{ - (\gamma - \|\beta\|_p^2) \|\Delta\|_q + 2 \|\beta^T \bar{X}_i\|_p \|\Delta\|_q \right\} 
\]
\[
= \left\{ \begin{array}{ll}
(\beta^T \bar{X}_i)^2 \gamma/(\gamma - \|\beta\|_p^2) & \text{if } \gamma > \|\beta\|_p^2, \\
+\infty & \text{if } \gamma \leq \|\beta\|_p^2.
\end{array} \right.
\] (28)

With this expression for \(\phi_\gamma(X_i, Y_i; \beta)\), we next investigate the right hand side of the duality relation in Proposition 1. As \(\phi_\gamma(x, y; \beta) = \infty\) when \(\gamma \leq \|\beta\|_p^2\), we obtain from the dual formulation in Proposition 1 that
\[
\sup_{P: D_n(P, P_n) \leq \delta} \mathbb{E}_P [l(X, Y; \beta)] = \inf_{\gamma \geq 0} \left\{ \gamma \delta + \frac{1}{n} \sum_{i=1}^n \phi_\gamma(X_i, Y_i; \beta) \right\} 
\]
\[
= \inf_{\gamma > \|\beta\|_p^2} \left\{ \gamma \delta + \frac{1}{\gamma - \|\beta\|_p^2} \frac{1}{n} \sum_{i=1}^n (\beta^T X_i)^2 \right\}. \] (29)

Now, see that \(\sum_{i=1}^n (\beta^T X_i)^2/n\) is nothing but the mean square error \(MSE_n(\beta)\). Next, as the right hand side of (29) is a convex function growing to \(\infty\) (when \(\gamma \to \infty\) or \(\gamma \to \|\beta\|_p^2\)), its global minimizer can be characterized uniquely via first order optimality condition. This, in turn, renders the right hand side of (29) as
\[
\sup_{P: D_n(P, P_n) \leq \delta} \mathbb{E}_P [l(X, Y; \beta)] = \left( \sqrt{MSE_n(\beta)} + \sqrt{\delta \|\beta\|_p^2} \right)^2.
\]
This completes the proof of Proposition 2.

Outline of a proof of Theorem 1. The proof of Theorem 1 is essentially the same as the proof of Proposition 2 except for adjusting for \(\infty\) in the definition of cost function \(N_q((x, y), (u, v))\) when \(y \neq v\) (as in the derivation leading to \(\phi_\gamma(X_i, Y_i; \beta)\) defined in (11)). First, see that
\[
\phi_\gamma(X_i, Y_i; \beta) = \sup_{x', y' \in \mathbb{R}^d} \left\{ (y'^T x'^2 - \gamma N_q((x', y'), (X_i, Y_i)) \right\}.
\]
As \(N_q((x', y'), (X_i, Y_i)) = \infty\) when \(y' \neq Y_i\), the supremum in the above expression is effectively over only \((x', y')\) such that \(y' = Y_i\). As a result, we obtain,
\[
\phi_\gamma(X_i, Y_i; \beta) = \sup_{x' \in \mathbb{R}^d} \left\{ (Y_i - \beta^T x'^2 - \gamma N_q((x', Y_i), (X_i, Y_i)) \right\}.
\]
Now, following same lines of reasoning as in the proof of Theorem 2 and the derivation leading to (28), we obtain
\[
\phi_\gamma(x, y; \beta) = \left\{ \begin{array}{ll}
\frac{\gamma}{\gamma - \|\beta\|_p^2} (Y_i - \beta^T X_i)^2 & \text{when } \lambda > \|\beta\|_p^2, \\
+\infty & \text{otherwise}.
\end{array} \right.
\]
The rest of the proof is same as in the proof of Proposition 2.
Proof of Theorem\footnote{2} As in the proof of Proposition\footnote{2} we apply the duality formulation in Proposition\footnote{1} to write the worst case expected log-exponential loss function as:

\[
\sup_{P: D_c(P, P_n) \leq \delta} \mathbb{E}_P[l(X, Y; \beta)] = \inf_{\lambda \geq 0} \left\{ \delta \lambda + \frac{1}{n} \sum_{i=1}^{n} \sup_x \left\{ \log \left( 1 + \exp(-Y_i \beta^T x) \right) - \lambda \|x - X_i\|_p \right\} \right\}.
\]

For each \((X_i, Y_i)\), following Lemma 1 in \cite{42}, we obtain

\[
\sup_x \left\{ \log \left( 1 + \exp(-Y_i \beta^T x) \right) - \lambda \|x - X_i\|_p \right\} = \begin{cases} 
\log \left( 1 + \exp(-Y_i \beta^T X_i) \right) & \text{if } \|\beta\|_q \leq \lambda, \\
+\infty & \text{if } \|\beta\|_q > \lambda.
\end{cases}
\]

Then we can write the worst case expected loss function as,

\[
\inf_{\lambda \geq 0} \left\{ \delta \lambda + \frac{1}{n} \sum_{i=1}^{n} \sup_x \left\{ \log \left( 1 + \exp(-Y_i \beta^T x) \right) - \lambda \|x - X_i\|_p \right\} \right\} = \inf_{\lambda \geq 0} \left\{ \delta \lambda + \frac{1}{n} \sum_{i=1}^{n} \left( \log \left( 1 + \exp(-Y_i \beta^T X_i) \right) 1_{\{\lambda \|\beta\|_q \leq \lambda\}} + \infty 1_{\{\lambda \|\beta\|_q > \lambda\}} \right) \right\}
\]

\[
= \inf_{\lambda \geq \|\beta\|_q} \left\{ \delta \lambda + \frac{1}{n} \sum_{i=1}^{n} \log \left( 1 + \exp(-Y_i \beta^T X_i) \right) \right\}
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \log \left( 1 + \exp(-Y_i \beta^T X_i) \right) + \delta \|\beta\|_q,
\]

which is equivalent to regularized logistic regression in the theorem statement.

For SVM with hinge loss function, let us apply the duality formulation in Proposition\footnote{1} to write the worst case expected Hinge loss function as:

\[
\sup_{P: D_c(P, P_n) \leq \delta} \mathbb{E}_P \left\{ (1 - Y \beta^T X)^+ \right\} = \inf_{\lambda \geq 0} \left\{ \delta \lambda + \frac{1}{n} \sum_{i=1}^{n} \sup_x \left\{ (1 - Y_i \beta^T x)^+ - \lambda \|x - X_i\|_p \right\} \right\}.
\]

For each \(i\), let us consider the maximization problem and for simplicity we denote \(\Delta_i = x - X_i\)

\[
\sup_{\Delta_i} \left\{ (1 - Y_i \beta^T (X_i + \Delta_i))^+ - \lambda \|\Delta_i\|_p \right\}
\]

\[
= \sup_{\Delta_i} \sup_{0 \leq \alpha \leq 1} \left\{ \alpha_i (1 - Y_i \beta^T (X_i + \Delta_i)) - \lambda \|\Delta_i\|_p \right\}
\]

\[
= \sup_{0 \leq \alpha_i \leq 1} \left\{ \alpha_i Y_i \beta^T \Delta_i - \lambda \|\Delta_i\|_p + \alpha_i (1 - Y_i \beta^T X_i) \right\}
\]

\[
= \sup_{0 \leq \alpha_i \leq 1} \left\{ \alpha_i \|\beta\|_q \|\Delta_i\|_p - \lambda \|\Delta_i\|_p + \alpha_i (1 - Y_i \beta^T X_i) \right\}
\]

\[
= \begin{cases} 
(1 - Y_i \beta^T X_i)^+ & \text{if } \|\beta\|_q \leq \lambda, \\
+\infty & \text{if } \|\beta\|_q > \lambda.
\end{cases}
\]

The first equality follows from the observation that \(x^+ = \sup_{0 \leq \alpha \leq 1} x\); second equality is because the function is concave in \(\Delta_i\), linear in \(\alpha\); as \(\alpha\) is in a compact set, we can apply minimax theorem to switch the order of maxima; third equality is due to applying Hölder inequality to the first term, and since the second term only depends on the norm of \(\Delta_i\) the equality holds for this
maximization problem. For the outer minimization, it is sufficient to restrict to \( \lambda \geq \| \beta \|_q \). As a result, we obtain

\[
\inf_{\lambda \geq \| \beta \|_q} \left\{ \delta \lambda + \frac{1}{n} \sum_{i=1}^{n} (1 - Y_i \beta^T X_i)^+ \right\} = \frac{1}{n} \sum_{i=1}^{n} (1 - Y_i \beta^T X_i)^+ + \delta \| \beta \|_q.
\]

This completes the proof. \( \square \)

A.2. Proofs of results on coverage properties.

**Proof of Proposition 6.** Let \( \hat{P} \) be a probability measure from the set,

\[ \{ P : D_e(P, P_n) \leq \delta, \ E_P[D^\beta l(X, Y; \beta)] = 0 \}, \]

which is non-empty, because \( \delta > R_n(\beta_*). \) Then,

\[
\inf_{\beta \in \mathbb{R}^d} \sup_{P: D_e(P, P_n) \leq \delta} E_P[l(X, Y; \beta)] \geq \inf_{\beta \in \mathbb{R}^d} E_{\hat{P}}[l(X, Y; \beta)] = E_{\hat{P}}[l(X, Y; \beta_*)].
\]

Moreover, since \( D_e(\cdot) \) is symmetric in its arguments, we have \( D_e(\hat{P}, P_n) \leq \delta. \) As a result,

\[
E_{P_n}[l(X, Y; \beta_*)] - \inf_{\beta} \sup_{P \in U_0(P_n)} E_P[l(X, Y; \beta)] \leq \sup_{P: D_e(P, \hat{P}) \leq \delta} E_P[l(X, Y; \beta)] - E_{\hat{P}}[l(X, Y; \beta_*)].
\]

(30)

On the other hand,

\[
\inf_{\beta} \sup_{P \in U_0(P_n)} E_P[l(X, Y; \beta)] - E_{P_n}[l(X, Y; \beta_*)] \leq \sup_{P: D_e(P, P_n) \leq \delta} E_P[l(X, Y; \beta)] - E_{P_n}[l(X, Y; \beta_*)],
\]

which can be bounded from above to result in the desired bound, \( C_1 \delta + C_2(n) \rho^{-2} \sqrt{\delta}, \) by substituting the regularized regression estimators derived in Theorem 1 (when \( \rho = 2 \)) and Theorem 2 (when \( \rho = 1 \)). Likewise, repeating the proofs of Theorems 1 and 2 for the case where the baseline distribution is set to be \( \hat{P} \) (instead of \( P_n) \), we obtain for any \( \beta \in \mathbb{R}^d \) that

\[
\sup_{P: D_e(P, \hat{P}) \leq \delta} E_P[l(X, Y; \beta)] - E_{\hat{P}}[l(X, Y; \beta)] = \delta \| \beta \|_p,
\]

for the logistic regression example in Theorem 2 and

\[
\sup_{P: D_e(P, \hat{P}) \leq \delta} E_P[l(X, Y; \beta)] - E_{\hat{P}}[l(X, Y; \beta)] = 2 \sqrt{\delta} \| \beta \|_p \sqrt{\sup_{P \in U_0(P_n)} E_P[(Y - \beta^T X)^2]} + \delta \| \beta \|_p^2
\]

\[
\leq 2 \sqrt{\delta} \| \beta \|_p \sqrt{\frac{\sup_{P \in U_0(P_n)} E_P[(Y - \beta^T X)^2]}{2}} + \delta \| \beta \|_p^2,
\]

\[
= 2 \sqrt{\delta} \| \beta \|_p \sup_{P \in U_0(P_n)} E_P[(Y - \beta^T X)^2] + 3 \delta \| \beta \|_p^2,
\]

for the linear regression example in Theorem 1. This verifies the upper bound for (30). \( \square \)

