Distributionally Robust Losses
for Latent Covariate Mixtures

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Abstract
While modern large-scale datasets often consist of heterogeneous subpopulations—for example, multiple demographic groups or multiple text corpora—the standard practice of minimizing average loss fails to guarantee uniformly low losses across all subpopulations. We propose a convex procedure that controls the worst-case performance over all subpopulations of a given size. Our procedure comes with finite-sample (nonparametric) convergence guarantees on the worst-off subpopulation. Empirically, we observe on lexical similarity, wine quality, and recidivism prediction tasks that our worst-case procedure learns models that do well against unseen subpopulations.

1 Introduction
When we train models over heterogeneous data, a basic goal is to train models that perform uniformly well across all subpopulations instead of just on average. For example, in natural language processing (NLP), large-scale corpora often consist of data from multiple domains, each domain varying in difficulty and frequently containing large proportions of easy examples [20]. Standard approaches optimize average performance, however, and yield models that accurately predict easy examples but sacrifice predictive performance on hard subpopulations [59].

The growing use of machine learning systems in socioeconomic decision-making problems, such as loan-servicing and recidivism prediction, highlights the importance of models that perform well over different demographic groups [6]. In the face of this need, a number of authors observe that optimizing average performance often yields models that perform poorly on minority subpopulations [3, 34, 39, 16, 63, 73]. When datasets contain demographic information, a natural approach is to optimize worst-case group loss or equalize losses over groups. But in many tasks—such as language identification or video analysis [73, 16]—privacy concerns preclude recording demographic or other sensitive information, limiting the applicability of methods that require knowledge of demographic identities. For example, lenders in the United States are prohibited from asking loan applicants for racial information unless it is to demonstrate compliance with anti-discrimination regulation [19, 21].

To address these challenges, we seek models that perform well on each sub-corpus rather than those that achieve good (average) performance by focusing on the easy examples and domains. Thus, in this paper we develop procedures that control performance over all large enough subpopulations, agnostic to the distribution of each subpopulation. We study a worst-case formulation over large enough subpopulations in the data, providing procedures that automatically focus on the difficult subsets of the dataset. Our procedure guarantees a uniform level of performance across subpopulations by hedging against unseen covariate shifts, potentially even in the presence of confounding.

In classical statistical learning and prediction problems, we wish to predict a target $Y \in \mathcal{Y}$ from a covariate vector $X \in \mathcal{X} \subset \mathbb{R}^d$ drawn from an underlying population $(X,Y) \sim P$, ...
measuring performance of a predictor $\theta$ via the loss $\ell : \Theta \times (X \times Y) \to \mathbb{R}_+$. The standard approach is to minimize the population expectation $\mathbb{E}_P[\ell(\theta; (X, Y))]$. In contrast, we consider an elaborated setting in which the observed data comes from a mixture model, and we evaluate model losses on a component (subpopulation) from this mixture. More precisely, we assume that for some mixing proportion $\alpha \in (0, 1)$, the data $X$ are marginally distributed as

$$X \sim P_X := \alpha Q_0 + (1 - \alpha)Q_1,$$

while the subpopulations $Q_0$ and $Q_1$ are unknown. The classical formulation does little to ensure equitable performance for data $X$ from both $Q_0$ and $Q_1$, especially for small $\alpha$. Thus for a fixed conditional distribution $P_{Y|X}$, we instead seek $\theta \in \Theta$ that minimizes the expected loss under the latent subpopulation $Q_0$

$$\min_{\theta \in \Theta} \mathbb{E}_{X \sim Q_0}[\mathbb{E}[\ell(\theta; (X, Y)) | X]]. \quad (1)$$

We call this loss minimization under mixture covariate shifts.

As the latent mixture weight and components are unknown, it is impossible to compute the loss (1) from observed data. Thus, we postulate a lower bound $\alpha_0 \in (0, \frac{1}{2})$ on the subpopulation proportion $\alpha$ and consider the set of potential minority subpopulations

$$\mathcal{P}_{\alpha_0, X} := \{Q_0 : P_X = \alpha Q_0 + (1 - \alpha)Q_1 \text{ for some } \alpha \geq \alpha_0 \text{ and distribution } Q_1 \text{ on } X\}.$$

Concretely, our goal is to minimize worst-case subpopulation risk $\mathcal{R}$,

$$\min_{\theta \in \Theta} \left\{ \mathcal{R}(\theta) := \sup_{Q_0 \in \mathcal{P}_{\alpha_0, X}} \mathbb{E}_{X \sim Q_0}[\mathbb{E}[\ell(\theta; (X, Y)) | X]] \right\}. \quad (2)$$

The worst-case formulation (2) is a distributionally robust optimization (DRO) problem [9, 67] where we consider the worst-case loss over mixture covariate shifts $Q_0 \in \mathcal{P}_{\alpha_0, X}$, and we term the methodology we develop around this formulation marginal distributionally robust optimization, as we seek robustness only to shifts in the marginals over the covariates $X$. For datasets with heterogeneous subpopulations (e.g. NLP corpora), the worst-case subpopulation corresponds to a group that is “hard” under the current model $\theta$. As we detail in the related work section, the approach (2) has connections with (among others) covariate shift problems, distributional robustness, fairness, and causal inference.

In some instances, the worst-case subpopulation (2) may be too conservative; the distribution of $X$ may shift only on some components, or we may only care to achieve uniform performance across one variable. As an example, popular computer-vision datasets draw images mostly from western Europe and the United States [65], but one may wish for models that perform uniformly well over different geographic locations. In such cases, when one wishes to consider distributional shifts only on a subset of variables $X_1$ (e.g. geographic location) of the covariate vector $X = (X_1, X_2)$, we may simply redefine $X$ as $X_1$, and $Y$ as $(X_2, Y)$ in the problem (2). All of our subsequent discussion generalizes to such scenarios.

On the other hand, because of confounding, the assumption that the conditional distribution $P_{Y|X}$ does not change across groups may be too optimistic. While the assumption is appropriate for machine learning tasks where human annotators use $X$ to generate the label $Y$, many problems include unmeasured confounding variables that affect the label $Y$ and vary across subpopulations. For example, in a recidivism prediction task, the feature $X$ may be the type of crime, the label $Y$ represents re-offending, and the subgroup may be race; without measuring
unobserved variables, such as income or location, \( P_{Y|X} \) is likely to differ between groups. To address this issue, in Section 5 we generalize our proposed worst-case loss (2) to incorporate worst-case confounding shifts via a robust optimization formulation, providing finite-sample upper bounds on worst-case loss whose tightness depends on the effect of the unmeasured confounders on the conditional risk \( E[\ell(\theta; (X, Y)) \mid X] \).

### 1.1 Overview of results

In the rest of the paper, we construct a tractable finite sample approximation to the worst-case problem (2), and show that it allows learning models \( \theta \in \Theta \) that do uniformly well over subpopulations. Our starting point is the duality result (see Section 2.1)

\[
R(\theta) := \sup_{Q_0 \in \mathcal{P}_{\alpha_0, X}} E_{X \sim Q_0} \left[ E[\ell(\theta; (X, Y)) \mid X] \right] = \inf_{\eta} \left\{ \frac{1}{\alpha_0} \sum_{P_X} \left[ (E[\ell(\theta; (X, Y)) \mid X] - \eta)_+ \right] + \eta \right\}.
\]

For convex losses, the dual form yields a single convex loss minimization in the variables \((\theta, \eta)\) for minimizing \( R(\theta) \). When we (approximately) know the conditional risk \( E[\ell(\theta; (X, Y)) \mid X] \)—for example, when we have access to replicate observations \( Y \) for each \( X \)—it is reasonably straightforward to develop estimators for the risk (2) (see Section 2.2).

Estimating the conditional risk via replication is infeasible in scenarios in which \( X \) corresponds to a unique individual (similar to issues in estimation of conditional treatment effects [42]). Our approach to this issue begins with the variational representation

\[
E[\ell(\theta; (X, Y)) \mid X] = \sup_{h: X \to [0, 1]} E_{P}[h(X)(\ell(\theta; (X, Y)) - \eta)].
\]

As the space \( \{ h: \mathcal{X} \to [0, 1] \} \) is too large to effectively estimate the quantity (3), we consider approximations via easier-to-control function spaces \( \mathcal{H} \subset \{ h: \mathcal{X} \to \mathbb{R} \} \) and study the problem

\[
\text{minimize} \left\{ \frac{1}{\alpha_0} \sup_{h \in \mathcal{H}} E_{P}[h(X)(\ell(\theta; (X, Y)) - \eta)] + \eta \right\}.
\]

By choosing \( \mathcal{H} \) appropriately—e.g. as a reproducing kernel Hilbert space [11, 24] or a collection of bounded Hölder continuous functions—we can develop analytically and computationally tractable approaches to minimizing Eq. (4) to approximate Eq. (2).

Since the variational approximation to the dual objective

\[
\theta \mapsto \inf_{\eta} \left\{ \frac{1}{\alpha_0} \sup_{h \in \mathcal{H}} E_{P}[h(X)(\ell(\theta; (X, Y)) - \eta)] + \eta \right\}
\]

is a lower bound on the worst-case subpopulation risk \( R(\theta) \), it does not (in general) provide uniform control over subpopulations \( Q_0 \in \mathcal{P}_{\alpha_0, X} \). Motivated by empirical observations that confirm the limitations of this approach, we propose and study a more “robust” formulation than the problem (2) that provides a natural upper bound on the worst-case subpopulation risk \( R(\theta) \). Our proposed formulation variational form analogous to Eq. (4) and is estimable.

If we consider a broader class of distributional shifts instead of simply considering subpopulations, we arrive at a more conservative formulation than the problem (2). In particular, a combination of our results and those of Shapiro [66] yields the following corollary. Recalling the Rényi divergence [75] of order \( q \), defined by

\[
D_q(P\|Q) := \frac{1}{q-1} \log \int \left( \frac{dP}{dQ} \right)^q dQ,
\]
then our Lemma 2.1 and Duchi and Namkoong [25, Section 3.2] show that defining
\[ \mathcal{P}_{\Delta, X, q} := \{ Q : D_q (Q | P_X) \leq \Delta \}, \]

then for \( 1/p + 1/q = 1 \) and \( p \in (1, \infty) \) we have
\[
\sup_{Q \in \mathcal{P}_{\Delta, X, q}} \mathbb{E} \left[ \mathbb{E}[\ell(\theta; (X, Y)) \mid X] \right] = \inf_{\eta} \left\{ \exp(\Delta/p) \mathbb{E}_{X \sim P_X} \left[ (\mathbb{E}[\ell(\theta; (X, Y)) \mid X] - \eta)_+^p \right]^{1/p} + \eta \right\}.
\]

Abstracting away the particular choice of uncertainty in \( P_X \), for \( p \in [1, \infty] \), the infimum
\[
\inf_{\eta \geq 0} \left\{ \frac{1}{\alpha_0} \mathbb{E}_{X \sim P_X} \left[ (\mathbb{E}[\ell(\theta; (X, Y)) \mid X] - \eta)_+^p \right]^{1/p} + \eta \right\}
\]
always upper bounds the basic uniform mixture performance risk (2). As we show in Section 4, for Lipschitz conditional risks \( x \mapsto \mathbb{E}[\ell(\theta; (X, Y)) \mid X = x] \), Eq. (5) is equal to a variant of the problem (4) where we take \( \mathcal{H} \) to be a particular collection of Hölder-continuous functions allowing estimation from data. Because our robustness approach in this paper is new, there is limited analysis—either empirical or theoretical—of similar problems. Consequently, we perform some initial empirical evaluation on simulations to suggest the appropriate approximation spaces \( \mathcal{H} \) in the dual form (4) (see Section 3). Our empirical analysis shows that the upper bound (5) provides good performance compared to other variational procedures based on (4), which informs our theoretical development and more detailed empirical evaluation to follow.