**Proof of Theorem 3.** Since \( \delta = n^{-\rho/2} \eta \) for some \( \eta \geq \eta_\alpha, \) we have from the definition of \( \eta_\alpha \), that,

\[
\lim_{n \to \infty} P(R_n(\beta_*) > \delta) = \lim_{n \to \infty} P(n^{\rho/2} R_n(\beta_*) > \eta) \leq \alpha,
\]

as \( n \to \infty. \) Then it follows from Proposition 6 that,

\[
E_{P_n}[l(X, Y; \beta_*)] - \inf_{\beta \in \mathbb{R}^d} \sup_{P \in U_0(P_n)} E_P[l(X, Y; \beta)] \leq C_1 \eta n^{-\rho/2} + C_2(n) \sqrt{\eta} 1_{(\rho=2)} n^{-\rho/4},
\]
with probability greater than or equal to $1 - \alpha$, as $n \to \infty$. Moreover, due to Chebyshev’s inequality, we obtain,

$$|\mathbb{E}_{P_n}[l(X, Y; \beta_n)] - \mathbb{E}_{P_n}[l(X, Y; \beta_*)]| \leq \frac{\sqrt{\text{Var}_{P_n}[l(X, Y; \beta_*)]}}{\alpha n},$$

and subsequently, $C_2(n)/(2(2\beta_*)_p) \leq \sqrt{\mathbb{E}_{P_n}[l(X, Y; \beta_n)]} + (\alpha^{-1}n^{-1}\text{Var}_{P_n}[l(X, Y; \beta_*)])^{1/4}$, with probability exceeding $1 - \alpha$. Since $\mathbb{E}_{P_n}[l(X, Y; \beta_*)] = \inf_{\beta} \mathbb{E}_{P_n}[l(X, Y; \beta)]$, the desired convergence in the statement of Theorem 4 follows from triangle inequality and an application of union bound to the above two inequalities. \hfill \Box

A.3. Proofs of asymptotic stochastic upper and lower bounds of RWP function in Section 3.3. We first use Proposition 3 to derive a dual formulation for $n^{\rho/2}R_n(\theta_*)$ which will be the starting point of our analysis. Due to Assumption A2), $\mathbb{E}[h(W, \theta_*)] = 0$. Combining this observation with the positive definiteness in Assumption A4), we have that 0 lies in the interior of convex hull of $\{h(u, \theta_*) : u \in \mathbb{R}^m\}$ by using a supporting hyperplane argument as in the proof of [10, Proposition 8]. Then, due to Proposition 3,

$$R_n(\theta_*) = \sup_{\lambda \in \mathbb{R}^r} \left\{ -\frac{1}{n} \sum_{i=1}^n \sup_{u \in \mathbb{R}^m} \left\{ \lambda^T h(u, \theta_*) - \|u - W_i\|_p^p \right\} \right\}.$$

In order to simplify the notation, throughout the rest of the proof we will write $h(W_i)$ instead of $h(W_i, \theta_*)$ and $D h(W_i)$ for $D_u h(W_i, \theta_*)$.

Letting $H_n = n^{-1/2} \sum_{i=1}^n h(W_i)$ and changing variables to $\Delta = u - W_i$, we obtain

$$R_n(\theta_*) = \sup_{\lambda} \left\{ -\frac{1}{n} \lambda^T H_n - \frac{1}{n} \sum_{i=1}^n \sup_{\Delta} \left\{ \lambda^T (h(W_i + \Delta) - h(W_i)) - \|\Delta\|_p^p \right\} \right\}.$$

Due to the fundamental theorem of calculus (using Assumption A3), we have that

$$h(W_i + \Delta) - h(W_i) = \int_0^1 Dh(W_i + u\Delta) \Delta du.$$

Now, redefining $\zeta = \lambda n^{(\rho - 1)/2}$ and $\Delta = \Delta/n^{1/2}$ we arrive at following representation

$$n^{\rho/2} R_n(\theta_*) = \sup_{\zeta} \left\{ -\zeta^T H_n - M_n(\zeta) \right\},$$

where

$$M_n(\zeta) = \frac{1}{n} \sum_{i=1}^n \sup_{\Delta} \left\{ \zeta^T \int_0^1 Dh \left( W_i + n^{-1/2} \Delta u \right) \Delta du - \|\Delta\|_q^q \right\}.$$  \hspace{1cm} (32)

The reformulation in (31) is our starting point of the analysis.

To proceed further, we first state a result which will allow us to apply a localization argument in the representation of $n^{\rho/2} R_n(\theta_*)$ in (31). Recall the definition of $M_n$ above in (32) and that $H_n = n^{-1/2} \sum_{i=1}^n h(W_i)$.

**Lemma 2.** Suppose that the Assumptions A2) to A4) are in force. Then, for every $\varepsilon > 0$, there exists $n_0 > 0$ and $b \in (0, \infty)$ such that

$$\mathbb{P} \left( \sup_{\|\zeta\|_p \geq b} \left\{ -\zeta^T H_n - M_n(\zeta) \right\} > 0 \right) \leq \varepsilon,$$

for all $n \geq n_0$. \hfill \Box
Proof of Lemma. Recall that $q > 1$ and $p = q/(q - 1)$. For $\zeta \neq 0$, we write $\bar{\zeta} = \zeta/\|\zeta\|_p$. Let us define the vector $V_i(\bar{\zeta}) = Dh(W_i)^T \bar{\zeta}$, and put

$$
\Delta'_i = \Delta'_i(\bar{\zeta}) = |V_i(\bar{\zeta})|^{p/q} \text{sgn} (V_i(\bar{\zeta})).
$$

(33)

Define the set $C_0 = \{w \in \mathbb{R}^m : \|w\|_p \leq c_0\}$, where $c_0$ will be chosen large enough momentarily. Then, for any $c > 0$, plugging in $\Delta = c\Delta'_i$, we have $\zeta^T Dh(W_i)\Delta = c\|\zeta^T Dh(W_i)\|_p\|\Delta'_i\|_q$, and therefore,

$$
\sup_{\Delta} \left\{ \zeta^T \int_0^1 Dh(W_i + n^{-1/2}\Delta t)\Delta du - \|\Delta\|_q^p \right\}
= \sup_{\Delta} \left\{ \zeta^T Dh(W_i)\Delta - \|\Delta\|_q^p + \zeta^T \int_0^1 \left[ Dh(W_i + n^{-1/2}\Delta u) - Dh(W_i) \right]\Delta du \right\}
\geq \max \left\{ c\|\zeta^T Dh(W_i)\|_p\|\Delta'_i\|_q - c^p\|\Delta'_i\|_q^p \right. \\
+ c\zeta^T \int_0^1 \left[ Dh(W_i + cn^{-1/2}\Delta'_i u) - Dh(W_i) \right]\Delta'_i du, 0 \right\} I(W_i \in C_0).
$$

(34)

Due to Hölder’s inequality,

$$
I(W_i \in C_0) \left| \zeta^T \int_0^1 \left[ Dh(W_i + cn^{-1/2}\Delta'_i u) - Dh(W_i) \right]\Delta'_i du \right|
\leq I(W_i \in C_0) \|\zeta\|_p \int_0^1 \left| \left[ Dh(W_i + cn^{-1/2}\Delta'_i u) - Dh(W_i) \right]\Delta'_i \right|_q du.
$$

Because of continuity $Dh(\cdot)$ and the fact that $W_i \in C_0$ (so the integrand is bounded), we have that the previous expression converges to zero as $n \to \infty$. Therefore, for given positive constants $c', c$ (note than convergence is uniform on $W_i \in C_0$), there exists $n_0$ such that for all $n \geq n_0
\quad cI(W_i \in C_0) \left| \zeta^T \int_0^1 \left[ Dh(W_i + cn^{-1/2}\Delta'_i u) - Dh(W_i) \right]\Delta'_i du \right| \leq c'\|\zeta\|_p.
$$

(35)

Next, as $\|\zeta^T Dh(W_i)\|_p^{p/q} = \|\Delta'_i\|_q$ and $1 + p/q = p,$

$$
c\|\zeta^T Dh(W_i)\|_p\|\Delta'_i\|_q - c^p\|\Delta'_i\|_q^p
= c\|\zeta\|_p\|\zeta^T Dh(W_i)\|_p^p - c^p\|\zeta^T Dh(W_i)\|_p^p.
$$

Consequently, it follows from (34) and (35) that

$$
M_n(\zeta) \geq \frac{1}{n} \sum_{i=1}^n \left\{ c\|\zeta\|_p\|\zeta^T Dh(W_i)\|_p^p - c^p\|\zeta^T Dh(W_i)\|_p^p - c'\|\zeta\|_p \right\} I(W_i \in C_0).
$$

(36)

Now, since the map $\bar{\zeta} \mapsto \|\zeta^T Dh(W_i)\|_p$ is Lipschitz continuous on $\|\zeta\|_p = 1$, we conclude that,

$$
\frac{1}{n} \sum_{i=1}^n \|\zeta^T Dh(W_i)\|_p^p I(W_i \in C_0) \to \mathbb{E} \left[ \|\zeta^T Dh(W)\|_p^p I(W \in C_0) \right],
$$

(37)

with probability one as $n \to \infty$. Moreover, due to Fatou’s lemma we have that the map $\bar{\zeta} \mapsto \mathbb{P} \left( \|\zeta^T Dh(W)\|_p > 0 \right)$ is lower semi-continuous. Therefore, by A4), we have that there exists $\delta > 0$ such that

$$
\inf_{\bar{\zeta}} \mathbb{E} \|\zeta^T Dh(W)\|_p^p > \delta.
$$

(38)
Consecutively, by selecting $c_0 > 0$ large enough, we conclude from (37) that for $n \geq N' (\delta)$,

$$\frac{1}{n} \sum_{i=1}^{n} \left\| \zeta^T D h (W_i) \right\|_p \mathbb{I} (W_i \in C_0) > \frac{\delta}{2} \tag{39}$$

Further, if we let $c_1 := \sup_{w \in C_0} \left\| \zeta^T D h (w) \right\|_p^{p/q} < \infty$, then

$$\frac{1}{n} \sum_{i=1}^{n} \left\| \zeta^T D h (W_i) \right\|_p^{\frac{p}{q}} I (W_i \in C_0) < c^2_1,$$

for all $n > N' (\delta)$. As a consequence, if $n \geq N' (\delta)$, it follows from (36) and (39) that

$$\sup_{\|\zeta\|_p > b} \left\{ - \zeta^T H_n - M_n (\zeta) \right\} \leq \sup_{\|\zeta\|_p > b} \left\{ - \zeta^T H_n - \left( \frac{e \delta \|\zeta\|_p}{2} - (cc_1)^p - cc_1 \|\zeta\|_p \right) \right\}

\leq \sup_{\|\zeta\|_p > b} \left\{ - \zeta^T H_n - \|\zeta\|_p \left( c \left( \frac{\delta}{2} - \epsilon' \right) - \frac{(cc_1)^p}{b} \right) \right\}. $$

Consequently, on the set $\|H_n\|_q \leq b'$, we obtain

$$\sup_{\|\zeta\|_p > b} \left\{ - \zeta^T H_n - M_n (\zeta) \right\} \leq \sup_{\|\zeta\|_p > b} \|\zeta\|_p \left[ b' - \left( c \left( \frac{\delta}{2} - \epsilon' \right) - \frac{(cc_1)^p}{b} \right) \right]. $$

Now, if we take $c > 4 (b' + 1) / \delta$, $\epsilon' = \delta / 4$ and $b$ to be large enough such that $b > (cc_1)^p$ then

$$b' - \left( c \left( \frac{\delta}{2} - \epsilon' \right) - \frac{(cc_1)^p}{b} \right) < 0. $$

Therefore, if $n \geq n_0$ (see (34)), then

$$\mathbb{P} \left( \max_{\|\zeta\|_p > b} \left\{ - \zeta^T H_n - M_n (\zeta) \right\} > 0 \right) \leq \mathbb{P} \left( \|H_n\|_q > b' \right) + \mathbb{P} \left( N' (\delta) > n_0 \right).$$

The result now follows immediately from the previous inequality by choosing $b'$ large enough so that $\mathbb{P} (\|H_n\|_q > b') \leq \epsilon / 2$ and later $n_0$ so that $\mathbb{P} (N' (\delta) > n_0) \leq \epsilon / 2$. The selection of $b'$ is feasible due to A2). This proves the statement of Lemma 2. \qed

**Lemma 3.** For any $b > 0$ and $c_0 \in (0, \infty)$,

$$\frac{1}{n} \sum_{i=1}^{n} \left\| \zeta^T D h (W_i) \right\|_p^{p/(p-1)} I (\|W_i\|_p \leq c_0) \to \mathbb{E} \left[ \left\| \zeta^T D h (W) \right\|_p^{p/(p-1)} I (\|W\|_p \leq c_0) \right],$$

uniformly over $\|\zeta\|_p \leq b$ in probability as $n \to \infty$.

**Proof of Lemma 3.** We first argue a suitable Lipschitz property for the map $\zeta \mapsto \left\| \zeta^T D h (W_i) \right\|_p^{p/(p-1)}$. It is elementary that for any $0 \leq a_0 < a_1$ and $\gamma > 1$

$$a_1^\gamma - a_0^\gamma = \gamma \int_{a_0}^{a_1} t^{\gamma-1} dt \leq \gamma a_1^{\gamma-1} (a_1 - a_0).$$
Applying this observation with
\[
\begin{align*}
a_1 &= \max \left( \| \zeta_1^T Dh(W_i) \|_p, \| \zeta_0^T Dh(W_i) \|_p \right), \\
a_0 &= \min \left( \| \zeta_1^T Dh(W_i) \|_p, \| \zeta_0^T Dh(W_i) \|_p \right), \\
\gamma &= \rho/(\rho - 1),
\end{align*}
\]
and using that \( \| \zeta_i^T Dh(W_i) \|_p \leq b \| Dh(W_i) \|_p \) for \( \| \zeta \|_p \leq b \), we obtain
\[
\left| \| \zeta_0^T Dh(W_i) \|_p^{\rho/(\rho-1)} - \| \zeta_1^T Dh(W_i) \|_p^{\rho/(\rho-1)} \right| \leq \frac{\rho}{\rho - 1} b^{1/(\rho-1)} \| Dh(W_i) \|_p^{\rho/(\rho-1)} \| \zeta_0 - \zeta_1 \|_p.
\]
Consequently, we have that
\[
\left| \frac{1}{n} \sum_{i=1}^{n} \| \zeta_i^T Dh(W_i) \|_p^{\rho/(\rho-1)} - \frac{1}{n} \sum_{i=1}^{n} \| \zeta_i^T Dh(W_i) \|_p^{\rho/(\rho-1)} \right| \leq \frac{\rho}{\rho - 1} \| \zeta_0 - \zeta_1 \|_p \frac{b^{1/(\rho-1)}}{n} \sum_{i=1}^{n} \| Dh(W_i) \|_p^{\rho/(\rho-1)}.
\]
Since \( Dh(\cdot) \) is continuous, \( \mathbb{E} \left[ \| Dh(W) \|_p^{\rho/(\rho-1)} I(\| W \|_p \leq c_0) \right] < \infty \), thus yielding the tightness of
\[
\frac{1}{n} \sum_{i=1}^{n} \| \zeta_i^T Dh(W_i) \|_p^{\rho/(\rho-1)} I(\| W_i \|_p \leq c_0),
\]
under the uniform topology on compact sets. The Strong Law of Large Numbers guarantees that finite dimensional distributions converge (for any choice of \( \zeta_1, \ldots, \zeta_k, k \geq 1 \), and, since the limit is deterministic, we obtain the desired convergence in probability. □

**Proof of Theorem** Let us first observe that \( R_n(\theta_*) \geq 0 \) (choosing \( \zeta = 0 \)). Then, as a consequence of Lemma there exists \( b > 0 \) such that the event
\[
\mathcal{A}_n = \left\{ \frac{n^{\rho/2} R_n(\theta_*)}{\| \zeta \|_p} = \max_{\| \zeta \|_p \leq b} \left\{ -\zeta^T H_n - M_n(\zeta) \right\} \right\},
\]
where the outer supremum is attained at some \( \| \zeta \|_p \leq b \), occurs with probability at least \( 1 - \varepsilon \), as long as \( n \geq n_0 \). In other words, \( \mathbb{P}(\mathcal{A}_n) \geq 1 - \varepsilon \) when \( n \geq n_0 \).

We first consider the case \( \rho > 1 \). For \( \zeta \neq 0 \), write \( \tilde{\zeta} = \zeta / \| \zeta \|_p \). Next, define the vector \( V_i(\tilde{\zeta}) \) via \( V_i(\tilde{\zeta}) = Dh(W_i)^T \tilde{\zeta} \) (that is, the \( j \)-th entry of \( V_i(\tilde{\zeta}) \) is the \( j \)-th entry of the vector \( Dh(W_i)^T \tilde{\zeta} \), and put
\[
\Delta_i' = \Delta_i'(\tilde{\zeta}) = \left| V_i(\tilde{\zeta}) \right|^{p/q} \text{sgn}(V_i(\tilde{\zeta})).
\]
Next, let \( \bar{\Delta}_i = c_i \Delta_i' \) with \( c_i \) chosen so that
\[
\| \bar{\Delta}_i \|_q = \left( \frac{1}{\rho} \| \zeta^T Dh(W_i) \|_p \right)^{1/(\rho-1)}.
\]
In such case we have that
\[
\max_{\Delta} \left\{ \zeta^T D_h(W_i) \Delta - \|\Delta\|_q \right\} = \max_{\|\Delta\|_q \geq 0} \left\{ \|\zeta^T D_h(W_i)\|_p \|\Delta\| - \|\Delta\|_q \right\} \\
= \zeta^T D_h(W_i) \Delta_i - \|\Delta_i\|_q
\]
\[
= \|\zeta^T D_h(W_i)\|_p^{\rho/(\rho-1)} \left( \frac{1}{\rho} \right)^{1/(\rho-1)} (1 - \frac{1}{\rho}) . \tag{42}
\]
Pick \(c_0 \in (0, \infty)\) and define \(C_0 = \{\|W_i\|_p \leq c_0\}\). Note that
\[
M_n(\zeta) \geq M_n'(\zeta, c_0),
\]
where
\[
M_n'(\zeta, c_0) = \frac{1}{n} \sum_{i=1}^{n} I(W_i \in C_0) \left\{ \zeta^T \int_0^1 D_h(W_i + n^{-1/2} \Delta_i u) \Delta_i du - \|\Delta\|_q \right\}^+. \tag{43}
\]
Define
\[
\tilde{M}_n(\zeta, c_0) = \frac{1}{n} \sum_{i=1}^{n} I(W_i \in C_0) \left\{ \zeta^T D_h(W_i) \Delta_i du - \|\Delta_i\|_q \right\}^+
\]
\[
= \frac{1}{n} \sum_{i=1}^{n} I(W_i \in C_0) \|\zeta^T D_h(W_i)\|_p^{\rho/(\rho-1)} \left( \frac{1}{\rho} \right)^{1/(\rho-1)} (1 - \frac{1}{\rho}), \tag{44}
\]
where the equality follows from (42). We then claim that
\[
\sup_{\|\zeta\|_p \leq b} \left| \tilde{M}_n(\zeta, c_0) - M_n'(\zeta, c_0) \right| \to 0.
\]
In order to verify (44), note, using the continuity of \(D_h(\cdot)\), that for any \(\varepsilon' > 0\) there exists \(n_0\) such that if \(n \geq n_0\) then (uniformly over \(\|\zeta\|_p \leq b\)),
\[
\left| \int_0^1 I(W_i \in C_0) \|\zeta^T \left[ D_h(W_i + n^{-1/2} \Delta_i u) - D_h(W_i) \right] \|_p \|\Delta_i\|_q du \right| \leq \varepsilon'.
\]
Therefore, if \(n \geq n_0\),
\[
\frac{1}{n} \sum_{i=1}^{n} I(W_i \in C_0) \left| \zeta^T \int_0^1 D_h(W_i + n^{-1/2} \Delta_i u) - D_h(W_i) \right| \|\Delta_i\|_q \|\Delta_i\|_q du \leq \varepsilon'.
\]
Since \(\varepsilon' > 0\) is arbitrary, (44) stands verified. Then, applying Lemma 3 we obtain
\[
\tilde{M}_n(\zeta, c_0) \to \mathbb{E} \left( \zeta^T D_h(W_i) \Delta_i du - \|\Delta_i\|_q^+ \right) I(W_i \in C_0),
\]
uniformly over \(\|\zeta\|_p \leq b\) as \(n \to \infty\), in probability. Therefore, applying the continuous mapping principle, we have that
\[
\max_{\|\zeta\|_p \leq b} \left\{ -\zeta^T H_n - M_n'(\zeta, c_0) \right\}
\]
\[
\Rightarrow \max_{\|\zeta\|_p \leq b} \left\{ -\zeta^T H - \kappa(\rho) \mathbb{E} \left[ \|\zeta^T D_h(W)\|_p^{\rho/(\rho-1)} \right] I \left( \|W\|_p \leq c_0 \right) \right\} , \tag{45}
\]
as \( n \to \infty \), where
\[
\kappa (\rho) = \left( \frac{1}{\rho} \right)^{1/\rho} \left( 1 - \frac{1}{\rho} \right),
\]
and \( H \sim \mathcal{N}(0, Cov[h(W; \theta_*)]) \). From (43) and the construction of (40), we can easily obtain that \( n^{p/2} R_n(\theta_*) \) is stochastically bounded (asymptotically) by
\[
\max_{\zeta} \left\{ -\zeta^T H - \kappa (\rho) \mathbb{E} \left[ \| \zeta^T D_h(W) \|_{p/(\rho-1)}^p \right] \right\},
\]
which verifies the first part of the theorem when \( \rho > 1 \).