We develop an empirical surrogate to the risk (5) in Section 4. Our main theoretical result—Theorem 2—shows that the model \( \hat{\theta}_n^{\text{rob}} \in \mathbb{R}^d \) minimizing this empirical surrogate achieves
\[
\sup_{Q_0 \in \mathcal{P}_{\alpha_0, X}} \mathbb{E}_{X \sim Q_0} \left[ \mathbb{E}[\ell(\hat{\theta}_n^{\text{rob}}; (X, Y)) \mid X] \right] \leq R_p^* + O \left( n^{-\frac{p-1}{p+1}} \right),
\]
with high probability, where
\[
R_p^* := \inf_{\theta \in \Theta, \eta \geq 0} \left\{ \frac{1}{\alpha_0} \mathbb{E}_{X \sim P_X} \left[ (\mathbb{E}[\ell(\theta; (X, Y)) \mid X] - \eta)_+^p \right]^{1/p} + \eta \right\}
\]
whenever \( x \mapsto \mathbb{E}[\ell(\theta; (X, Y)) \mid X = x] \) is suitably smooth. In a rough sense, then, we expect that \( p \) trades between approximation (via \( R_p^* \)) and estimation error.

While our convergence guarantee gives a nonparametric rate \( O(n^{-\frac{p-1}{p+1}}) \), we empirically observe that our procedure achieves low worst-case losses even when the dimension \( d \) is large. We conjecture that this is due to the fact that our empirical approximation to the \( L^p \) norm bound (5) is an upper bound with error only \( O(n^{-\frac{1}{2}}) \), but a lower bound at the conservative rate \( O(n^{-\frac{1}{2p+1}}) \). Such results—which we present at the end of Section 4—seem to point to the conservative nature of our convergence guarantee in practical scenarios. In our careful empirical evaluation on different semantic similarity assessment and recidivism prediction tasks (Section 6), we observe that our procedure learns models that do uniformly well across unseen subpopulations of difficult examples and minority groups.

**1.2 Related work**

Several important issues within statistics and machine learning are closely related to our goals of uniform performance across subpopulations. We briefly touch on a few of these connections here and hope that further linking them may yield alternative approaches and deeper insights.
Covariate shifts  A number of authors have studied the case where a target distribution of interest is different from the data-generating distribution—known as covariate shift or sample selection bias \cite{68, 8, 72}. Much of the work focuses on the domain adaptation setting where the majority of the observations come from a source population (and corresponding domain) \( P \). These methods require (often unsupervised) samples from an a priori fixed target domain, and apply importance weight methods to reweight the observations when training a model for the target \cite{71, 13, 33, 41}. For multiple domains, representation based methods can identify sufficient statistics not affected by covariate shifts \cite{38, 32}.

On the other hand, our worst-case formulation assumes no knowledge of the latent group distribution \( Q_0 \) (unknown target) and controls performance on the worst subpopulation of size larger than \( \alpha_0 \). Kernel-based adversarial losses \cite{76, 50, 51} minimize the worst-case loss over importance weighted distributions, where the importance weights lie within a reproducing kernel Hilbert space. These methods are similar in that they consider a worst-case loss, but these worst-case weights provide no guarantees (even asymptotically) for latent subpopulations.

Distributionally robust optimization  A large body of work on distributionally robust optimization (DRO) methods \cite{10, 12, 47, 55, 26, 56, 28, 64, 15, 69, 48, 30, 14, 31, 46, 70, 45} solves a worst-case problem over the joint distribution on \((X, Y)\). On the other hand, our marginal DRO formulation \( (2) \) studies distributional shifts in the marginal covariate distribution \( X \sim P_X \). Concretely, we can formulate an analogue \cite{10, 56} of our marginal formulation \( (2) \) by letting

\[
P_{\alpha_0, (X, Y)} := \{ Q_0 : P = \alpha Q_0 + (1 - \alpha) Q_1 \text{ for some } \alpha \geq \alpha_0 \text{ and probability } Q_1 \text{ on } \mathcal{X} \times \mathcal{Y} \}.\]

The joint DRO objective

\[
\sup_{Q_0 \in P_{\alpha_0, (X, Y)}} \mathbb{E}_{(X,Y) \sim Q_0} [\ell(\theta; (X,Y))]
\]

upper bounds the marginal worst-case formulation \( (2) \). The joint DRO objective \( (7) \) is frequently too conservative (see Section 2). By providing a tighter bound on the worst-case loss \( (2) \) under mixture covariate shifts, our proposed finite-sample procedure \( (20) \) achieves better performance on unseen subpopulations (see Sections 4 and 6). For example, the joint DRO bound \( (7) \) applied to zero-one loss for classification may result in a degenerate non-robust estimator that upweights all misclassified examples \cite{40}, but our marginal DRO formulation mitigates these issues by using the underlying metric structure.

Similar to our formulation \( (2) \), distributionally robust methods defined with appropriate Wasserstein distances—those associated with cost functions that are infinity when values of \( Y \) differ—also considers distributional shifts in the marginal covariate distribution \( X \sim P_X \). Such formulations allow incorporating the geometry of \( X \), and consider local perturbations in the covariate vector (with respect to some metric on \( \mathcal{X} \)). Our worst-case subpopulation formulation \( (2) \) departs from these methods by considering all large enough mixture components (subpopulations) of \( P_X \), giving strong fairness and tail-performance guarantees for learning problems.

Fairness  A growing literature recognizes the challenges of fairness within statistical learning \cite{27, 35, 44, 43, 36, 21}, which motivates our approach as well. Among the many approaches to this problem, researchers have proposed that models with similar behavior across demographic subgroups are fair \cite{27, 43}. The closest approach to our work is the use of Lipschitz
constraints as a way to constrain the labels predicted by a model \([27]\). Rather than directly constraining the prediction space, we use the Lipschitz continuity of the conditional risk to derive upper bounds on model performance. The gap between joint DRO and marginal DRO relates to “gerrymandering” \([43]\): fair models can be unreasonably pessimistic by guaranteeing good performance against minority subpopulations with high observed loss—which can be a result of random noise—rather than high expected loss \([27, 43, 37]\). Our marginal DRO approach alleviates such gerrymandering behavior relative to the joint DRO formulation \((7)\); see Section 4 for a more detailed discussion.

**Causal inference** Learning models that perform well under interventions is a common goal in causal inference, and one formulation of causality is as a type of invariance across environmental changes \([58]\). In this context, our formulation seeking models \(\theta\) with low loss across marginal distributions on \(X\) is an analogue of observational studies in causal inference. Bühlmann, Meinshausen, and colleagues have proposed a number of procedures similar in spirit to our marginal DRO formulation \((2)\), though the key difference in their approaches is that they assume that underlying environmental changes or groups are known. Their maximin effect methods find linear models that perform well over heterogeneous data relative to a fixed baseline with known or constrained population structure \([53, 61, 18]\), while anchor regression \([62]\) fits regression models that perform well under small perturbations to feature values. Heinze-Deml and Meinshausen \([38]\) consider worst-case covariate shifts, but assume a decomposition between causal and nuisance variables, with replicate observations sharing identical causal variables. Peters et al. \([58]\) use heterogeneous environments to discover putative causal relationships in data, identifying robust models and suggesting causal links. Our work, in contrast, studies models that are robust to mixture covariate shifts, a new type of restricted interventions over all large enough subpopulations.

## 2 Performance Under Mixture Covariate Shift

We begin by reformulating the worst-case loss over mixture covariate shifts \((2)\) via its dual (Section 2.1). We then consider a simpler setting in which we can collect replicate labels \(Y\) for individual feature vectors \(X\)—essentially, the analogue of a randomized study in causal inference problems—showing that in this case appropriate sample averages converge quickly to the worst-case loss \((2)\) (Section 2.2). Although this procedure provides a natural gold standard when \(x \mapsto \mathbb{E}[\ell(\theta; (x, Y)) \mid X = x]\) is estimable, it is impossible to implement when large sets of replicate labels are unavailable. This motivates empirical fitting procedure we propose in Eq. \((20)\) to come, which builds out of the tractable upper bounds we present in Section 4.

### 2.1 Upper bounds for mixture covariate shift

Taking the dual of the inner maximization problem over covariate shifts \((2)\) gives the below result.

**Lemma 2.1.** If \(\mathbb{E}[\mathbb{E}[\ell(\theta; (X, Y)) \mid X]] < \infty\), then

\[
\sup_{Q_0 \in \mathcal{P}_{\alpha_0 \times X}} \mathbb{E}_{X \sim Q_0} \left[ \mathbb{E}[\ell(\theta; (X, Y)) \mid X] \right] = \inf_{\eta \in \mathbb{R}} \left\{ \frac{1}{\alpha_0} \mathbb{E}_{X \sim \mathcal{P}_X} \left[ (\mathbb{E}[\ell(\theta; (X, Y)) \mid X] - \eta)_+ \right] + \eta \right\}. \tag{8}
\]

If additionally \(0 \leq \mathbb{E}[\ell(\theta; (X, Y)) \mid X] \leq M\) w.p. 1, the infimizing \(\eta\) lies in \([0, M]\).
Observed data
Marginal DRO worst-case
Joint DRO worst-case

(a) Data for a 1-dimensional regression problem (circle) and the worst case distribution $Q_0$ for joint and marginal DRO (triangle/square).

(b) Best fit lines according to each loss. Only marginal DRO selects a line which fits both the $X > 0$ and $X < 0$ groups.

(c) Loss under different regression coefficients. Unlike Marginal DRO, ERM dramatically underestimates and joint DRO overestimates the worst case loss (2).

**Figure 1:** Toy problem of $L_1$ regression through origin.

See Appendix A.1 for the proof. The dual form (8) is the conditional-value-at-risk (CVaR) of the conditional risk $E[\ell(\theta; (X,Y)) | X]$; CVaR is a common measure of risk in the portfolio and robust optimization literatures [60, 67], but there it applies to an unconditional loss, making it (as we discuss below) conservative for the problems we consider.

The marginal DRO formulation (8) makes clear that the joint DRO problem (7) is conservative, as an identical calculation gives that Eq. (7) is equal to $\inf_{\eta} \left\{ \frac{1}{\alpha_0} E[\ell(\theta; (X,Y)) - \eta]_+ + \eta \right\}$, which is greater than the marginal DRO (8) unless $Y$ is a deterministic function of $X$. In Section 4, we provide an approximation to the marginal DRO dual form (8), and one of our contributions is to show that our procedure has better theoretical and empirical performance than conservative estimators using the joint DRO objective (7).

To illustrate the advantages of the marginal distributionally robust approach, consider a misspecified linear regression problem, where we predict $\hat{Y} = X\theta$ and use absolute the loss $\ell(\theta; (x,y)) = |\theta x - y|$. Letting $\varepsilon \sim N(0,1)$, the following mixture model generates the data

$$Z \sim \text{Bernoulli}(0.15), \quad X = (1 - 2Z) \cdot \text{Uniform}([0,1]), \quad Y = |X| + 1 \{X \geq 0\} \cdot \varepsilon \quad (9)$$

so that the subpopulation $Q_0(\cdot) := P(\cdot | Z = 1)$ has minority proportion 15%. We plot observations from this model in Figure 1a, where 85% of the points are on the right, and have high noise. The model with the best uniform performance is near $\theta = 0$, which incurs similar losses between left and right groups. In contrast, the empirical risk minimizer ($\theta = 1$) incurs a high loss of 1 on the left group and $\sqrt{2/\pi}$ on the right one.

Empirical risk minimization tends to ignore the (left) minority group, resulting in high loss on the minority group $X < 0$ (Figure 1b). The joint DRO solution (7) minimizes losses over a worst-case distribution $Q_0$ consisting of examples which receive high loss (blue triangles), which tend to be samples on $X > 0$ due to noise. This results in a loose upper bound on the true worst-case risk as seen in Figure 1c. Our proposed estimator selects a worst-case distribution consisting of examples with high conditional risk $E[\ell(\theta; (X,Y)) | X]$ (Figure 1a, orange squares). This worst-case distribution is not affected by the noise level, and results in a close approximation to the true loss (Figure 1c).