Now, for \( \rho = 1 \), we will follow very similar steps. Again, due to Lemma 2 we concentrate on the region \( \| \zeta \|_p \leq b \) for some \( b > 0 \). For the upper bound, define \( \Delta_i' \) as in (41). Using a localization technique similar to that described in the proof of Lemma 2 in which the set \( C_0 \) as introduced we might assume that \( \| W_i \|_p \leq c_0 \) for some \( c_0 > 0 \). Then, for a given constant \( c > 0 \), setting \( \Delta_i = c \Delta_i' \), we obtain that
\[
\max_{\| \zeta \|_p \leq b} \left\{ -\zeta^T H_n - \frac{1}{n} \sum_{i=1}^n \sup_{\Delta_i} \left\{ \zeta^T \int_0^1 D_h(W_i + \Delta_i u/n^{1/2}) \Delta_i du - \| \Delta_i \|_q \right\} \right\}
\leq \max_{\| \zeta \|_p \leq b} \left\{ -\zeta^T H_n - \frac{1}{n} \sum_{i=1}^n \left( c \zeta^T \int_0^1 D_h(W_i + c \Delta_i' u/n^{1/2}) \Delta_i' du - c \| \Delta_i' \|_q \right) I(W_i \in C_0) \right\}.
\]
As in the case \( \rho > 1 \) we have that
\[
\frac{1}{n} \sum_{i=1}^n I(W_i \in C_0) \int_0^1 \zeta^T \left[ D_h(W_i + c \Delta_i' u/n^{1/2}) - D_h(W_i) \right] \Delta_i' du \to 0
\]
in probability uniformly on \( \zeta \)-compact sets. Similarly, in addition, for any \( c > 0 \) and any \( b > 0 \)
\[
\max_{\| \zeta \|_p \leq b} \left\{ -\zeta^T H_n - \frac{1}{n} \sum_{i=1}^n \left( c \zeta^T D_h(W_i) \Delta_i' du - c \| \Delta_i' \|_q \right) I(W_i \in C_0) \right\}
\]
\[
= \max_{\| \zeta \|_p \leq b} \left\{ -\zeta^T H_n - \frac{1}{n} \sum_{i=1}^n c \left( \| \zeta^T D_h(W_i) \|_p - 1 \right)^+ \| \Delta_i' \|_q I(\| W_i \|_p \leq c_0) \right\}
\]
\[
\Rightarrow \max_{\| \zeta \|_p \leq b} \left\{ -\zeta^T H - c \mathbb{E} \left[ \left( \| \zeta^T D_h(W) \|_p - 1 \right)^+ \| \zeta^T D_h(W) \|_p^{p/q} I(\| W \|_p \leq c_0) \right] \right\},
\]
because \( \| \Delta_i' \|_q = \| \zeta^T D_h(W_i) \|_p^p \). Next, as the constant \( c \) can be arbitrarily large, we obtain a stochastic upper bound of the form
\[
\max_{\| \zeta \|_p \leq b: P(\| \zeta^T D_h(W) \|_p \leq 1)} \left\{ -\zeta^T H \right\} \leq \max_{\zeta: P(\| \zeta^T D_h(W) \|_p \leq 1)} \left\{ -\zeta^T H \right\}.
\]
This completes the proof of Theorem 3.

**Proof of Proposition 4** We follow the notation introduced in the proof of Theorem 3. Recall from (31) and (32) that
\[
n^{1/2} R_n(\theta_*) = \sup_{\zeta} \left\{ \zeta^T H_n - \frac{1}{n} \sum_{k=1}^n \sup_{\Delta} \left\{ \int_0^1 \zeta^T D_h \left( W_i + \Delta u/n^{1/2} \right) \Delta du - \| \Delta \|_q \right\} \right\}.
\]
Let $A := \{\zeta : \text{esssup} \left\| \zeta^T D\theta (w) \right\|_p \leq 1\}$, where the essential supremum is taken with respect to the Lebesgue measure. Then, due to Hölder’s inequality, if $\zeta \in A$,

$$
\sup_{\Delta} \left\{ \int_0^1 \zeta^T D\theta \left( W_i + \Delta u/n^{1/2} \right) \Delta du - \left\| \Delta \right\|_q \right\}
\leq \sup_{\Delta} \left\{ \int_0^1 \left\| \zeta^T D\theta \left( W_i + \Delta u/n^{1/2} \right) \right\|_p \left\| \Delta \right\|_q du - \left\| \Delta \right\|_q \right\}
\leq \sup_{\Delta} \left\| \Delta \right\|_q \left\{ \int_0^1 \left( \left\| \zeta^T D\theta \left( W_i + \Delta u/n^{1/2} \right) \right\|_p - 1 \right) du \right\} \leq 0.
$$

Consequently,

$$
n^{1/2} R_n (\theta_*) \geq \sup_{\zeta \in A} \zeta^T H_n.
$$

Letting $n \to \infty$ we conclude that

$$
\sup_{\zeta \in A} \zeta^T H_n \Rightarrow \sup_{\zeta \in A} \zeta^T H.
$$

Because $W_i$ is assumed to have a density with respect to the Lebesgue measure it follows that $P \left( \left\| \zeta^T D\theta \left( W_i \right) \right\|_p \leq 1 \right) = 1$ if and only if $\zeta \in A$ and the result follows. \(\Box\)

Finally, we provide the proof of Proposition 5.

**Proof of Proposition 5** Recall from (31) and (32) that

$$
n^{1/2} R_n (\theta_*) = \sup_{\zeta} \left\{ \zeta^T H_n - \frac{1}{n} \sum_{k=1}^n \sup_{\Delta} \left\{ \int_0^1 \zeta^T D\theta \left( W_i + \Delta u/n^{1/2} \right) \Delta du - \| \Delta \|_q \right\} \right\}. \quad (46)
$$

As in the proof of Theorem 3 due to Lemma 2 we might assume that $\| \zeta \|_p \leq b$ for some $b > 0$.

The strategy will be to split the inner supremum in values of $\| \Delta \|_q \leq \delta n^{1/2}$ and values $\| \Delta \|_q > \delta n^{1/2}$ for a suitably small positive constant $\delta$. In Step 1, we shall show that the supremum is achieved with high probability in the former region. Then, in Step 2, we analyze the region in which $\| \Delta \|_q \leq \delta n^{1/2}$ and argue that the integrals inside the summation in (46) can be replaced by $\zeta^T D\theta (W_i) \Delta$. Once this substitution is performed we can solve the inner maximization problem explicitly in Step 3 and, finally, we will apply a weak convergence result on $\zeta$-compact sets to conclude the result. We now proceed to execute this strategy.

**Execution of Step 1:** Pick $\delta > 0$ small, to be chosen in the sequel, then note that A5) implies (by redefining $\kappa$ if needed, due to the continuity of $D\theta (\cdot)$) that

$$
\| D\theta (w) \|_p \leq \kappa \left( 1 + \| w \|_q^{\rho - 1} \right).
$$

Therefore, for $\zeta$ such that $\| \zeta \|_p \leq b$,

$$
\sup_{\| \Delta \|_q \leq \delta n^{1/2}} \left\{ \int_0^1 \left| \zeta^T D\theta \left( W_i + \Delta u/n^{1/2} \right) \Delta du - \left\| \Delta \right\|_q \right\}
\leq \sup_{\| \Delta \|_q \geq \delta n^{1/2}} \left\{ b \kappa \left( 1 + \int_0^1 \| W_i + \Delta u/n^{1/2} \|_q^{\rho - 1} \| du \right) \left\| \Delta \right\|_q - \left\| \Delta \right\|_q \right\}.
$$
Note that if \( \rho \in (1, 2) \), then \( 0 < \rho - 1 < 1 \), and therefore by the triangle inequality and concavity
\[
\left\| W_i + \Delta u/n^{1/2} \right\|^\rho_q \leq \left( \left\| W_i \right\| + \left\| \Delta/n^{1/2} \right\| \right)^{\rho-1} \leq \left\| W_i \right\|^{\rho-1} + \left\| \Delta/n^{1/2} \right\|^{\rho-1}.
\]
On the other hand, if \( \rho \geq 2 \), then \( \rho - 1 \geq 1 \) and the triangle inequality combined with Jensen’s inequality applied as follows:
\[
\|a + c\|^\rho - 1 \leq 2^{\rho - 1} \left( \frac{1}{2} \|a\|^\rho - 1 + \frac{1}{2} \|c\|^\rho - 1 \right) = 2^{\rho - 2} \left( \|a\|^\rho - 1 + \|c\|^\rho - 1 \right),
\]
yields
\[
\left\| W_i + \Delta u/n^{1/2} \right\|^\rho_q \leq 2^{\rho - 2} \left( \| W_i \|^\rho - 1 + \left\| \Delta/n^{1/2} \right\|^\rho - 1 \right).
\]
So, in both cases we can write
\[
\sup_{\|\Delta\|_q \geq \delta n^{1/2}} \left\{ \int_0^1 \zeta^T D\theta(W_i + \Delta u/n^{1/2}) \Delta \right\} \left[ du - \|\Delta\|^\rho_q \right] \\
\leq \sup_{\|\Delta\|_q \geq \delta n^{1/2}} \left\{ b\kappa \left( 1 + 2^{\rho - 1} \left( \| W_i \|^\rho - 1 + \left\| \Delta/n^{1/2} \right\|^\rho - 1 \right) \right) \right\} \|\Delta\|_q - \|\Delta\|^\rho_q \}
\leq \sup_{\|\Delta\|_q \geq \delta n^{1/2}} \left\{ b\kappa \left( \|\Delta\|_q + 2^{\rho - 1} \| W_i \|^\rho - 1 \|\Delta\|_q + 2^{\rho - 1} \left\| \Delta/n^{(\rho - 1)/2} \right\| - \|\Delta\|^\rho_q \right) \right\}.
\]
Next, as \( \mathbb{E}\|W_n\|^\rho < \infty \), we have that for any \( \varepsilon' > 0 \),
\[
\mathbb{P} \left( \|W_n\|^\rho_q \geq \varepsilon' n \text{ i.o.} \right) = 0,
\]
therefore we might assume that there exists \( n_0 \) such that for all \( i \leq n \) and \( n \geq n_0 \), \( \| W_i \|^\rho_q - 1 \leq \left( \varepsilon' n \right)^{(\rho - 1)/\rho} \). Therefore, if \( \left( \varepsilon' \right)^{(\rho - 1)/\rho} \leq \delta^{\rho - 1} / \left( b\kappa 2^\rho \right) \), we conclude that if \( \|\Delta\|_q \geq \delta n^{1/2} \) and \( n > n_0 \),
\[
b\kappa 2^{\rho - 1} \| W_i \|^\rho - 1 \|\Delta\|_q \leq b\kappa 2^{\rho - 1} \left( \varepsilon' n \right)^{(\rho - 1)/\rho} \|\Delta\|_q \leq \frac{1}{2} \delta^{\rho - 1} n^{(\rho - 1)/\rho} \|\Delta\|_q \leq \frac{1}{2} \|\Delta\|^\rho_q .
\]
Similarly, choosing \( n \) sufficiently large we can guarantee that
\[
b\kappa \left( \|\Delta\|_q + 2^{\rho - 1} \left\| \Delta/n^{(\rho - 1)/\rho} \right\| \right) \leq \frac{1}{2} \|\Delta\|^\rho_q .
\]
Therefore, we conclude that for any fixed \( \delta > 0 \),
\[
\sup_{\|\Delta\|_q \geq \delta \sqrt{n}} \left\{ \int_0^1 \zeta^T D\theta(W_i + \Delta u/n^{1/2}) \Delta \right\} \left[ du - \|\Delta\|^\rho_q \right] \leq 0 \tag{47}
\]
provided \( n \) is large enough, thus achieving the desired result over the region \( \|\Delta\|_q \geq \delta \sqrt{n} \).
Execution of Step 2: Next, we let $\varepsilon'' > 0$, and note that

$$\sup_{\|\Delta\|_q \leq \delta \sqrt{n}} \left\{ \int_0^1 \zeta^T D_h(W_i + \Delta u/n^{1/2}) \Delta du - \|\Delta\|_q^{\rho} \right\}$$

$$\leq \sup_{\|\Delta\|_q \leq \delta \sqrt{n}} \left\{ \int_0^1 \zeta^T \left[ D_h(W_i + \Delta u/n^{1/2}) - D_h(W_i) \right] \Delta du - \varepsilon'' \|\Delta\|_q^{\rho} \right\}$$

$$+ \sup_{\|\Delta\|_q \leq \delta \sqrt{n}} \left\{ \zeta^T D_h(W_i) \Delta - (1 - \varepsilon'') \|\Delta\|_q^{\rho} \right\}.$$  

We now argue locally, using A6), a bound for the first term in the right hand side of (48):

$$\sup_{\|\Delta\|_q \leq \delta \sqrt{n}} \left\{ \int_0^1 \zeta^T \left[ D_h(W_i + \Delta u/n^{1/2}) - D_h(W_i) \right] \Delta du - \varepsilon'' \|\Delta\|_q^{\rho} \right\}$$

$$\leq \sup_{\|\Delta\|_q \leq \delta \sqrt{n}} \left\{ \|\zeta\|_{p,0} \bar{\kappa}(W_i) \|\Delta\|_q^{2} n^{1/2} - \varepsilon'' \|\Delta\|_q^{\rho} \right\}$$

$$\leq \sup_{\|\Delta\|_q \leq 1} \left\{ \bar{\kappa}(W_i) \|\Delta\|_q^{2} n^{1/2} - \varepsilon'' \|\Delta\|_q^{\rho} \left( \delta n^{1/2} \right)^{\rho} \right\}.$$  

As $\sup_{x \in [0,1]} \{ a_n x^2 - b_n x^p \} \leq (\rho - 2)^+ (a_n^{\rho} / b_n^{2 \rho})^{1/(\rho - 2)} / \rho$ when $b_n > a_n$, we have, for all $n$ sufficiently large, that

$$\sup_{\|\Delta\|_q \leq \delta \sqrt{n}} \left\{ \int_0^1 \zeta^T \left[ D_h(W_i + \Delta u/n^{1/2}) - D_h(W_i) \right] \Delta du - \varepsilon'' \|\Delta\|_q^{\rho} \right\} \leq \frac{(\rho - 2)^+}{\rho} \left( \frac{b \bar{\kappa}(W_i)}{\varepsilon'' \sqrt{n}} \right)^{\rho/(\rho - 2)}.$$  

Since $E[\bar{\kappa}(W_i)^2] < \infty$ (from Assumption A6)), we have that $P(\bar{\kappa}(W_i) > \varepsilon'' \sqrt{i} \text{ i.o.}) = 0$ for any $\varepsilon'' > 0$. Consecutively, $\bar{\kappa}(W_i) < \varepsilon'' \sqrt{i}$ for all $i$ large enough, and therefore,

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^{n} \sup_{\|\Delta\|_q \leq \delta \sqrt{n}} \left\{ \int_0^1 \zeta^T \left[ D_h \left( W_i + \Delta u/n^{1/2} \right) - D_h \left( W_i \right) \right] \Delta du - \varepsilon'' \|\Delta\|_q^{\rho} \right\}$$

$$\leq \frac{(\rho - 2)^+}{\rho} \lim_{n \rightarrow \infty} \left( \frac{b}{\varepsilon''} \right)^{\rho/(\rho - 2)} \frac{1}{n} \sum_{i=1}^{n} \left( \bar{\kappa}(W_i) \right)^{\rho/(\rho - 2)}$$

$$\leq \frac{(\rho - 2)^+}{\rho} \left( \frac{b \varepsilon''}{\varepsilon''} \right)^{\rho/(\rho - 2)},$$  

which can be made arbitrarily small by choosing $\varepsilon''$ arbitrarily small. Therefore, for any fixed $\varepsilon'', \delta > 0,$

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^{n} \sup_{\|\Delta\|_q \leq \delta \sqrt{n}} \left\{ \int_0^1 \zeta^T \left[ D_h \left( W_i + \Delta u/n^{1/2} \right) - D_h \left( W_i \right) \right] \Delta du - \varepsilon'' \|\Delta\|_q^{\rho} \right\} = 0. \quad (50)$$
Execution of Step 3: Next, it follows from [47], [48] and [50] that for any fixed \( \varepsilon'' \), \( \delta > 0 \), there exists \( N_0 \) such that if \( n \geq N_0 \),
\[
\frac{1}{n} \sum_{i=1}^{n} \sup_{\Delta} \left\{ \int_0^1 \zeta^T Dh \left( W_i + \Delta u/n^{1/2} \right) \Delta du - \|\Delta\|_q^p \right\} \\
\leq \frac{1}{n} \sum_{i=1}^{n} \sup_{\Delta \leq \delta \sqrt{n}} \left\{ \zeta^T Dh(W_i) \Delta du - (1 - \varepsilon'') \|\Delta\|_q^p \right\} + \delta \\
\leq \frac{1}{n} \sum_{i=1}^{n} \min \left\{ \kappa(\rho, \varepsilon'') \|\zeta^T Dh(W_i)\|_{\rho/(\rho-1)}, c_n \right\} + \delta,
\]
where
\[
\kappa(\rho, \varepsilon'') = \left( \frac{1}{\rho(1-\varepsilon'')} \right)^{1/(\rho-1)} \left( 1 - \frac{1}{\rho} \right),
\]
and \( c_n \to \infty \) as \( n \to \infty \) (the exact value of \( c_n \) is not important).

Next, note that A5) implies that
\[
\|Dh(W_i)\|_{\rho/(\rho-1)} I (\|W_i\| \geq 1) \leq \kappa I (\|W_i\| \geq 1) \|W_i\|_q^p \leq \kappa \|W_i\|_q^p
\]
and, therefore, since \( Dh(\cdot) \) is continuous (therefore locally bounded) and \( \mathbb{E} \|W_i\|_q^p < \infty \) also by A5), we have that
\[
\mathbb{E} \|Dh(W)\|_{\rho/(\rho-1)} < \infty.
\]
Then, an argument similar to Lemma 3 shows that
\[
\sup_{\|\zeta\|_{\rho} \leq b} \left\{ \zeta^T H_n - \frac{1}{n} \sum_{i=1}^{n} \left\{ \kappa(\rho, \varepsilon'') \|\zeta^T Dh(W_i)\|_{\rho/(\rho-1)}, c_n \right\} \right\} \\
\Rightarrow \sup_{\|\zeta\|_{\rho} \leq b} \left\{ \frac{1}{n} \sum_{i=1}^{n} \kappa(\rho, \varepsilon'') \mathbb{E} \|\zeta^T Dh(W_i)\|_{\rho/(\rho-1)} \right\},
\]
as \( n \to \infty \) (where \( \Rightarrow \) denotes weak convergence). Finally, we can send \( \varepsilon'', \delta \to 0 \) and \( b \to \infty \) to obtain the desired asymptotic stochastic lower bound.

A4. Proofs of RWP function limit theorems for linear and logistic regression examples. We first obtain the dual formulation of the respective RWP functions for linear and logistic regressions using Proposition 3. Let \( \mathbb{E}[h(x; y; \beta)] = 0 \) be the estimating equation under consideration \( h(x; y; \beta) = (y - \beta^T x) x \) for linear regression and \( h(x; y; \beta) \) as in (27) for logistic regression. Recall that the cost function is \( c(\cdot) = N_q(\cdot) \). Due to the duality result in Proposition 3 we obtain
\[
R_n(\beta_*) = \inf \left\{ D_\epsilon(P, P_n) : \mathbb{E}_P[h(X, Y; \beta_*)] = 0 \right\} \\
= \sup_{\lambda} \left\{ -\frac{1}{n} \sum_{i=1}^{n} \sup_{(x', y')} \left\{ \lambda^T h(x', y'; \beta_*) - N_q((x', y'), (X_i, Y_i)) \right\} \right\}.
\]
As \( N_q((x', y'), (X_i, Y_i)) = \infty \) when \( y' \neq Y_i \), the above expression simplifies to,
\[
R_n(\beta_*) = \sup_{\lambda} \left\{ -\frac{1}{n} \sum_{i=1}^{n} \sup_{x'} \left\{ \lambda^T h(x', Y_i; \beta_*) - \|x' - X_i\|_q^p \right\} \right\},
\]
where \( \rho = 2 \) for the case of linear regression (Theorem 3) and \( \rho = 1 \) for the case of logistic regression (Theorem 4). As RWP function here is similar to the RWP function for general
Lemma 5. If $H$ where

Assumptions:

A2') Suppose that $\beta* \in \mathbb{R}^d$ satisfies $\mathbb{E}[h(X,Y;\beta*)] = 0$ and $\mathbb{E}[\|h(X,Y;\beta*)\|^2_2] < \infty$ (While we do not assume that $\beta*$ is unique, the results are stated for a fixed $\beta*$ satisfying $\mathbb{E}[h(X,Y;\beta*)] = 0$.)

A4') Suppose that for each $\xi \neq 0$, the partial derivative $D_x h(x,y;\beta*)$ satisfies,

$$P\left(\|\xi^T D_x h(X,Y;\beta*)\|_p > 0\right) > 0.$$

A6') Assume that there exists $\tilde{\kappa}: \mathbb{R}^m \to \infty$ such that

$$\|D_x h(x + \Delta, y; \beta*) - D_x h(x, y; \beta*)\|_p \leq \tilde{\kappa}(x, y)\|\Delta\|_q,$$

for all $\Delta \in \mathbb{R}^d$, and $\mathbb{E}[\tilde{\kappa}(X,Y)^2] < \infty$.

Lemma 4. If $\rho \geq 2$, under Assumptions A2', A4' and A6'), we have,

$$nR_n(\beta*; \rho) \Rightarrow \bar{R}(\rho),$$

where

$$\bar{R}(\rho) = \sup_{\xi \in \mathbb{R}^d} \left\{ \rho \xi^T H - (\rho - 1)\mathbb{E}\|\xi^T D_x h(X,Y;\beta*)\|_p^{\rho/(\rho - 1)} \right\},$$

with $H \sim \mathcal{N}(0, \text{Cov}[h(X,Y;\beta*)])$ and $1/p + 1/q = 1$.