### 2.2 Estimation via replicates

A natural approach to estimating the dual form (8) is a two phase strategy, where we draw $X_1, \ldots, X_n \overset{\text{iid}}{\sim} P_X$ and then—for each $X_i$ in the sample—draw a secondary sample of size $m$
i.i.d. from the conditional $Y \mid X = X_i$. We then use these empirical samples to estimate $E[\ell(\theta; (X, Y)) \mid X = X_i]$. While it is not always possible to collect replicate labels for a single $X$, human annotated data, which is common in machine learning applications [52, 5], allows replicate measurement, where we may ask multiple annotators to label the same $X$.

We show this procedure can yield explicit finite sample bounds with error at most $O(n^{-1/2} + m^{-1/2})$ for the population marginal robust risk (2) when the losses are bounded.

**Assumption A1.** For $M < \infty$, we have $\ell(\theta; (x, y)) \in [0, M]$ for all $\theta \in \Theta, x \in \mathcal{X}, y \in \mathcal{Y}$.

The following estimate approximates the worst-case loss (2) for a fixed value of $\theta$.

**Proposition 1.** Let Assumption A1 hold. There exists a universal constant $C$ such that for any fixed $\theta \in \Theta$, with probability at least $1 - \delta$

$$\left| \sup_{Q_0 \in \mathcal{P}_{\alpha_0, X} \sim Q_0} E[\ell(\theta; (X, Y)) \mid X] - \inf_{\eta \in [0, M]} \left\{ \frac{1}{\alpha_0 n} \sum_{i=1}^{n} \left( \frac{1}{m} \sum_{j=1}^{m} \ell(\theta; (X_i, Y_{i,j})) - \eta \right) + \eta \right\} \right| \leq C \frac{M}{\alpha_0} \sqrt{\frac{1 + \log \frac{1}{\delta}}{\min\{m, n\}}}.$$ 

See Appendix A.2 for the proof. The estimator in Proposition 1 approximates the worst-case loss (2) well for large enough $m$ and $n$. However—similar to the challenges of making causal inferences from observational data and estimating conditional treatment effects—it is frequently challenging or impossible to collect replicates for individual observations $X$, as each $X$ represents an unrepeatable unique measurement. Consequently, the quantity in Proposition 1 is a type of gold standard, but achieving it is likely practically challenging.

## 3 Variational Approximation to Worst-Case Loss

The difficulty of collecting replicate data, coupled with the conservativeness of the joint DRO objective (7) for approximating the worst-case loss $\mathcal{R}(\theta)$, impel us to study tighter approximations that do not depend on replicates. Recalling the variational representation (3), our goal is to minimize

$$\mathcal{R}(\theta) = \frac{1}{\alpha_0} \sup_{h \in \mathcal{H}} \mathbb{E}_{P}[h(X)(\ell(\theta; (X, Y)) - \eta)] + \eta.$$ 

As we note in the introduction, this quantity is challenging to work with, so we restrict $h$ to subsets $\mathcal{H} \subset \{ h : \mathcal{X} \to [0, 1] \}$, developing many possible approximations. The advantage of this formulation and its related relaxations (4) is that it replaces the dependence on the conditional risk with an expectation over the joint distribution on $(X, Y)$, which we may estimate using the empirical distribution, as we describe in the next section. In this case, the lack of a "standard" choice motivates us to perform experiments to direct our development; we provide several example approximations in the next section, evaluating each empirically, and then perform a more careful theoretical analysis of the procedure providing the best empirical performance.

### 3.1 Example approximations and empirical variants

Each choice of a collection of functions $\mathcal{H} \subset \{ h : \mathcal{X} \to [0, 1] \}$ to approximate the variational form (3) in the formulation (4) yields a new optimization problem. For each choice of $\mathcal{H}$
we propose below, we consider an empirical approximation \( \hat{\mathcal{H}} \), the subset of \( \mathcal{H} \) restricted to mapping \( \{X_1, \ldots, X_n\} \rightarrow \mathbb{R} \) instead of \( \mathcal{X} \rightarrow \mathbb{R} \), solving the empirical alternative

\[
\min_{\theta \in \Theta, \eta} \left\{ \frac{1}{\alpha_0} \sup_{h \in \hat{\mathcal{H}}} \mathbb{E}_{\mathcal{R}_n}[h(X)(\ell(\theta; (X, Y)) - \eta)] + \eta \right\}.
\]  

(10)

We design our proposals so the dual of the inner supremum (10) is computable. When the conditional risk \( x \rightarrow \mathbb{E}[\ell(\theta; (X, Y)) \mid X = x] \) is smooth, we can provide generalization bounds for our procedures. We omit detailed development for our first two procedures—which we believe are natural proposals, justifying a bit of discussion—as neither is as effective as the last procedure in our empirical evaluations, which controls the \( L^p \) upper bound (5) on \( R(\theta) \).

**Reproducing Hilbert kernel spaces (RKHS)**

Let \( K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}_+ \) be a reproducing kernel \([11, 4]\) generating the reproducing kernel Hilbert space \( \mathcal{H}_K \) with associated norm \( \| \cdot \|_K \). For any \( R \in \mathbb{R}_+ \), we can define a norm ball

\[
\mathcal{H}_{K,R} := \{ h \in \mathcal{H}_K : \| h \|_K \leq R, h \in [0, 1] \}
\]

and consider the variational approximation (4) with \( \mathcal{H} = \mathcal{H}_{K,R} \). To approximate the population variational problem \( \sup_{h \in \mathcal{H}_{K,R}} \mathbb{E}[h(X)(\ell(\theta; (X, Y)) - \eta)] \), we consider a restriction of the same kernel \( K \) to the sample space \( \{X_1, \ldots, X_n\} \). Let \( K_n = \{K(X_i, X_j)\}_{1 \leq i, j \leq n} \) be the Gram matrix evaluated on samples \( X_1, \ldots, X_n \), and define the empirical approximation

\[
\hat{\mathcal{H}}_{K,R} := \left\{ h \in [0, 1]^n : h = K_n \xi \text{ for some } \xi \in \mathbb{R}^n \text{ such that } \frac{1}{n^2} \xi^\top K_n \xi \leq R \right\}.
\]

(Recall that if \( h(x) = \sum_{i=1}^n K(x, X_i) \xi_i \), then \( \| h \|_K^2 = \frac{1}{n} \xi^\top K_n \xi \)). To compute the empirical problem (10) with \( \hat{\mathcal{H}} = \hat{\mathcal{H}}_{K,R} \), we take the dual of the inner supremum. Simplifying the dual form—whose derivation is a standard exercise in convex optimization—we get

\[
\min_{\theta \in \Theta, \eta \in \mathbb{R}, \beta \in \mathbb{R}_+} \left\{ \frac{1}{\alpha_0 n} \sum_{i=1}^n (\ell(\theta; (X_i, Y_i)) - \eta + \beta_i)_+ + \frac{1}{n} \sqrt{R^{-1} \beta^\top K_n \beta} \right\}.
\]

(11)

For convex losses \( \ell(\theta; (X, Y)) \), this is a convex optimization problem in \( (\theta, \beta, \eta) \).

**Hölder continuous functions (bounded Hölder)**

Recall that a function \( f : \mathcal{X} \rightarrow \mathbb{R} \) is \((\alpha, c)\)-Hölder continuous for \( \alpha \in (0, 1] \) and \( c > 0 \) if \( |f(x) - f(x')| \leq c \|x - x'\|_\alpha \) for all \( x, x' \in \mathcal{X} \). Instead of the space of bounded functions, we restrict attention to Hölder continuous functions

\[
\mathcal{H}_{L,p} := \{ h : \mathcal{X} \rightarrow [0, 1] \mid h \text{ is } (p - 1, L^{p-1})\text{-Hölder continuous} \},
\]

where the particular scaling with respect to \( p \in (1, 2] \) and \( L > 0 \) is for notational convenience in the next section. Noting that the empirical plug-in of \( \mathcal{H}_{L,p} \) is

\[
\hat{\mathcal{H}}_{L,p} := \{ h : \{X_1, \ldots, X_n\} \rightarrow [0, 1] \mid h \text{ is } (p - 1, L^{p-1})\text{-Hölder continuous} \},
\]

the empirical plug-in of the variational problem (4) with \( \mathcal{H} = \mathcal{H}_{L,p} \) is given by the procedure (10) with \( \hat{\mathcal{H}} = \hat{\mathcal{H}}_{L,p} \). Taking the dual of the inner supremum problem, we have the following equivalent dual formulation of the empirical variational problem

\[
\min_{\theta \in \Theta, \eta, B \in \mathbb{R}_+^{n \times n}} \left\{ \frac{1}{\alpha_0 n} \sum_{i=1}^n \left( \ell(\theta; (X_i, Y_i)) - \frac{1}{n} \sum_{j=1}^n (B_{ij} - B_{ji}) - \eta \right)_+ + \frac{L^{p-1}}{n^2} \sum_{i,j=1}^n \|X_i - X_j\|^{p-1} B_{ij} \right\}.
\]
For convex losses \( \theta \mapsto \ell(\theta; (X, Y)) \), this is again a convex optimization problem in \((\theta, B, \eta)\), and is always smaller than the empirical joint DRO formulation (7).

By definition, the population Hölder continuous variational approximation provides the lower bound on the worst-case loss

\[
R_{L,p}(\theta) := \inf_{\eta} \sup_{h \in \mathcal{H}_{L,p}} \left\{ \frac{1}{\alpha_0} \mathbb{E}_P[h(X)(\ell(\theta; (X, Y)) - \eta)] + \eta \right\} \leq R(\theta).
\]

As a consequence, \( R_{L,p} \) cannot upper bound the subpopulation loss \( \mathbb{E}_{X \sim Q_0}[\mathbb{E}[\ell(\theta; (X, Y)) \mid X]] \) uniformly over \( Q_0 \in \mathcal{P}_{\alpha_0,X} \). Nonetheless, for any subpopulation \( Q_0 \in \mathcal{P}_{\alpha_0,X} \) with Lipschitz density \( \frac{dQ_0}{dP} : \mathcal{X} \to \mathbb{R}_+ \), then \( R_{L,2}(\theta) \) does provide a valid upper bound on \( \mathbb{E}_{X \sim Q_0}[\mathbb{E}[\ell(\theta; (X, Y)) \mid X]] \):

**Lemma 3.1.** Let \( Q_0 \in \mathcal{P}_{\alpha_0,X} \) be any distribution with \( L \)-Lipschitz density \( \frac{dQ_0}{dP} : \mathcal{X} \to \mathbb{R}_+ \). Then

\[
\mathbb{E}_{X \sim Q_0}[\mathbb{E}[\ell(\theta; (X, Y)) \mid X]] \leq R_{L,2}(\theta) \leq R(\theta).
\]

See Section A.3 for a proof. For example, if \( P \) and \( Q_0 \in \mathcal{P}_{\alpha_0,X} \) both have Lipschitz log densities, then \( \frac{dQ_0}{dP} \) is also Lipschitz, as the following example shows.

**Example 1:** Let \( P \) be absolutely continuous with respect to some \( \sigma \)-finite measure \( \mu \), denote \( p(X) := \frac{dP}{d\mu}(X) \) and \( q_0(X) := \frac{dQ_0}{d\mu}(X) \) and assume \( \log p \) and \( \log q_0 \) are \( L \)-Lipschitz. Let \( h(x) := \frac{q_0(x)}{p(x)} \), and consider any fixed \( x, x' \in \mathcal{X} \). If we assume that without loss of generality that \( h(x) > h(x') \), then

\[
\frac{|h(x) - h(x')|}{\|x - x'\|} = \frac{h(x)}{\|x - x'\|} \left( 1 - \exp\left( \log \frac{p(x)}{q_0(x)} - \log \frac{p(x')}{q_0(x')} \right) \right) \leq \frac{L}{\alpha_0},
\]

where the final inequality follows because \( h(x) = q_0(x)/p(x) \leq 1/\alpha_0 \) and \( \exp(x) \geq 1 + x \). Consequently, then \( x \mapsto q_0(x)/p(x) \) is \((L/\alpha_0)\)-Lipschitz. \( \diamond \)

\( L^p \) norm bounded Hölder functions (\( L^p \) Hölder) We consider the closely related function class consisting of \( L^p \) bounded Hölder functions. This class of functions, which we motivate via an \( L^p \)-norm bound (5) on the first term of the dual objective (8). For any \( p \in (1, \infty) \) and \( q = \frac{p}{p-1} \) we have

\[
\mathbb{E}_{X \sim P_X} \left[ (\mathbb{E}[\ell(\theta; (X, Y)) \mid X] - \eta)^+ \right] \leq \left( \mathbb{E}_{X \sim P_X} \left[ (\mathbb{E}[\ell(\theta; (X, Y)) \mid X] - \eta)^p \right] \right)^{1/p} = \sup_h \{ \mathbb{E} [h(X)(\ell(\theta; (X, Y)) - \eta)] \mid h : \mathcal{X} \to \mathbb{R}_+, \mathbb{E}[h(X)] \leq 1 \}.
\]

If \( x \mapsto \mathbb{E}[\ell(\theta; (X, Y)) \mid X = x] \) is Hölder continuous, then the function

\[
h^*(x) := \frac{(\mathbb{E}[\ell(\theta; (X, Y)) \mid X = x] - \eta)^{p-1}}{\left( \mathbb{E}_{X \sim P_X} \left[ (\mathbb{E}[\ell(\theta; (X, Y)) \mid X] - \eta)^p \right] \right)^{1/q}}
\]

attaining the supremum in the variational form (12) is Hölder continuous with constant dependent on the magnitude of the denominator. In this case, carefully selecting the smoothness constant and \( L^p \) norm radius allows us to ensure that \( \mathcal{H} \) contains \( h^* \) and to derive guarantees for the resulting estimator (see Section 4 for more).

Minimizing the \( L^p \) upper bound rather than the original variational objective (alternatively, seeking higher-order robustness than the CVaR of the conditional risk \( \mathbb{E}[\ell(\theta; (X, Y)) \mid X] \) as in
our discussion of the quantity (5)) incurs approximation error. In practice, our experience is that this gap has limited effect, and the following lemma—whose proof we defer to Section A.4—quantifies the approximation error in inequality (12).

**Lemma 3.2.** Let Assumption A1 hold and \( Z(X) = \mathbb{E}[\ell(\theta; (X, Y)) \mid X] \). For \( \eta \in [0, M] \)

\[
(\mathbb{E}_{X \sim P_X} [(Z(X) - \eta)_+^p])^{1/p} \leq \min \left\{ (M - \eta)^{1/q} (\mathbb{E} (Z(X) - \eta)_+)^{1/p}, \right.
\]

\[
\mathbb{E} (Z(X) - \eta)_+ + p^{1/p} (M - \eta)^{1/q} (\mathbb{E} |(Z(X) - \eta)_+ - \mathbb{E} [(Z(X) - \eta)_+]|)^{1/p} \right\}.
\]

Empirically, we find in the next subsection that this function class performs favorably to the other potential approximations; we consequently focus on it in the sequel.

### 3.2 Empirical Comparison of Variational Procedures

**A priori** it is unclear whether one class or another in our choices in Section 3.1 should yield better performance; at least at this point, our theoretical understanding provides similarly limited guidance. To that end, we perform a small simulation study to direct our coming deeper theoretical and empirical evaluation, discussing the benefits and drawbacks of various choices of \( \mathcal{H} \) through the example we introduce in Figure 1a, Section 2.1.

We consider an elaborated version of the data mechanism (9) to incorporate higher dimensionality, with the data generating distribution

\[
Z \sim \text{Bern}(0.15), \quad X_1 = (1 - 2Z) \cdot \text{Uni}([0, 1]), \quad X_2, \ldots, X_d \overset{\text{iid}}{\sim} \text{Uni}([-1, 1])
\]

\[
Y = |X_1| + 1 \{X_1 \geq 0\} \cdot \varepsilon, \quad \varepsilon \sim \text{N}(0, 1). \tag{14}
\]

Our goal is to predict \( Y \) via \( \hat{Y} = \theta^T X \), and we use the absolute loss \( \ell(\theta; (x, y)) = |y - \theta^T x| \).

We provide details of the experimental setup, such as the estimators and optimizers, in Section 6. In brief, we perform a grid search over all hyperparameters (Lipschitz estimates and kernel scales) for each method over 4 orders of magnitude; for the RKHS-based estimators, we test Gaussian, Laplacian, and Matern kernels, none of which have qualitative differences from one another, so we present results only for the Gaussian kernel \( K(x, x') = \exp(-\frac{1}{2\sigma^2} \|x - x'\|_2^2) \).

**Dimension dependence** We first investigate the dimension dependence of the estimators, increasing \( d \) in the model (14) from \( d = 2 \) to 50 with a fixed sample size \( N = 5000 \).

Under model (14), we consider marginal distributionally robust objective (2) and evaluate the excess risk \( R(\theta) - \inf_\theta R(\theta) \) for the choice \( \alpha_0 = .15 \), the hardest 15% of the data. As \( d \) grows, we expect estimation over Hölder continuous functions to become more difficult, and for the RKHS-based estimator to outperform the others. Figure 2 bears out this intuition (plotting the excess risk): high dimensionality induces less degradation in the RKHS approach than the others. Yet the absolute performance of the Hölder-based methods is better, which is unsurprising, as we are approximating a discontinuous indicator function.

**Sample size dependence** We also consider the sample dependence of the estimators, fitting models using losses with robustness level set to \( \alpha_0 = .15 \), then evaluating their excess risk \( R(\hat{\theta}) - \inf_\theta R(\theta) \) using \( \alpha_0 \in \{.05, .15\} \), so that we can see the effects of misspecification, as it is unlikely in practice that we know the precise minority population size against which to
evaluate. Unlike the $L^p$-Hölder class (Eq. (12)), the bounded $c$-Hölder continuous function class (11) can approximate the population optimum of the original variational problem (3) as $n \to \infty$ and $c \to \infty$. Because of this, we expect that as the sample size grows, and $c$ is set optimally, the bounded Hölder class will perform well.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure2.png}
\caption{Variational estimates based on RKHS are less affected by the dimensionality of the problems, but perform worse than the Hölder continuous function approaches overall.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure3.png}
\caption{Performance of the function classes in low dimensional high sample size settings with well-specified robustness level (left) and misspecified robustness level (right).}
\end{figure}

On example (9) with $d = 1$, we observe in Figure 3a that both Hölder continuous class estimators with constants set via a hold-out set perform well as $n$ grows, achieving negligible excess error. In contrast, the RKHS approach incurs high loss even with large sample sizes. Although both Hölder class approaches perform similarly when the robustness level $\alpha_0$ is set properly, we find that the $L^p$-Hölder class is substantially better when the test time robustness level changes. The $L^p$-Hölder based estimator is the only one which provides reasonable estimators when training with $\alpha_0 = 0.15$ and testing with $\alpha_0 = 0.05$ (Figure 3b). Motivated by these practical benefits, we study finite sample properties of the $L^p$-bound estimator in what follows.

\section{Tractable Risk Bounds for $L^p$ Variational Problem}

In this section, we focus on the $L^p$ norm bounded Hölder class and formally develop and analyze a marginal DRO estimator $\tilde{\theta}^{\text{rob}}_n$. We derive this estimator by solving an empirical approximation of the upper bound (12) and we provide a number of generalization guarantees
for this procedure.

4.1 A restricted variational formulation

Recall that the $L^p$ variational form provides a tractable upper bound to the worst-case loss for Lipschitzian conditional risks. We formally state this upper bound, and derive its empirical counterpart.

**Assumption A2.** $(x,y) \mapsto \ell(\theta; (x,y))$ and $x \mapsto \mathbb{E}[\ell(\theta; (x,Y)) \mid X = x]$ are $L$-Lipschitz for all $\theta \in \Theta$.

Recall that a function $f : \mathcal{X} \to \mathbb{R}$ is $(\alpha, c)$-Hölder continuous for $\alpha \in (0, 1]$ and $c < \infty$ if $|f(x) - f(x')| \leq c \|x - x'\|^\alpha$ for all $x, x' \in \mathcal{X}$. To ease notation let $\mathcal{H}_{L,p}$ denote the space of Hölder continuous functions

$$\mathcal{H}_{L,p} := \{ h : \mathcal{X} \to \mathbb{R}, (p - 1, L^{p-1})\text{-Hölder continuous} \} .$$

As we show below, if Assumption A2 holds and the denominator in the expression (13) has lower bound $\epsilon > 0$, then $c^* \in \mathcal{H}_{L,p}$, and we can approximate the variational form (12) by solving an analogous problem over smooth functions. Otherwise, we can bound the $L^p$-norm (12) by $\epsilon^{q-1}$, which is small for small values of $\epsilon$. Hence, if we define a variational objective over smooth functions $\mathcal{H}_{L,p}$

$$R_{p,\epsilon,L}(\theta, \eta) := \sup_{h \in \mathcal{H}_{L,p}} \left\{ \mathbb{E} \left[ \frac{h(X)}{\epsilon} (\ell(\theta; (X,Y)) - \eta) \right] \middle| \ h \geq 0, \ (\mathbb{E}[h(X)^q])^{1/q} \leq \epsilon \right\} ,$$

we arrive at a tight approximation to the variational form (12), which we prove in Section A.5.

**Lemma 4.1.** Let Assumptions A1, A2 hold and let $p \in (1, 2]$. Then, for any $\theta \in \Theta$ and $\eta \in \mathbb{R}$,

$$\left( \mathbb{E}_{X \sim P_X} \left[ (\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)^p \right] \right)^{1/p} = \inf_{\epsilon \geq 0} \{ R_{p,\epsilon,L}(\theta, \eta) \vee \epsilon^{q-1} \}$$

and for any $\epsilon > 0$, $(R_{p,\epsilon,L}(\theta, \eta) \vee \epsilon^{q-1}) - \epsilon^{q-1} \leq \left( \mathbb{E}_{X \sim P_X} \left[ (\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)^p \right] \right)^{1/p}$.

4.2 The empirical estimator

Since the variational approximation $R_{p,\epsilon,L}$ does not use the conditional risk $\mathbb{E}[\ell(\theta; (X,Y)) \mid X]$, its empirical plug-in is a natural finite-sample estimator. Defining

$$\widehat{\mathcal{H}}_{L,p} := \left\{ h \in \mathbb{R}^n : h(X_i) = h(X_j) \leq L^{p-1}\|X_i - X_j\|^{p-1} \text{ for all } i, j \in [n] \right\} ,$$

we consider the estimator

$$\widehat{R}_{p,\epsilon,L}(\theta, \eta) := \sup_{h \in \widehat{\mathcal{H}}_{L,p}} \left\{ \mathbb{E}_{P_\theta} \left[ \frac{h(X)}{\epsilon} (\ell(\theta; (X,Y)) - \eta) \right] \middle| \ h \geq 0, \ (\mathbb{E}_{P_\theta}[h^q(X)])^{1/q} \leq \epsilon \right\} .$$

The following lemma shows that the plug-in $\widehat{R}_{p,\epsilon,L}(\theta, \eta)$ is the infimum of a convex objective. 