Lemma 5. If $\rho = 1$, in addition to assuming A2', A4'), suppose that $D_x h(\cdot, y; \beta*)$ is continuous for every $y$ in the support of probability distribution of $Y$. Also suppose that $X$ has a positive probability density (almost everywhere) with respect to the Lebesgue measure. Then,

$$nR_n(\beta*; 1) \Rightarrow \bar{R}(1),$$

where

$$\bar{R}(1) = \sup_{\xi \in \mathbb{P}(\|\xi^T D_x h(X,Y;\beta*)\|_p > 1)} \left\{ \xi^T H \right\},$$

with $H \sim \mathcal{N}(0, \text{Cov}[h(X,Y;\beta*)])$.

The proof of Lemma 4 and 5 follows closely the proof of our results in Section 3 and therefore it is omitted. We prove Theorem 5 and 6 as a quick application of these lemmas.

Proof of Theorem 5. To show that the RWP function dual formulation in (51) converges in distribution, we verify the assumptions of Lemma 4 with $h(x,y;\beta) = (y - \beta^T x)x$. Under the null hypothesis $H_0$, $Y - \beta_x^T X = e$ is independent of $X$, has zero mean and finite variance $\sigma^2$. Therefore,

$$\mathbb{E}[h(X,Y;\beta)] = \mathbb{E}[eX] = 0,$$

and

$$\mathbb{E}[\|h(X,Y;\beta)\|^2_2] = \mathbb{E}[e^2 X^T X] = \sigma^2 \mathbb{E}\|X\|_2^2,$$

which is finite, because trace of the covariance matrix $\Sigma$ is finite. This verifies Assumption A2'.

Further,

$$D_x h(X,Y;\beta*) = (y - \beta_x^T X)I_d - X\beta_x^T = eI_d - X\beta_x^T,$$

where $I_d$ is the $d \times d$ identity matrix. For any $\xi \neq 0$,

$$P\left(\|\xi^T D_x h(X,Y;\beta*)\|_p = 0\right) = P(e\xi = (\xi^T X)\beta) = 0,$$
thus satisfying Assumption A4') trivially. In addition,
\[ \|D_x h(x + \Delta, y; \beta_*) - D_x h(x, y; \beta_*)\|_p = \|\beta_*^T \Delta I_d - \Delta \beta_*^T\|_p \leq c \|\Delta\|_q, \]
for some positive constant \(c\). This verifies Assumption A6'). As all the assumptions imposed in Lemma 4 are easily satisfied, using \(\rho = 2\), we obtain the following convergence in distribution as a consequence of Lemma 4:

\[ R_n(\beta_*) \Rightarrow \sup_{\xi \in \mathbb{R}^d} \left\{ 2\xi^T H - E \|e\xi - (\xi^T X)\beta_*\|_p^2 \right\}, \]

as \(n \to \infty\). Here, \(H \sim \mathcal{N}(0, \text{Cov}[h(X, Y; \beta_*)])\). As \(\text{Cov}[h(X, Y; \beta_*)] = E [e^2 X X^T] = \sigma^2 \Sigma\), if we let \(Z = H/\sigma\), by solving the inner optimization problem in Lemma 4 are easily satisfied, using \(\rho = 2\), we obtain the following limit law,

\[ L_1 = \sup_{\xi \in \mathbb{R}^d} \left\{ 2\sigma \xi^T Z - E \|e\xi - (\xi^T X)\beta_*\|_p^2 \right\}, \]

where \(Z \sim \mathcal{N}(0, \Sigma)\), as in the statement of the theorem.

**Proof of the stochastic upper bound in Theorem 5.** For the stochastic upper bound, let us consider the asymptotic distribution \(L_1\) and rewrite the maximization problem as,

\[ L_1 = \sup_{\|\xi\|_p = 1} \inf_{\alpha \geq 0} \left\{ 2\sigma \alpha \xi^T Z - \alpha^2 E \|e\xi - (\xi^T X)\beta_*\|_p^2 \right\} \]

\[ \leq \sup_{\|\xi\|_p = 1} \inf_{\alpha \geq 0} \left\{ 2\sigma \alpha \|Z\|_q - \alpha^2 E \|e\xi - (\xi^T X)\beta_*\|_p^2 \right\}, \]

because of H"{o}lder's inequality. By solving the inner optimization problem in \(\alpha\), we obtain

\[ L_1 \leq \sup_{\|\xi\|_p = 1} \frac{\sigma^2 \|Z\|_q^2}{E \|e\xi - (\xi^T X)\beta_*\|_p^2} = \frac{\sigma^2 \|Z\|_q^2}{\inf_{\|\xi\|_p = 1} E \|e\xi - (\xi^T X)\beta_*\|_p^2}. \]

Next, consider the minimization problem in the denominator: Due to triangle inequality,

\[ \inf_{\|\xi\|_p = 1} E \|e\xi - (\xi^T X)\beta_*\|_p^2 \geq \inf_{\|\xi\|_p = 1} \left\{ E |e| \|\xi\|_p - \|\xi^T X\| \|\beta_*\|_p \right\}^2 \]

\[ = E |e|^2 + \inf_{\|\xi\|_p = 1} \left\{ \|\beta_*\|_p^2 \left( E |\xi^T X| \right)^2 - 2 \|\beta_*\|_p E |e| E |\xi^T X| \right\} \]

\[ \geq E |e|^2 + \inf_{\|\xi\|_p = 1} \left\{ \|\beta_*\|_p^2 \left( E |\xi^T X| \right)^2 - 2 \|\beta_*\|_p E |e| E |\xi^T X| \right\} \]

\[ = E |e|^2 - (E |e|)^2 + \inf_{\|\xi\|_p = 1} \left\{ \|\beta_*\|_p E |\xi^T X| - E |e| \right\}^2 \]

\[ \geq E |e|^2 - (E |e|)^2 = \text{Var} \left[ |e| \right]. \]

Combining the above inequality with (52), we obtain,

\[ \sup_{\xi \in \mathbb{R}^d} \left\{ \sigma^2 \xi^T Z - E \|e\xi - (\xi^T X)\beta_*\|_p^2 \right\} \leq \frac{\sigma^2 \|Z\|_q^2}{\text{Var} |e|}. \]

Consequently,

\[ nR_n(\beta_*) D \rightarrow L_1 := \max_{\xi \in \mathbb{R}^d} \left\{ \sigma \xi^T Z - E \|e\xi - (\xi^T X)\beta_*\|_p^2 \right\} \leq \frac{E |e|^2}{E |e|^2 - (E |e|)^2} \|Z\|_q^2. \]
If random error $e$ is normally distributed, then
\[ nR_n(\beta_s) \lesssim_D \frac{\pi}{\sqrt{2}} \|Z\|_q^2, \]
thus establishing the desired upper bound.

**Proof of Theorem 2.** Under null hypothesis $H_0$, the training samples $(X_1, Y_1), \ldots, (X_n, Y_n)$ are produced from the logistic regression model with parameter $\beta_s$. As $\beta_s$ minimizes the expected log-exponential loss $l(x, y; \beta)$, the corresponding optimality condition is $\mathbb{E}[h(X, Y; \beta_s)] = 0$, where
\[ h(x, y; \beta_s) = \frac{-yx}{1 + \exp(y \beta_s x)}. \]
As $\mathbb{E}\|h(X, Y; \beta_s)\|^2 \leq \mathbb{E}\|X\|^2$ is finite, Assumption A2$'$ is satisfied. Let $I_d$ denote $d \times d$ identity matrix. While
\[ D_xh(x, y; \beta_s) = \frac{-yI_d}{1 + \exp(y \beta_s^T x)} + \frac{x \beta_s^T}{(1 + \exp(y \beta_s^T x))(1 + \exp(-y \beta_s^T x))} \]
is continuous (as a function of $x$) for every $y$, it is also true that
\[ \mathbb{P} \left( \left\| \xi^T D_x h(X, Y; \beta_s) \right\|_p = 0 \right) = \mathbb{P} \left( Y (1 + \exp(-Y \beta_s^T X)) \xi = (\xi^T X) \beta = 0 \right), \]
for any $\xi \neq 0$, thus satisfying Assumption A4$'$. As all the conditions required for the convergence in distribution in Lemma 5 are satisfied, we obtain,
\[ \sqrt{n}R_n(\beta_s) \Rightarrow \sup_{\xi \in A} \xi^T Z, \]
where $Z \sim \mathcal{N}(0, \mathbb{E}[X X^T/(1 + \exp(Y \beta_s^T X))^2])$ as a consequence of Lemma 5. Here, the set $A = \{ \xi \in \mathbb{R}^d : \text{ess sup} \|\xi^T D_x h(X, Y; \beta_s)\|_p \leq 1 \}$.

**Proof of the stochastic upper bound in Theorem 2.** First, we claim that $A$ is a subset of the norm ball $\{ \xi \in \mathbb{R}^d : \|\xi\|_p \leq 1 \}$. To establish this, we observe that,
\[ \|\xi^T D_x h(X, Y; \beta_s)\|_p \geq \left\| \frac{-y \xi}{1 + \exp(Y \beta_s^T X)} \right\|_p - \left\| \frac{(\xi^T X) \beta_s}{(1 + \exp(Y \beta_s^T X))(1 + \exp(-Y \beta_s^T X))} \right\|_p \]
\[ \geq \left( \frac{1}{1 + \exp(Y \beta_s^T X)} - \frac{\|X\|_q \|\beta_s\|_p}{(1 + \exp(Y \beta_s^T X))(1 + \exp(-Y \beta_s^T X))} \right) \|\xi\|_p, \tag{53} \]
because $Y \in \{+1, -1\}$, and due to H"older's inequality $|\xi^T X| \leq \|\xi\|_p \|X\|_q$. If $\xi \in \mathbb{R}^d$ is such that $\|\xi\|_p = (1 - \epsilon)^{-2} > 1$ for a given $\epsilon > 0$, then following (53), $\|\xi^T D_x h(X, Y)\|_p > 1$, whenever
\[ (X, Y) \in \Omega_\epsilon := \left\{ (x, y) : \frac{\|x\|_q \|\beta_s\|_p}{1 + \exp(-y \beta_s^T x)} \leq \frac{\epsilon}{2}, \frac{1}{1 + \exp(y \beta_s^T x)} \geq 1 - \frac{\epsilon}{2} \right\}. \]
Since $X$ has positive density almost everywhere, the set $\Omega_\epsilon$ has positive probability for every $\epsilon > 0$. Thus, if $\|\xi\|_p > 1$, $\|\xi^T D_x h(X, Y; \beta_s)\|_p > 1$ with positive probability. Therefore, $A$ is a subset of $\{ \xi : \|\xi\|_p \leq 1 \}$. Consequently,
\[ L_3 := \sup_{\xi \in A} \xi^T Z \lesssim_D \sup_{\xi : \|\xi\|_p \leq 1} \xi^T Z = \|Z\|_q. \]
If we let \( \tilde{Z} \sim \mathcal{N}(0, \text{E}[XX^T]) \), then \( \text{Cov}[\tilde{Z}] - \text{Cov}[Z] \) is positive definite. As a result, \( L_3 \) is stochastically dominated by \( L_4 := \|Z\|_q \), thus verifying the desired stochastic upper bound in the statement of Theorem 6.