13
We now turn to uniform convergence guarantees based on concentration of Wasserstein distances, which show that the empirical minimizer population distributions converges at rate for in (18) is at most the $W$ distance to its population counterpart at the rate solution to the population bound (5). First, we prove that the empirical plug-in (18) converges.

Our final bound follows from the fact that the Wasserstein distance between empirical and population distributions converges at rate $n^{-(p-1)/(d+1)}$. (See Appendix A.8 for proof.)
Theorem 2. Let Assumptions A1, A2 hold. If $p \in (1, 2]$, $d > 1$, and \( \text{diam}(\mathcal{X}) + \text{diam}(\mathcal{Y}) \leq R \), then for any $t > 0$, with probability at least $1 - c_1 \exp \left(-c_2 n \left( \frac{d+1}{p} + \ell^2 \right) \right)$

\[
\sup_{Q_0(z) \in \mathcal{P}_{\mathcal{X}, \mathcal{X}}} \mathbb{E}_{X \sim Q_0} \left[ \mathbb{E}[\ell(\hat{\theta}_{rob}^n, (X, Y)) \mid X] \right]
\leq \inf_{\eta \in [0, M]} \left\{ \frac{1}{\alpha_0} \left( \mathbb{E} \left[ \left( \mathbb{E}[\ell(\hat{\theta}_{rob}^n, (X, Y)) \mid X] - \eta \right)^p \right]^{1/p} + \eta \right) \right\}
\leq \inf_{\theta \in \Theta, \eta \in [0, M]} \left\{ \frac{1}{\alpha_0} \left( \mathbb{E} \left[ \left( \mathbb{E}[\ell(\theta; (X, Y)) \mid X] - \eta \right)^p \right]^{1/p} + \eta \right) \right\} + \frac{c^q - 1}{\alpha_0} + \frac{2Bt}{\alpha_0}
\]

where $c_1$ and $c_2$ are positive constants that depend on $M, d, p$.

Our concentration bounds exhibit tradeoffs for the worst case loss (2) under mixture covariate shifts; in Theorem 2, the power $p$ trades between approximation and estimation error. As $p \downarrow 1$, the value $R^*_p$ defined by expression (6) approaches the optimal value $\inf_{\theta \in \Theta} \sup_{Q_0(z) \in \mathcal{P}_{\mathcal{X}, \mathcal{X}}} \mathbb{E} \left[ \mathbb{E}[\ell(\theta; (X, Y)) \mid X] \right]$ so that approximation error goes down, but estimation becomes more difficult.

**Upper bounds at faster rates**  Theorem 2 shows the empirical estimator $\hat{\theta}_{rob}^n$ is approximately optimal with respect to the $L^p$-bound (5), but with a conservative $O(n^{-\frac{q-1}{q+1}})$-rate of convergence. On the other hand, we can still show that $\hat{\theta}_{rob}^n$ provides an upper bound to the worst-case loss under mixture covariate shifts (2) at the faster rate $O(n^{-\frac{3}{2}})$. This provides a conservative estimate on the performance under the worst-case subpopulation.

Proposition 3. Let Assumptions A1 and A2 hold. There exist numerical constants $c_1, c_2 < \infty$ such that the following holds. Let $\theta \in \Theta$, $\epsilon > 0$, and $p \in (1, 2]$. Then with probability at least $1 - 2\gamma$, uniformly over $\eta \in [0, M]$

\[
\mathbb{E}[\left( \mathbb{E}[\ell(\theta; (X, Y)) \mid X] - \eta \right)^p]^{1/p} \leq \max \left\{ \epsilon^{q-1}, (1 + \tau_n)^{q-1} \hat{R}_{p, \epsilon, L_{\gamma}}(\theta, \eta) + \frac{c_1 M^2}{\epsilon q-1} \sqrt{\frac{1}{n} \log \frac{1}{\gamma}} \right\}
\]

where $\tau_n := c_2 M^2 \epsilon^{-q} \sqrt{\frac{1}{n} \log \frac{1}{\gamma}}$ and $L_{\gamma}(\gamma) := L(1 + \tau_n(\gamma, \epsilon))^{-1/q}$.

See Section A.9 for the proof. We can similarly prove a uniform variant of Proposition 3 with respect to $\theta \in \Theta$, but we omit the details for brevity.

5  Risk bounds under confounding

Our assumption that $P_{Y \mid X}$ is fixed for each of our marginal populations over $X$ is analogous to the frequent assumptions in causal inference that there are no unmeasured confounders [42]. When this is true—for example, in machine learning tasks where the label $Y$ is a human annotation of the covariate $X$—minimizing worst-case loss over covariate shifts is natural, but the assumption may fail in other real-world problems. For example, in predicting crime recidivism $Y$ based on the type $X$ of crime committed and race $Z$ of the individual, unobserved confounders $C$ (e.g. income, location, education) likely vary with race. Consequently, we provide a parallel to our earlier development that provides a sensitivity analysis to unmeasured (hidden) confounding.
Let us formalize. Let $C \in \mathbb{C}$ be a random variable, and in analogy to (2) we define
\[ P_{\alpha_{0}, (X,C)} := \{ Q_{0} : \exists \alpha \geq \alpha_{0} \text{ and measure } Q_{1} \text{ on } (X \times C) \text{ s.t. } P_{(X,C)} = \alpha Q_{0} + (1 - \alpha) Q_{1} \} \] .

Our goal is then to minimize the worst-case loss under mixture covariate shifts
\[ \min_{\theta \in \Theta} \sup_{Q_{0} \in P_{\alpha_{0}, (X,C)}} \mathbb{E} \left[ \mathbb{E}[\ell(\theta; (X,Y)) \mid X,C] \right] . \tag{23} \]

Since the confounding variable $C$ is unobserved, we extend our robustness approach assuming a bounded effect of confounding, and derive conservative upper bounds on the worst-case loss.

We make the following boundedness definition and assumption on the effects of $C$.

**Definition 1.** The triple $(X,Y,C)$ is at most $\delta$-confounded for the loss $\ell$ if
\[ \| \mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \mathbb{E}[\ell(\theta; (X,Y)) \mid X,C] \|_{L_{\infty}(P)} \leq \delta . \]

**Assumption A3.** The triple $(X,Y,C)$ is at most $\delta$-confounded for the loss $\ell$.

Paralleling earlier developments, we derive a variational bound on the worst-case confounded risk (23).

**Confounded variational problem** Under confounding, a development completely parallel to Lemma 2.1 and Hölder’s inequality yields the dual
\[ \sup_{Q_{0} \in P_{\alpha_{0}, (X,C)}} \mathbb{E} \left[ \mathbb{E}[\ell(\theta; (X,Y)) \mid X,C] \right] \leq \inf_{\eta \in \mathbb{R}} \left\{ \frac{1}{\alpha_{0}} \left( \mathbb{E}[\ell(\theta; (X,Y)) \mid X,C - \eta]_{+}^{p} \right)^{\frac{1}{p}} + \eta \right\} \]
for all $p \geq 1$. Taking the variational form of the $L^{p}$-norm for $p \in (1, 2]$ yields
\[ \left( \mathbb{E}_{P_{X,C}} \left[ (\mathbb{E}[\ell(\theta; (X,Y)) \mid X,C - \eta]_{+})^{p} \right] \right)^{1/p} = \sup_{h} \left\{ \mathbb{E} \left[ h(X,C) \mathbb{E}[\ell(\theta; (X,Y)) \mid X,C - \eta] \right] \mid h \geq 0, \mathbb{E}[h^{q}(X,C)] \leq 1 \right\} . \tag{24} \]

Instead of the somewhat challenging variational problem over $h$, we reparameterize problem (24) as $h(X) + f(X,C)$, where $h$ is smooth and $f$ is a bounded residual term, which—by taking the worst case over bounded $f$—allows us to provide an upper bound on the worst-case problem (22). Let $H_{L_{p}}$ be the space of Hölder functions (15) and $F_{\delta,p}$ be the space of bounded functions
\[ F_{\delta,p} := \{ f : X \times C \rightarrow \mathbb{R} \text{ measurable, } \| f(X,C) \|_{L_{\infty}(P)} \leq \delta^{p-1} \} . \]

Then defining the analogue of the unconfounded variational objective (16)
\[ R_{p,\epsilon,\delta}(\theta, \eta) := \sup_{h+f \geq 0} \left\{ \mathbb{E} \left[ \frac{h(X) + f(X,C)}{\epsilon} \ell(\theta; (X,Y)) - \eta \right] \mid h \in H_{L_{p}}, f \in F_{\delta,p}, \| h + f \|_{L_{p}(P)} \leq \epsilon \right\} , \]
the risk $R_{p,\epsilon,\delta}$ is $\epsilon$-close to the variational objective (24). See Appendix A.10 for proof.

**Lemma 5.1.** Let Assumptions A1, A2, and A3 hold. Then, for any $\theta \in \Theta$ and $\eta \in \mathbb{R}$, we have
\[ \left( \mathbb{E}_{P_{X,C}} \left[ (\mathbb{E}[\ell(\theta; (X,Y)) \mid X,C - \eta]_{+})^{p} \right] \right)^{1/p} = \inf_{\epsilon \geq 0} \left\{ R_{p,\epsilon,\delta}(\theta, \eta) \vee \epsilon^{q-1} \right\} \]
and for any $\epsilon > 0$, $R_{p,\epsilon,\delta}(\theta, \eta) \vee \epsilon^{q-1} - \epsilon^{q-1} \leq \left( \mathbb{E}_{P_{X,C}} \left[ (\mathbb{E}[\ell(\theta; (X,Y)) \mid X,C - \eta]_{+})^{p} \right] \right)^{1/p} . \tag{25} \]
Confounded estimator. By replacing \( \mathcal{H}_{L,p} \) with the empirical version \( \hat{\mathcal{H}}_{L,p} \) (the set of Hölder functions on the empirical distribution) and \( \mathcal{F}_{\delta,p} \) with the empirical counterpart \( \mathcal{F}_{\delta,p,n} := \{ f \in \mathbb{R}^n \mid \max_{i \leq n} |f(X_i, C_i)| \leq \delta^{p-1} \} \), we get the obvious empirical plug-in \( \hat{R}_{p,\epsilon,L,\delta}(\theta, \eta) \) of the population quantity \( R_{p,\epsilon,L,\delta}(\theta, \eta) \). In this case, a duality argument provides the following analogue of Lemma 4.2, which follows because the class \( \mathcal{F}_{\delta,p,n} \) simply corresponds to an \( \| \cdot \|_\infty \) constraint on a vector in \( \mathbb{R}^n \).

Lemma 5.2. For any \( \epsilon > 0 \) and \( (X_1, Y_1), \ldots, (X_n, Y_n) \), we have

\[
\hat{R}_{p,\epsilon,L,\delta}(\theta, \eta) = \inf_{B \in \mathbb{R}^\times_n^+} \left\{ \left( \frac{p-1}{n} \sum_{i=1}^n \left( \ell(\theta; (X_i, Y_i)) - \frac{1}{n} \sum_{j=1}^n (B_{ij} - B_{ji}) - \eta \right)_+^p \right)^{1/p} + \frac{L^{p-1}}{en^2} \sum_{i,j=1}^n \|X_i - X_j\|_B B_{ij} + \frac{2L^{p-1}}{en^2} \sum_{i,j=1}^n |B_{ij}| \right\}.
\]

See Appendix A.12 for the proof. The lemma is satisfying in that it smoothly interpolates, based on the degree of confounding \( \delta \), between marginal distributionally robust optimization (when \( \delta = 0 \), as in Lemma 4.2) and the fully robust joint DRO setting as \( \delta \uparrow \infty \), which results in the choice \( B = 0 \).

Upper bound on confounded objective. In analogy with Proposition 3, the empirical plug-in \( \hat{R}_{p,\epsilon,L,\delta}(\theta, \eta) \) is an upper bound on the population objective under confounding. Although our estimator only provides an upper bound, it provides practical procedures for controlling the worst-case loss (22) when Assumption A3 holds, as we observe in the next section. The next proposition, whose proof we provide in Section A.11, shows the upper bound.

Proposition 4. Let Assumptions A1, A2, and A3 hold. There exist universal constants \( c_1, c_2 < \infty \) such that the following holds. Let \( \theta \in \Theta, \epsilon > 0 \), and \( p \in (1,2] \). Then with probability at least \( 1 - 2\gamma \), uniformly in \( \eta \in [0,M] \)

\[
\left( \mathbb{E}_{P_X, C} \left( \mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta \right)_+^q \right)^{1/p} \leq \max \left\{ \epsilon^{q-1}, \left( 1 + \tau_n(\gamma, \epsilon) \right)^{1/q} \hat{R}_{p,\epsilon,L,\delta_n(\gamma)}(\theta, \eta) + \frac{c_1M^2}{\epsilon^{q-1}} \sqrt{\frac{\log \frac{1}{\gamma}}{n}} \right\}
\]

where \( \tau_n(\gamma, \epsilon) := \frac{c_2M^2}{\epsilon^{q-1}} \sqrt{\frac{1}{n} \log \frac{1}{\gamma}} \), \( \delta_n(\gamma) := \delta(1 + \tau_n(\gamma, \epsilon))^{-1/q} \), and \( L_n(\gamma) := L(1 + \tau_n(\gamma, \epsilon))^{-1/q} \).

6 Experiments

We now present empirical investigations of the procedure (20), focusing on two main aspects of our results. First, our theoretical results exhibit nonparametric rates of convergence, so it is important to understand whether these upper bounds on convergence rates govern empirical performance and the extent to which the procedure is effective. Second, on examples with high conditional risk \( \mathbb{E}[\ell(\theta; (X, Y)) \mid X] \), we expect our procedure to improve performance on minority groups and hard subpopulations when compared against joint DRO and empirical risk minimization (ERM).

To investigate both of these issues, we begin by studying simulated data (Section 6.1) so that we can evaluate true convergence precisely. We see that in moderately high dimensions,
our procedure outperforms both ERM and joint DRO on worst-off subpopulations; we perform a parallel simulation study in Section 6.2 for the confounded case (minimizing $\hat{R}_{p,\epsilon,L,\delta}(\theta, \eta)$ of Lemma 5.2). After our simulation study, we continue to assess efficacy of our procedure on real data, using our method to predict semantic similarity (Section 6.3), wine quality (Section 6.4) and crime recidivism (Section 6.5). In all of these experiments, our results are consistent with our expectation that our procedure (20) typically improves performance over unseen subpopulations.

Hyperparameter choice is important in our procedures. We must choose a Lipschitz constant $L$, worst-case group size $\alpha_0$, risk level $\epsilon$, and moment parameter $p$. In our experiments, we see that cross-validation is attractive and effective. We treat the value $L/\epsilon$ as a single hyperparameter to estimate via a hold-out set or, in effort to demonstrate sensitivity to the parameter, plot results across a range of $L/\epsilon$. As the objective (20) is convex standard methods apply; we use (sub)gradient descent to optimize the problem parameters over $\theta, \eta, B$. Each experiment, we compare our marginal DRO method against two baselines: empirical risk minimization (ERM) and joint DRO (7). ERM minimizes the empirical risk $\min_{\theta \in \Theta} \mathbb{E}_{P_n} [\ell(\theta; (X,Y))]$, and provides very weak guarantees on subpopulation performance. The joint DRO formulation (7) is the only existing method that provides an upper bound to the worst-case risk. We evaluate empirical plug-ins of the dual formulation ($p \geq 1$)

$$\inf_{\eta \in \mathbb{R}} \left\{ \frac{1}{\alpha_0} \mathbb{E}[\ell(\theta; (X,Y)) - \eta]^p_+^{1/p} + \eta \right\}, \quad (26)$$

which is the joint DRO counterpart of our marginal DRO procedure (20) for the same value of $p$. Joint DRO formulations over other uncertainty sets (e.g. Wasserstein balls [45]) do not provide guarantees on subpopulation performance as they protect against different distributional shifts, including adversarial attacks [69].

### 6.1 Simulation study: the unconfounded case

Our first simulation study focuses on the unconfounded procedure (20), where the data follows the distribution (14), and the known ground truth allows us to carefully measure the effects of the problem parameters ($n, d, \alpha$) and sensitivity to the smoothness assumption $L$. We focus on the regression example from Sec. 3.2 with loss $\ell(\theta; x, y) = |\theta^T x - y|$, so
the procedure (20) is an empirical approximation to minimizing the worst-case objective
\[ \sup_{Q_0 \in P_{\alpha_0}, X \sim Q_0} \mathbb{E}_{X \sim Q_0} \left[ \mathbb{E}[|\theta^T X - Y| \mid X] \right]. \]

The simulation distribution (14) captures several aspects of loss minimization in the presence of heterogeneous subpopulations. The subpopulations \( X_1 \geq 0 \) and \( X_1 < 0 \) constitute a majority and minority group, and minimizing the risk of the majority group comes at the expense of risk for the minority group. The two subpopulations also define an oracle model that minimizes the maximum loss over the two groups. As the uniform distribution exhibits the slowest convergence of empirical distributions for Wasserstein distance [29]—and as Wasserstein convergence underpins our \( n^{-1/d} \) rates in Lemma 4.3—we use the uniform distribution over covariates \( X \). We train all DRO models with worst-case group size \( \alpha_0 = 0.3 \) and choose the estimated Lipschitz parameter \( L/\epsilon \) by cross-validation on a replicate-based estimate of the worst-case loss (27) (below) using a held-out set of 1000 examples and 100 repeated measurements of \( Y \). We do not regularize as \( d \ll n \).

**Effect of the \( p \)-norm bound** We evaluate the difference in model quality as a function of \( p \), which controls the tightness of the \( p \)-norm upper bound. Our convergence guarantees in Theorem 2 are looser for \( p \) near 1, though such values achieve smaller asymptotic bias to the true sub-population risk, while values of \( p \) near 2 suggest a more favorable sample size dependence in the theorem.

In Figure 4, we plot the results of experiments for each suggested procedure, where the horizontal axes index sample size and the vertical axes an empirical approximation to the worst-case loss
\[ R_{\alpha_0}(\theta) := \sup_{Q_0 \in P_{\alpha_0}, X \sim Q_0} \mathbb{E}_{X \sim Q_0} \left[ |\theta^T X - Y| \mid X \right] \] (27)
over the worst 5% of the population (test-time \( \alpha_0 = 0.05 \)); the plots index dimensions \( d = 1, 10, 50 \). We evaluate a worst-case error smaller than the true mixture proportion to measure our procedure’s robustness within the minority subgroup. The plots suggest that the choice \( p = 2 \) (Marginal DRO) outperforms \( p = 1 \) (Linf Marginal DRO), and performance generally seems to degrade as \( p \downarrow 1 \). We consequently focus on the \( p = 2 \) case for the remainder of this section.

**Sample size and dimension dependence** We use the same experiment to also examine the pessimistic \( O(n^{-1/d}) \) convergence rate of our estimator (20); this is substantially worse than that for ERM and joint DRO (7), both of which have convergence rates scaling at worst as \( 1/\sqrt{n} \) [25]. In low dimensions (\( d = 1 \) to \( d = 10 \)) convergence to the optimal function value—which we can compute exactly—is relatively fast, and marginal DRO becomes substantially better with as few as 500 samples (Figure 4). In higher dimensions (\( d = 50 \)), marginal DRO convergence is slower, but it is only worse than the joint DRO solution when \( n = d = 100 \). At large sample sizes \( n > 1000 \), marginal DRO begins to strictly outperform the two baselines as measured by the worst-case 5% loss (27).

**Sensitivity to robustness level** We rarely know the precise minority proportion \( \alpha_{\text{true}} \), so that in practice one usually provides a postulated lower bound \( \alpha_0 \); we investigate sensitivity to its specification. We fix the data generating distribution \( \alpha_{\text{true}} = 0.15 \) and train DRO models with \( \alpha_0 = 0.3 \), while evaluating them using varying test-time worst case group size \( \alpha_0 \) in Eq. 27. We show the results of varying the test-time worst-case group size in Figure 5a. Marginal DRO
obtains a loss within 1.2 times the oracle model regardless of the test-time worst-case group size, while both ERM and joint DRO incur substantially higher losses on the tails.

**Sensitivity to Lipschitz constant** Finally, the empirical bound (22) requires an estimate of the Lipschitz constant of the conditional risk. We vary the estimate \( L/\epsilon \) in Figure 5, showing that the marginal robustness formulation has some sensitivity to the parameter, though there is a range of several orders of magnitude through which it outperforms the joint DRO procedures. The behavior that it exhibits is expected, however: the choice \( L = 0 \) reduces the marginal DRO procedure to ERM in the bound (22), while the choice \( L = \infty \) results in the joint DRO approach.

### 6.2 Simulation study: the confounded case

To complement our results in the unconfounded case, we extend our simulation experiment by adding unmeasured confounders, investigating the risk upper bounds of Lemma 5.2 and Proposition 4. We generate data nearly identically to model (14), introducing a confounder \( C \):

\[
Z \sim \text{Bern}(0.15), \quad X_1 = (1 - 2Z) \cdot \text{Uni}([0, 1]), \quad X_2, \ldots, X_d \text{ iid } \text{Uni}([0, 1])
\]

\[
Y = |X_1| + 1 \{X_1 \geq 0\} \cdot C, \quad C \sim \text{Uni}([-1, 0.5, 0, 0.5, 1]).
\]

To evaluate a putative parameter \( \theta \), we approximate the worst-case risk

\[
R_{\alpha_0}(\theta, c) := \sup_{Q_0 \in \mathcal{P}_{\alpha_0}, X} \mathbb{E}_{X \sim Q_0} \left[ \|\theta^\top X - Y\| \mid X, C = c \right] . \tag{28}
\]

via the plug-in replicate estimate in Proposition 1, using a sample of size \( n = 2000 \), \( m = 10 \) replicates, and test-time worst-case group size \( \alpha_0 = 0.05 \). The gap in the conditional risk from \( \delta \)-confounding (i.e. \( \mathbb{E}[\ell(\theta; (X, Y)) \mid X] - \mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] \)) in Definition 1 varies monotonically with \(|c|\). To construct estimates \( \hat{\theta} \), we minimize the dual representation of the empirical confounded risk \( \hat{R}_{p,\epsilon,L,\delta}(\theta, \eta) \) in Lemma 5.2, varying the postulated level \( \delta \) of confounding while fixing the training time worst-case group size \( \alpha_0 = 0.1 \). We present results in Fig. 6, which compares the worst-case loss (28) as \( c \) varies (vertical axis) for different methods to select \( \hat{\theta} \) (horizontal axis). We compare marginal DRO (20) (which assumes no confounding \( \delta = 0 \)), the procedure minimizing empirical confounded risk \( \hat{R}_{p,\epsilon,L,\delta}(\theta, \eta) \) as we vary \( \delta \), and the
joint DRO procedure (26) (full confounding) with \( p = 1, 2, \) and empirical risk minimization (ERM). The figure shows the (roughly) expected result that the confounding-aware risks achieve lower worst-case loss (28) as the postulated confounding level \( \delta \) increases with the actual amount of confounding, with joint DRO and ERM achieving worse performance.

Figure 6. Worst-case losses (Eq. 28) incurred by each model (column) when varying the influence of the unobserved confounder \( c \) (rows). Adjusting marginal DRO to account for the level of confounding (Lemma 5.2) by varying \( \delta \) improves worst-case loss.