**Proof of Theorem 7.** Instead of characterizing the exact weak limit, we will find a stochastic upper bound for \( R_n(\beta_*) \). The RWP function, as in the proof of Theorem 5, admits the following dual representation (see (51)):

\[
R_n(\beta_*) = \sup_\lambda \left\{ -\frac{1}{n} \sum_{i=1}^n \sup_{x'} \left\{ \lambda^T (Y_i - \beta_0^T x') x' - \|x' - X_i\|_\infty^2 \right\} \right\}
\]

\[
= \sup_\lambda \left\{ -\lambda^T \frac{Z_n}{\sqrt{n}} - \frac{1}{n} \sum_{i=1}^n \sup_{\Delta} \left\{ e_i \lambda^T \Delta - (\beta_*^T \Delta)(\lambda^T X_i) - \left( \|\Delta\|_\infty^2 + (\beta_*^T \Delta)(\lambda^T \Delta) \right) \right\} \right\},
\]

where \( Z_n = n^{-1/2} \sum_{i=1}^n e_i X_i \), \( e_i = Y_i - \beta_*^T X_i \). In addition, we have changed the variable from \( x' - X_i = \Delta \). If we let \( \zeta = \sqrt{n} \lambda \), then

\[
nR_n(\beta_*) = \sup_\zeta \left\{ -\zeta^T Z_n - \frac{1}{n \sqrt{n}} \sum_{i=1}^n \sup_{\Delta} \left\{ e_i \zeta^T \Delta - (\beta_*^T \Delta)(\zeta^T X_i) - \left( \sqrt{n}\|\Delta\|_\infty^2 + (\beta_*^T \Delta)(\zeta^T \Delta) \right) \right\} \right\}
\]

\[
\leq \sup_\zeta \left\{ -\zeta^T Z_n - \frac{1}{n \sqrt{n}} \sum_{i=1}^n \sup_{\|\Delta\|_\infty} \left\{ \|e_i \zeta^T - \zeta^T X_i \beta_*^T \|_1 \|\Delta\|_\infty - \sqrt{n} \left( 1 + \frac{\|\beta_*\| \|\zeta\|_1}{\sqrt{n}} \right) \|\Delta\|_\infty^2 \right\} \right\},
\]

where we have used Hölder’s inequality thrice to obtain the upper bound. If we solve the inner supremum over the variable \( \|\Delta\|_\infty \), we obtain,

\[
nR_n(\beta_*) \leq \sup_\zeta \left\{ -\zeta^T Z_n - \frac{1}{n \sqrt{n}} \sum_{i=1}^n \frac{\|e_i \zeta - \zeta^T X_i \beta_*\|_1^2}{4} \right\}
\]

\[
\leq \sup_{a \geq 0} \sup_{\zeta: \|\zeta\|_1 = 1} \left\{ -a \zeta^T Z_n - \frac{a^2}{4(1 + a \|\beta_*\|_1 n^{-1/2})} n \sum_{i=1}^n \|e_i \zeta - \zeta^T X_i \beta_*\|_1^2 \right\},
\]

where we have split the optimization into two parts: one over the magnitude (denoted by \( a \)), and another over all unit vectors \( \zeta \). Further, due to Hölder’s inequality, we have \( |\zeta^T Z_n| \leq \|Z_n\|_\infty \) as \( \|\zeta\|_1 = 1 \). Therefore, letting \( c_1(n) = \|Z_n\|_\infty \), \( c_2(n) = \inf_{\zeta: \|\zeta\|_1 = 1} \frac{1}{n} \sum_{i=1}^n \|e_i \zeta - \zeta^T X_i \beta_*\|_1^2 \) and \( c_3(n) = 1 + a \|\beta_*\|_1^2 n^{-1/2} \), observe that

\[
nR_n(\beta_*) \leq \sup_{a \geq 0} \left\{ c_1(n) a - \frac{c_2(n)}{4 c_3(n)} a^2 \right\} = \frac{c_1(n)}{c_2(n)} \left( 1 + o(1) \right) = \frac{\|Z_n\|_\infty^2 \left( 1 + o(1) \right)}{\inf_{\zeta: \|\zeta\|_1 = 1} \frac{1}{n} \sum_{i=1}^n \|e_i \zeta - \zeta^T X_i \beta_*\|_1^2}.
\]

Since \( \|e_i \zeta - \zeta^T X_i \beta_*\|_1^2 \geq \left( \|e_i\| \|\zeta\|_1 - \|\zeta^T X_i \| \|\beta_*\|_1 \right)^2 \), the denominator, \( c_2(n) \), can be lower bounded as follows:

\[
c_2(n) := \inf_{\zeta: \|\zeta\|_1 = 1} \mathbb{E}_{\mathbb{P}_n} \left[ \|e\zeta - \zeta^T X \beta_*\|_1^2 \right] \geq \inf_{\zeta: \|\zeta\|_1 = 1} \mathbb{E}_{\mathbb{P}_n} \left[ \left( \|e\| - \|\zeta^T X\| \|\beta_*\|_1 \right)^2 \right] \geq \mathbb{E}_{\mathbb{P}_n} \left[ \mathbb{E}_{\mathbb{P}_n} \left[ \left( \|e\| - \|\zeta\| \|X\| \|\beta_*\|_1 \right)^2 \right] \right] \geq \mathbb{E}_{\mathbb{P}_n} \left[ \inf_{c \in \mathbb{R}} \mathbb{E}_{\mathbb{P}_n} \left[ \left( \|e\| - c \right)^2 \right] \right].
\]

Since \( e_i \) and \( X_i \) are independent and \( \min_c \mathbb{E}[(Z - c)^2] = \text{Var}[Z] \) for any random variable \( Z \), we obtain that \( c_2(n) \geq \text{Var}_n |e| \). Therefore \( nR_n(\beta_*) \leq \|Z_n\|_\infty^2 \left( 1 + o(1) \right) / \text{Var}_n |e| \). \( \square \)
APPENDIX B. STRONG DUALITY FOR THE LINEAR SEMI-INFINITE PROGRAM RESULTING FROM THE RWP FUNCTION

In the main body of the paper, we have utilized strong duality of linear semi-infinite programs to derive a dual representation of the RWP function in order to perform asymptotic analysis (see Proposition 3). Establishing strong duality in this context relies on the following well-known result on problem of moments ([23, 30]).

The problem of moments. Let $\Omega$ be a nonempty Borel measurable subset of $\mathbb{R}^m$, which, in turn, is endowed with the Borel sigma algebra $\mathcal{B}_\Omega$. Let $X$ be a random vector taking values in the set $\Omega$, and $f = (f_1, \ldots, f_k) : \Omega \rightarrow \mathbb{R}^k$ be a vector of moment functionals. Let $\mathcal{P}_\Omega$ and $\mathcal{M}_{\Omega}^+$ denote, respectively, the set of probability and non-negative measures, respectively on $(\Omega, \mathcal{B}_\Omega)$ such that the Borel measurable functionals $\phi, f$ denote, respectively, the set of probability and non-negative measures, respectively on $(\Omega, \mathcal{B}_\Omega)$ such that the Borel measurable functionals $\phi, f_1, f_2, \ldots, f_k$, defined on $\Omega$, are all integrable. Given a real vector $q = (q_1, \ldots, q_k)$, the objective of the problem of moments is to find the worst-case bound,

$$v(q) := \sup \{ \mathbb{E}_\mu[\phi(X)] : \mathbb{E}_\mu[f(X)] = q, \mu \in \mathcal{P}_\Omega \}.$$  \hfill (54)

If we let $f_0 = 1_{\Omega}$, it is convenient to add the constraint, $\mathbb{E}_\mu[f_0(X)] = 1$, by appending $\hat{f} = (f_0, f_1, \ldots, f_k)$, $\hat{q} = (1, q_1, \ldots, q_k)$, and consider the following reformulation of the above problem:

$$v(q) := \sup \left\{ \int \phi(x)d\mu(x) : \int \hat{f}(x)d\mu(x) = \hat{q}, \mu \in \mathcal{M}_{\Omega}^+ \right\}. \hfill (55)$$

Then, under the assumption that a certain Slater’s type of condition is satisfied, one has the following equivalent dual representation for the moment problem \hfill (55). See Theorem 1 (and the discussion of Case [I] following Theorem 1) in [23] for a proof of the following result:

**Proposition 7.** Let $Q_f = \{ \int \hat{f}(x)d\mu(x) : \mu \in \mathcal{M}_{\Omega}^+ \}$. If $\hat{q} = (1, q_1, \ldots, q_k)$ is an interior point of $Q_f$, then

$$v(q) = \inf \left\{ \sum_{i=0}^{k} a_i q_i : a_i \in \mathbb{R}, \sum_{i=0}^{k} a_i \phi_i(x) \geq \phi(x) \text{ for all } x \in \Omega \right\}.$$ 

In the rest of this section, we recast the dual reformulation of RWP function (in (3)) and the dual reformulation of the distributional representation in Proposition 1 as particular cases of the dual representation of the problem of moments in Proposition 7.

**Dual representation of RWP function.** Recall from Section 3.2 that $W$ is a random vector taking values in $\mathbb{R}^m$ and $h(\cdot, \theta)$ is Borel measurable.

**Proof of Proposition 3.** For simplicity, we do not write the dependence on parameter $\theta$ in $h(u, \theta)$ and $R_n(\theta)$ in this proof; nevertheless, we should keep in mind that the RWP function is a function of parameter $\theta$. Given estimating equation $\mathbb{E}[h(W)] = 0$, recall the definition of the corresponding RWP function,

$$R_n := \inf \{ D_c(\mathbb{P}_n, \mathbb{P}_n) : \mathbb{E}_{\mathbb{P}}[h(W)] = 0 \}$$

$$= \inf \{ \mathbb{E}_{\pi}[c(U, W)] : \mathbb{E}_{\pi}[h(U)] = 0, \pi_w = \mathbb{P}_n, \pi \in \mathcal{P}(\mathbb{R}^m \times \mathbb{R}^m) \},$$

where $\pi_w$ denotes the marginal distribution of $W$ and $\mathbb{P}_n$ is the empirical distribution formed from distinct samples $\{W_1, \ldots, W_n\}$. To recast this as a problem of moments as in \hfill (3), let
Further, let $\phi(u,w) = -c(u,w)$, for all $(u,w) \in \Omega$. Then, 

$$R_n = -\inf_{a_i \in \mathbb{R}} \left\{ \frac{1}{n} \sum_{i=1}^{n} a_i : \sum_{i=1}^{n} a_i 1_{(u=w)}(u,w) + \sum_{i=n+1}^{k} a_i h_i(u) \geq -c(u,w), \text{for all } (u,w) \in \Omega \right\}$$

$$= -\inf_{a_i \in \mathbb{R}} \left\{ \frac{1}{n} \sum_{i=1}^{n} a_i : a_i \geq \sup_{u \in \Omega} \left\{ \sum_{i=n+1}^{k} a_i h_i(u) \right\} \right\}.$$ 

As the inner supremum is not affected even if we take supremum over $\{u : c(u,W_i) = \infty\}$, after letting $\lambda = (a_{n+1}, \ldots, a_k)$ for notational convenience, we obtain 

$$R_n = \sup_{\lambda} \left\{ \frac{1}{n} \sum_{i=1}^{n} \inf_{u \in \mathbb{R}^m} \left\{ c(u,W_i) + \lambda^T h(u) \right\} \right\}. \quad (56)$$

As $\lambda$ is a free variable, we flip the sign of $\lambda$ to arrive at the statement of Proposition 8. This completes the proof.  