6.3 Semantic similarity prediction

We now present the first of our real-world evaluations of the marginal DRO procedure (20), focusing on a setting where we have multiple measured outcome labels \( Y \) for each covariate \( X \), so it is possible to accurately estimate the worst-case loss over covariate shifts. We consider the WS353 lexical semantic similarity prediction dataset [2] where the features are pairs of words, and labels are a set of 13 human annotations rating the word similarity on a 0–10 scale. In this task, our goal is to use noisy human annotations of word similarities to learn a robust model that accurately predicts word similarities over a large set of word pairs.

We represent each word pair as the difference \((x_1 - x_2)\) of the word vectors \(x_1\) and \(x_2\) associated to each word in GloVe [57] and cast this as a standard metric learning task of predicting a scalar similarity \( Y \) with a word-pair vector \( X \) via the quadratic model \( x \mapsto x^\top \theta_1 x + \theta_2 \), \( \theta_1 \in \mathbb{R}^{d \times d} \), \( \theta_2 \in \mathbb{R} \). We use the absolute deviation loss \( |y - x^\top \theta_1 x + \theta_2| \). The training set consists of 1989 individual annotations of word similarities (ignoring any replicate structure), and we fit the marginal DRO model with \( p = 2 \), joint DRO models (26) with \( p = 1, 2 \), and an ERM model. All methods use the same ridge regularizer tuned for the ERM model. We train all DRO procedures using \( \alpha_0 = 0.3 \) and tune the Lipschitz constant via a held out set using the empirical estimate to the worst-case loss based on replicate annotations (as in Proposition 1).

To evaluate each model \( \theta = (\theta_1, \theta_2) \), we take an empirical approximation to the worst-case loss over the word pairs with respect to the averaged human annotation

\[
R_{\alpha_0}(\theta) := \sup_{Q_0 \in \mathcal{P}_{\alpha_0}} \mathbb{E}_{X \sim Q_0} \left[ |X^\top \theta_1 X + \theta_2 - \mathbb{E}[Y | X]| \right].
\]
This is a worst-case version of the standard word similarity evaluation [57], where we also use averaged replicate human annotations as the ground truth \( \mathbb{E}[Y \mid X] \) in our evaluations, and consider test-time worst-case group sizes \( \alpha_0 \) ranging from 0.01 to 1.0.

Figure 7. Semantic similarity prediction task, with worst-case prediction error \( R_{\alpha_0}(\theta) \) (Eq. 29) over subgroups (y-axis) evaluated over varying test time worst-case group sizes \( \alpha_0 \) (x-axis).

All methods achieve low average error over the entire dataset, but ERM, joint DRO and marginal DRO exhibit disparate behaviors for small subgroups. ERM incurs large errors at \( \sim 5\% \) of the test set, resulting in near random prediction. Applying the joint DRO estimator reduces error by nearly half and marginal DRO reduces this even further (Figure 7).

6.4 Distribution shifts in wine quality prediction

Next, we show that marginal DRO (\( p = 2 \)) can yield improvements outside of the worst-case subgroup assumptions we have studied thus far. The UCI wine dataset [23] is a regression task with 4898 examples and 12 features, where each example is a wine with measured chemical properties and the label \( y \in \mathbb{R} \) is a subjective quality assessment; the data naturally splits into subgroups of white and red wines. We consider a distribution shift problem where the regression model is trained on red wines but tested on (subsets of) white wines. Unlike the earlier examples, the test set here does not correspond to subpopulations of the training distribution, and the chemical features of red wine are likely distinct from those for white wines, violating naive covariate shift assumptions.

We minimize the absolute deviation loss \( \ell(\theta; x, y) = |\theta^\top x - y| \) for linear predictions, tuning baseline parameters (e.g. ridge regularization) on a held-out set that is i.i.d. with the training distribution. Our training distribution is 1500 samples of red wines and the test distribution is all white wines. We evaluate models via their loss over worst-case subgroups of the white wines, though in distinction from earlier experiments, we have no replicate labels. Thus we measure the joint DRO loss (7), i.e.

\[
R_{\alpha_0, \text{joint}}(\theta) := \sup_{Q_0 \in \mathcal{P}_{\alpha_0}(X_w,Y_w)} \mathbb{E}_{X_w,Y_w \sim Q_0} \left[ |\theta^\top X_w - Y_w| \right],
\]

so that the worst-case loss \( R_{\alpha_0, \text{joint}}(\theta) \) measures the subgroup losses under the white wine distribution.

Figure 8 shows the worst-case loss \( R_{\alpha_0, \text{joint}}(\theta) \) over the test set as a function of \( \alpha_0 \). Here, Marginal DRO with Lipschitz constants \( L/\epsilon \) varying over 0.1 to 300 and \( \alpha_0 = 0.15 \) provides improvements over both joint DRO and ERM baselines across the entire range of test-time \( \alpha_0 \).
Worst-case Loss $R_{\alpha_0,\text{joint}}(\theta)$

**Figure 8.** Marginal DRO improves worst-case loss $R_{\alpha_0,\text{joint}}(\theta)$ for the wine quality prediction task under a real world red to white wine distribution shift. The gain holds on a wide range of Lipschitz constants from $L/\epsilon = 0.1$ (left) to 300 (right).

![Graph showing the improvement in worst-case loss](image)

**Table 1.** Worst-case error of recidivism prediction models across demographic subgroups. The ERM row shows baseline worst-case error; subsequent rows show error differences from baseline (negatives indicate lower error).

| Method               | Old   | Young | Black | Hispanic | Other race | Female | Misdemeanor |
|----------------------|-------|-------|-------|----------|------------|--------|-------------|
| ERM                  | 37.7 ± 0.8 | 44.6 ± 1.0 | 37.7 ± 0.8 | 37.9 ± 1.1 | 37.5 ± 0.9 | 37.6 ± 0.8 |
| Joint ($p = 2$) - ERM| 10.0 ± 2.0 | 4.0 ± 1.7 | 9.7 ± 1.7 | 9.6 ± 1.8 | 10.9 ± 2.3 | 9.2 ± 1.8 | 9.0 ± 1.6 |
| Joint ($p = 1$) - ERM| 5.8 ± 1.7 | 1.2 ± 1.7 | 5.2 ± 1.5 | 7.4 ± 1.9 | 6.6 ± 2.1 | 5.9 ± 1.7 | 5.1 ± 1.5 |
| Marginal L=0.01 - ERM| -0.7 ± 0.7 | 1.4 ± 1.1 | -1.0 ± 0.7 | -1.7 ± 0.9 | -2.4 ± 1.1 | -1.5 ± 0.8 | -1.5 ± 0.7 |
| Marginal L=0.001 - ERM| -1.1 ± 0.7 | 0.4 ± 1.1 | -1.4 ± 0.7 | -2.1 ± 0.9 | -2.6 ± 1.1 | -1.9 ± 0.8 | -1.8 ± 0.7 |

Marginal DRO improves losses both for the pure distribution shift from red to white wines (test-time group size $\alpha = 1.0$) as well as for the more pessimistic groups with small test-time proportion $\alpha_0$. Distribution shift from red to white wines appears difficult to capture for the pessimistic joint DRO methods.

### 6.5 Recidivism prediction

Finally, we show that marginal DRO ($p = 2$) can control the loss over a minority group on a recidivism prediction task. The COMPAS recidivism dataset [22] is a classification task where examples are individual convicts, features consist of binary demographic labels (such as African American or not) and description of their crimes, and the label is whether they commit another crime after release (recidivism). We use the fairML toolkit version of this dataset [1]. Classification algorithms for recidivism have systematically discriminated against minority groups, and this dataset illustrates such discrimination [6]. We consider this dataset from the perspective of achieving uniform performance across various groups. There are 10 binary variables in data, each indicating a potential split of the data into minority and majority group (e.g. young vs. not young, or Black vs. non-Black), of which 7 have enough ($n > 10$) observations in each split to make reasonable error estimates. We train a model over the full population (using all the features), and for each of the 7 demographic indicator variables and evaluate the held-out 0-1 loss over both the associated majority group and minority group.

Our goal is to ensure that the classification accuracy remains high without explicitly splitting the data on particular demographic labels (though we include them in our models as they have predictive power). We use the binary logistic loss with linear models and a 70/30 train/test split. We set $\alpha_0 = 0.4$ for all DRO methods, and apply ridge regularization to all models with regularization parameter tuned for the ERM model.
Table 1 presents the 0-1 loss on the seven demographic splits over 100 random train/test splits. For each attribute (table column) we split the test set into examples for which the attribute is true and false and report the average 0-1 loss on the worst of the two groups. The first row gives the average worst-case error and associated 95% standard error for the ERM model. For the DRO based models (remaining rows), we report the average differences with respect to the baseline ERM model and standard error intervals. Unlike our earlier regression tasks, joint DRO (both $L_2$ and $L_1$) performs worse than ERM on almost all demographic splits. On the other hand, we find that marginal DRO with the appropriate smoothness constant $L \in \{10^{-2}, 10^{-3}\}$ reduces classification errors between 1–2% on the worst-case group across various demographics, with the largest error reduction of 3% occurring in the young vs. old demographic split.

**References**

[1] J. A. Adebayo. Fairml : Toolbox for diagnosing bias in predictive modeling. Master’s thesis, Massachusetts Institute of Technology, 2016.

[2] E. Agirre, E. Alfonseca, K. Hall, J. Kravalova, M. Pasca, and A. Soroa. A study on similarity and relatedness using distributional and wordnet-based approaches. In Proceedings of the North American Chapter of the Association for Computational Linguistics (NAACL-HLT), 2009.

[3] D. Amodei, S. Ananthanarayanan, R. Anubhai, J. Bai, E. Battenberg, C. Case, J. Casper, B. Catanzaro, Q. Cheng, and G. Chen. Deep speech 2: end-to-end speech recognition in English and Mandarin. In Proceedings of the 33rd International Conference on Machine Learning, pages 173–182, 2016.

[4] N. Aronszajn. Theory of reproducing kernels. Transactions of the American Mathematical Society, 68(3):337–404, May 1950.

[5] A. Asuncion and D. J. Newman. UCI machine learning repository, 2007. URL http://www.ics.uci.edu/~mlearn/MLRepository.html.

[6] S. Barocas and A. D. Selbst. Big data’s disparate impact. 104 California Law Review, 3:671–732, 2016.

[7] P. L. Bartlett and S. Mendelson. Rademacher and Gaussian complexities: Risk bounds and structural results. Journal of Machine Learning Research, 3:463–482, 2002.

[8] S. Ben-David, J. Blitzer, K. Crammer, and F. Pereira. Analysis of representations for domain adaptation. In Advances in Neural Information Processing Systems 20, pages 137–144, 2007.

[9] A. Ben-Tal, L. E. Ghaoui, and A. Nemirovski. Robust Optimization. Princeton University Press, 2009.

[10] A. Ben-Tal, D. den Hertog, A. D. Waegenaere, B. Melenberg, and G. Rennen. Robust solutions of optimization problems affected by uncertain probabilities. Management Science, 59(2):341–357, 2013.

[11] A. Berlinet and C. Thomas-Agnan. Reproducing Kernel Hilbert Spaces in Probability and Statistics. Kluwer Academic Publishers, 2004.
[12] D. Bertsimas, V. Gupta, and N. Kallus. Data-driven robust optimization. *Mathematical Programming, Series A*, 167(2):235–292, 2018. URL http://arxiv.org/abs/1401.0212.

[13] S. Bickel, M. Brückner, and T. Scheffer. Discriminative learning for differing training and test distributions. In *Proceedings of the 24th International Conference on Machine Learning*, 2007.

[14] J. Blanchet, Y. Kang, F. Zhang, and K. Murthy. Data-driven optimal transport cost selection for distributionally robust optimization. *arXiv:1705.07152 [stat.ML]*, 2017.

[15] J. Blanchet, Y. Kang, and K. Murthy. Robust Wasserstein profile inference and applications to machine learning. *Journal of Applied Probability*, 56(3):830–857, 2019.