**Appendix C. Exchange of sup and inf in the DRO formulation**

The inf-sup exchange in Proposition 8 below is obtained by suitably modifying the inf-sup exchange in [10, Theorem 2] and its proof to accommodate more relaxed assumptions than in [10]. The sequence of steps in the proof of Proposition 8 is similar to that of [10, Theorem 2] and is given here for completeness.

**Proposition 8.** For a given probability distribution $Q$, define 

$$g(\beta) := \sup_{P : D_\alpha(P,Q) \leq \delta} \mathbb{E}_P \left[ l(X,Y;\beta) \right],$$ 

for $\beta \in \mathbb{R}^d$. Suppose that $g(\cdot)$ is real-valued and the level set $\{\beta \in \mathbb{R}^d : g(\beta) \leq b\}$ is bounded for every $b \in \mathbb{R}$. In addition, suppose that $\mathbb{E}_P \left[ l(X,Y;\beta) \right]$ is convex and lower semicontinuous in the variable $\beta$, for every $P \in \mathcal{U}_d(Q) := \{P : D_\alpha(P,Q) \leq \delta\}$. Then,

$$\inf_{\beta \in \mathbb{R}^d} \sup_{P : D_\alpha(P,Q) \leq \delta} \mathbb{E}_P \left[ l(X,Y;\beta) \right] = \sup_{P : D_\alpha(P,Q) \leq \delta} \inf_{\beta \in \mathbb{R}^d} \mathbb{E}_P \left[ l(X,Y;\beta) \right].$$
Proof. We begin by defining the sequence of approximation problems,
\[ g_N(\beta) := \sup_{P \in \mathcal{U}^N_\delta(Q)} \mathbb{E}_P [I(X,Y;\beta)], \]
where \( N = 1, 2, \ldots, \) and
\[ \mathcal{U}^N_\delta(Q) = \{ P \in \mathcal{P}(\mathcal{K}_N) : \mathcal{D}_c(P,Q) \leq \delta \}, \]
with \( \mathcal{P}(\mathcal{K}_N) \) denoting the set of probability distributions over the set \( \mathcal{K}_N := \{ x : \|x\|_2 \leq N \}. \)
Then, due to the compactness of the set \( \mathcal{U}^N_\delta(Q) \), we obtain
\[
\inf_{\beta \in \mathbb{R}^d} g_N(\beta) = \inf_{\beta \in \mathbb{R}^d} \sup_{P \in \mathcal{U}^N_\delta(Q)} \mathbb{E}_P [I(X,Y;\beta)] = \sup_{P \in \mathcal{U}^N_\delta(Q)} \inf_{\beta \in \mathbb{R}^d} \mathbb{E}_P [I(X,Y;\beta)],
\]
as a consequence of Sion’s minimax theorem [45]. Therefore, with \( g_N(\cdot) \) being an increasing sequence of functions, we have
\[
\lim_{N \to \infty} \inf_{\beta \in \mathbb{R}^d} g_N(\beta) = \inf_{N \geq 1} \sup_{\beta \in \mathbb{R}^d} \mathbb{E}_P [I(X,Y;\beta)] = \sup_{P \in \mathcal{U}^N_\delta(Q)} \inf_{\beta \in \mathbb{R}^d} \mathbb{E}_P [I(X,Y;\beta)] \leq \sup_{P \in \mathcal{U}^N_\delta(Q)} \mathbb{E}_P [I(X,Y;\beta)] \leq \inf_{\beta \in \mathbb{R}^d} \mathbb{E}_P [I(X,Y;\beta)] \quad (57)
\]
\[
= \inf_{\beta \in \mathbb{R}^d} g(\beta).
\]
The rest of the proof is divided into three technical steps:

**Step 1:** In this step, we show that the sequence of functions \( \{g_N(\cdot) : N \geq 1\} \) converges pointwise to the function \( g(\cdot) \), as \( N \to \infty \). Since \( g_N(\beta) \) is increasing in \( N \), we have that \( g_N(\beta) \) converges as \( N \to \infty \), for every \( \beta \). Let the function \( g^*(\cdot) \) denote the pointwise limit, \( g^*(\cdot) = \lim_{N \to \infty} g_N(\cdot) \). With \( g_N(\cdot) \leq g(\cdot) \) for every \( N \), we have \( g^*(\beta) \leq g(\beta) \). Since \( g(\cdot) \) is real-valued, we consequently have \( g^*(\beta) \leq g(\beta) < +\infty \), for every \( \beta \in \mathbb{R}^d \).

To show that \( g^*(\beta) \) necessarily equals \( g(\beta) \) for every \( \beta \), we argue via contradiction as follows: Suppose that \( \varepsilon := g(\beta) - g^*(\beta) > 0 \) for some \( \beta \in \mathbb{R}^d \). Consider any \( P' \in \mathcal{U}_\delta(\mathcal{P}_n) \) such that \( \mathbb{E}_{P'} [I(X,Y;\beta)] < (g(\beta) - \varepsilon/2, g(\beta)] \). With \( g(\beta) \) being finite, there exists \( N_0 \) sufficiently large such that
\[
\mathbb{E}_{P'} [I(X,Y;\beta)] \mathbb{I}([\|X\|_2 > N]) < \varepsilon/4 \quad \text{and} \quad [1 - \mathbb{P}'(\mathcal{K}_N)] \mathbb{E}_Q [I(X,Y;\beta)] \mathbb{I}([\|X\|_2 \leq N]) > -\varepsilon/4,
\]
for all \( N > N_0 \). From \( P' \), we construct a measure \( P'_N \in \mathcal{U}^N_\delta(Q) \) by letting,
\[
P'_N(\cdot) = P'(\cdot) + [1 - \mathbb{P}'(\mathcal{K}_N)] \frac{Q(\cdot)}{Q(\mathcal{K}_N)},
\]
for all \( N \) large enough such that \( Q(\mathcal{K}_N) > 0 \). Then,
\[
g^*(\beta) \geq g_N(\beta) \geq \mathbb{E}_{P'_N} [I(X,Y;\beta)] > \mathbb{E}_{P'} [I(X,Y;\beta)] - \varepsilon/2,
\]
for all \( N > N_0 \). With \( \mathbb{E}_{P'} [I(X,Y;\beta)] \in (g(\beta) - \varepsilon/2, g(\beta)] \), we then have \( g^*(\beta) > g(\beta) - \varepsilon \), which leads to a contradiction to the assumption that \( \varepsilon := g(\beta) - g^*(\beta) > 0 \). This verifies that the pointwise limit \( g^*(\cdot) = g(\cdot) \).

**Step 2:** In this next step, we show that the sequence of functions \( \{g_N(\cdot) : N \geq 1\} \) epiconverges to the function \( g(\cdot) \), as \( N \to \infty \). See, for example, [39] Definition 7.1 for a definition of epiconvergence. To accomplish this step, we first see that for every sequence \( \{\beta_N : N \geq 1\} \) satisfying \( \beta_N \to \beta \in \mathbb{R}^d \),
\[
\liminf_{N \to \infty} g_N(\beta_N) \geq \liminf_{N \to \infty} g_M(\beta_N) \geq g_M(\beta),
\]
for any positive integer $M$. Indeed, this is because $g_N(\cdot)$ is an increasing sequence of functions and $g_M(\cdot)$, being pointwise maxima of lower semicontinuous functions, is lower semicontinuous. Letting $M \to \infty$, we then have

$$\liminf_{N \to \infty} g_N(\beta_N) \geq g(\beta),$$

due to the pointwise convergence concluded in Step 1. Next, for any $\beta \in \mathbb{R}^d$, if we pick the sequence $\beta_N = \beta$, we have $\lim_{N \to \infty} g_N(\beta_N) = \lim_{N \to \infty} g_N(\beta) = g(\beta)$. We therefore have from the epiconvergence characterization in [39, Proposition 7.1] that the sequence $\{g_N : N \geq 1\}$ epiconverges to the function $g(\cdot)$.

**Step 3:** In this final step, we show that the optimal values $\inf_{\beta \in \mathbb{R}^d} g_N(\beta)$ converge to $\inf_{\beta \in \mathbb{R}^d} g(\beta)$, as $N \to \infty$. With $\mathbb{E}_P[l(X, Y; \beta)]$ being convex in the variable $\beta$, we have that the pointwise maximum $g(\cdot)$ is convex. Combining this observation with the level-boundedness of the limiting function $g(\cdot)$, we have from [39, Exercise 7.32(c)] that the sequence $\{g_N(\beta) : N \geq 1\}$ is eventually level-bounded. Further, since the functions $g_N(\cdot), g(\cdot)$ are lower semicontinuous and proper, we obtain the desired optimal value convergence,

$$\inf_{\beta \in \mathbb{R}^d} g_N(\beta) \to \inf_{\beta \in \mathbb{R}^d} g(\beta),$$

as a consequence of [39, Theorem 7.33].

The conclusion in Step 3 forces the inequalities in (57) to be equalities, thus rendering the desired inf-sup interchange in the statement of Proposition S.

**Proof of Lemma I.** Let us consider linear regression loss function first. Under the null hypothesis, $\mathbb{E}\|X\|_2^2 < \infty$ and $\mathbb{E}[c^2] < \infty$. Therefore, for any $\beta \in \mathbb{R}^d$, $\mathbb{E}[l(X, Y; \beta)] = \mathbb{E}[(Y - \beta^T X)^2] < \infty$. Further, as the loss function $l(x, y; \beta)$ is a convex and continuous in the variable $\beta$, we have that $\mathbb{E}_P[l(X, Y; \beta)]$ is convex and lower semicontinuous for any $\mathbb{P} \in \mathcal{U}_d(\mathbb{P}_n)$. Next, the distributionally robust representation in Theorem I

$$g(\beta) = \sup_{\mathbb{P} \in \mathcal{U}_d(\mathbb{P}_n)} \mathbb{E}_P[l(X, Y; \beta)] = \left( \sqrt{\mathbb{E}_{\mathbb{P}_n}[(Y - \beta^T X)^2]} + \sqrt{\mathbb{E}_{\mathbb{P}_n}[(Y - \beta^T X)^2]} \right)^2$$

allows us to conclude that $g(\beta)$ is finite for every $\beta \in \mathbb{R}^d$. Further, as $g(\beta) \to \infty$ when $\|\beta\|_p \to \infty$ and $g(\beta)$ is convex and continuous in $\mathbb{R}^d$, the level sets $\{\beta : g(\beta) \leq b\}$ are compact and nonempty for every $b > (\sqrt{\mathbb{E}_{\mathbb{P}_n}[(Y - \beta^T X)^2]} + \sqrt{\mathbb{E}_{\mathbb{P}_n}[(Y - \beta^T X)^2]})^2$. This verifies the level-boundedness requirement in the statement of Proposition S. As all the conditions in Proposition S are satisfied, the sup and inf in the DRO formulation S can be exchanged in the linear regression example as a consequence of Proposition S. Exactly similar reasoning applies for logistic regression loss function when $\mathbb{E}\|X\|_2^2$ is finite. \qed