[16] S. L. Blodgett, L. Green, and B. O’Connor. Demographic dialectal variation in social media: A case study of African-American English. In *Proceedings of Empirical Methods for Natural Language Processing*, pages 1119–1130, 2016.

[17] S. Boucheron, G. Lugosi, and P. Massart. *Concentration Inequalities: a Nonasymptotic Theory of Independence*. Oxford University Press, 2013.

[18] P. Bühlmann and N. Meinshausen. Magging: maximin aggregation for inhomogeneous large-scale data. *Proceedings of the IEEE*, 104(1):126–135, 2016.

[19] C. F. P. Bureau. Using publicly available information to proxy for unidentified race and ethnicity: a methodology and assessment, 2014. Available at https://www.consumerfinance.gov/data-research/research-reports/usingpublicly-available-information-to-proxy-for-unidentified-race-and-ethnicity/.

[20] D. Cer, M. Diab, E. Agirre, I. Lopez-Gazpio, and L. Specia. Semeval-2017 task 1: Semantic textual similarity multilingual and cross-lingual focused evaluation. In *Proceedings of the 10th International Workshop on Semantic Evaluation (SemEval 2017)*, 2017.

[21] J. Chen, N. Kallus, X. Mao, G. Svacha, and M. Udell. Fairness under unawareness: Assessing disparity when protected class is unobserved. In *Proceedings of the Conference on Fairness, Accountability, and Transparency*, pages 339–348. ACM, 2019.

[22] A. Chouldechova. A study of bias in recidivism prediction instruments. *Big Data*, pages 153–163, 2017.

[23] P. Cortez, A. Cerdeira, F. Almeida, T. Matos, and J. Reis. Modeling wine preferences by data mining from physicochemical properties. *Decision Support Systems*, 47(4):547–553, 2009.

[24] N. Cristianini and J. Shawe-Taylor. *Kernel Methods for Pattern Analysis*. Cambridge University Press, 2004.

[25] J. C. Duchi and H. Namkoong. Learning models with uniform performance via distributionally robust optimization. *arXiv:1810.08750 [stat.ML]*, 2018.

[26] J. C. Duchi, P. W. Glynn, and H. Namkoong. Statistics of robust optimization: A generalized empirical likelihood approach. *arXiv:1610.03425 [stat.ML]*, 2016.

[27] C. Dwork, M. Hardt, T. Pitassi, O. Reingold, and R. Zemel. Fairness through awareness. In *Innovations in Theoretical Computer Science (ITCS)*, pages 214–226, 2012.
[28] P. M. Esfahani and D. Kuhn. Data-driven distributionally robust optimization using the Wasserstein metric: Performance guarantees and tractable reformulations. *Mathematical Programming, Series A*, 171(1–2):115–166, 2018.

[29] N. Fournier and A. Guillin. On the rate of convergence in Wasserstein distance of the empirical measure. *Probability Theory and Related Fields*, 162(3-4):707–738, 2015.

[30] R. Gao and A. J. Kleywegt. Distributionally robust stochastic optimization with Wasserstein distance. *arXiv:1604.02199 [math.OC]*, 2016.

[31] R. Gao, X. Chen, and A. Kleywegt. Wasserstein distributional robustness and regularization in statistical learning. *arXiv:1712.06050 [cs.LG]*, 2017.

[32] M. Gong, K. Zhang, T. Liu, D. Tao, C. Glymour, and B. Schölkopf. Domain adaptation with conditional transferable components. In *Proceedings of the 33rd International Conference on Machine Learning*, pages 2839–2848, 2016.

[33] A. Gretton, A. Smola, J. Huang, M. Schmittfull, K. Borgwardt, and B. Schölkopf. Covariate shift by kernel mean matching. In J. Q. nonero Candela, M. Sugiyama, A. Schwaighofer, and N. D. Lawrence, editors, *Dataset Shift in Machine Learning*, chapter 8, pages 131–160. MIT Press, 2009.

[34] P. J. Grother, G. W. Quinn, and P. J. Phillips. Report on the evaluation of 2d still-image face recognition algorithms. *NIST Interagency/Internal Reports (NISTIR)*, 7709, 2010.

[35] M. Hardt, E. Price, and N. Srebro. Equality of opportunity in supervised learning. In *Advances in Neural Information Processing Systems 29*, 2016.

[36] T. Hashimoto, M. Srivastava, H. Namkoong, and P. Liang. Fairness without demographics in repeated loss minimization. In *Proceedings of the 35th International Conference on Machine Learning*, 2018.

[37] Ú. Hébert-Johnson, M. P. Kim, O. Reingold, and G. N. Rothblum. Calibration for the (computationally-identifiable) masses. *arXiv:1711.08513 [cs.LG]*, 2017.

[38] C. Heinze-Deml and N. Meinshausen. Grouping-by-id: Guarding against adversarial domain shifts, 2017.

[39] D. Hovy and A. Søgaard. Tagging performance correlates with author age. In *Proceedings of the 53rd Annual Meeting of the Association for Computational Linguistics (Short Papers)*, volume 2, pages 483–488, 2015.

[40] W. Hu, G. Niu, I. Sato, and M. Sugiyama. Does distributionally robust supervised learning give robust classifiers? In *Proceedings of the 35th International Conference on Machine Learning*, 2018.

[41] J. Huang, A. Gretton, K. M. Borgwardt, B. Schölkopf, and A. J. Smola. Correcting sample selection bias by unlabeled data. In *Advances in Neural Information Processing Systems 20*, pages 601–608, 2007.

[42] G. Imbens and D. Rubin. *Causal Inference for Statistics, Social, and Biomedical Sciences*. Cambridge University Press, 2015.

[43] M. Kearns, S. Neel, A. Roth, and Z. S. Wu. Preventing fairness gerrymandering: Auditing and learning for subgroup fairness. *arXiv:1711.05144 [cs.LG]*, 2018.
[44] N. Kilbertus, M. R. Carulla, G. Parascandolo, M. Hardt, D. Janzing, and B. Schölkopf. Avoiding discrimination through causal reasoning. In Advances in Neural Information Processing Systems 30, 2017.

[45] D. Kuhn, P. M. Esfahani, V. A. Nguyen, and S. Shafieezadeh-Abadeh. Wasserstein distributionally robust optimization: Theory and applications in machine learning. In Operations Research & Management Science in the Age of Analytics, pages 130–166. INFORMS, 2019.

[46] H. Lam and H. Qian. Combating conservativeness in data-driven optimization under uncertainty: A solution path approach. arXiv:1909.06477 [math.OC], 2019.

[47] H. Lam and E. Zhou. Quantifying input uncertainty in stochastic optimization. In Proceedings of the 2015 Winter Simulation Conference. IEEE, 2015.

[48] J. Lee and M. Raginsky. Minimax statistical learning and domain adaptation with Wasserstein distances. arXiv:1705.07815 [cs.LG], 2017.

[49] J. Lei. Convergence and concentration of empirical measures under Wasserstein distance in unbounded functional spaces. arXiv:1804.10556 [math.ST], 2018.

[50] A. Liu and B. Ziebart. Robust classification under sample selection bias. In Advances in Neural Information Processing Systems 27, pages 37–45, 2014.

[51] A. Liu and B. Ziebart. Robust covariate shift prediction with general losses and feature views. arXiv:1712.10043 [cs.LG], 2017. URL https://arxiv.org/abs/1712.10043.

[52] M. Marcus, B. Santorini, and M. Marcinkiewicz. Building a large annotated corpus of English: the Penn Treebank. Computational Linguistics, 19:313–330, 1994.

[53] N. Meinshausen and P. Bühlmann. Maximin effects in inhomogeneous large-scale data. The Annals of Statistics, 43(4):1801–1830, 2015.

[54] G. J. Minty. On the extension of lipschitz, lipschitz-hölder continuous, and monotone functions. Bulletin of the American Mathematical Society, 76(2):334–339, 1970.

[55] T. Miyato, S.-i. Maeda, M. Koyama, K. Nakae, and S. Ishii. Distributional smoothing with virtual adversarial training. arXiv:1507.00677 [stat.ML], 2015.

[56] H. Namkoong and J. C. Duchi. Variance regularization with convex objectives. In Advances in Neural Information Processing Systems 30, 2017.

[57] J. Pennington, R. Socher, and C. D. Manning. Glove: Global vectors for word representation. In Proceedings of Empirical Methods for Natural Language Processing, 2014.

[58] J. Peters, P. Bühlmann, and N. Meinshausen. Causal inference by using invariant prediction: identification and confidence intervals. Journal of the Royal Statistical Society, Series B, 78(5):947–1012, 2016.

[59] P. Rajpurkar, R. Jia, and P. Liang. Know what you don’t know: Unanswerable questions for squad. In Proceedings of the Annual Meeting of the Association for Computational Linguistics, 2018.

[60] R. T. Rockafellar and S. Uryasev. Optimization of conditional value-at-risk. Journal of Risk, 2:21–42, 2000.
[61] D. Rothenhäusler, N. Meinshausen, and P. Bühlmann. Confidence intervals for maximin effects in inhomogeneous large-scale data. In *Statistical Analysis for High-Dimensional Data*, pages 255–277. Springer, 2016.

[62] D. Rothenhäusler, P. Bühlmann, N. Meinshausen, and J. Peters. Anchor regression: heterogeneous data meets causality. *arXiv:1801.06229 [stat.ME]*, 2018.

[63] P. Sapiezynski, V. Kassarnig, and C. Wilson. Academic performance prediction in a gender-imbalanced environment. In *Proceedings of the Eleventh ACM Conference on Recommender Systems*, volume 1, pages 48–51, 2017.

[64] S. Shafieezadeh-Abadeh, P. M. Esfahani, and D. Kuhn. Distributionally robust logistic regression. In *Advances in Neural Information Processing Systems 28*, pages 1576–1584, 2015.

[65] S. Shankar, Y. Halpern, E. Breck, J. Atwood, J. Wilson, and D. Sculley. No classification without representation: Assessing geodiversity issues in open data sets for the developing world. *arXiv:1711.08536 [stat.ML]*, 2017.

[66] A. Shapiro. Distributionally robust stochastic programming. *SIAM Journal on Optimization*, 27(4):2258–2275, 2017.

[67] A. Shapiro, D. Dentcheva, and A. Ruszczyński. *Lectures on Stochastic Programming: Modeling and Theory*. SIAM and Mathematical Programming Society, 2009.

[68] H. Shimodaira. Improving predictive inference under covariate shift by weighting the log-likelihood function. *Journal of Statistical Planning and Inference*, 90(2):227–244, 2000.

[69] A. Sinha, H. Namkoong, and J. Duchi. Certifying some distributional robustness with principled adversarial training. In *Proceedings of the Sixth International Conference on Learning Representations*, 2018.

[70] M. Staib and S. Jegelka. Distributionally robust optimization and generalization in kernel methods. In *Advances in Neural Information Processing Systems 32*, pages 9134–9144, 2019. URL *https://arxiv.org/abs/1905.10943*.

[71] A. J. Storkey and M. Sugiyama. Mixture regression for covariate shift. In *Advances in Neural Information Processing Systems 19*, pages 1337–1344, 2006.

[72] M. Sugiyama, M. Krauledat, and K.-R. Müller. Covariate shift adaptation by importance weighted cross validation. *Journal of Machine Learning Research*, 8:985–1005, 2007.

[73] R. Tatman. Gender and dialect bias in YouTube’s automatic captions. In *First Workshop on Ethics in Natural Language Processing*, volume 1, pages 53–59, 2017.

[74] A. W. van der Vaart and J. A. Wellner. *Weak Convergence and Empirical Processes: With Applications to Statistics*. Springer, New York, 1996.

[75] T. van Erven and P. Harremoës. Rényi divergence and Kullback-Leibler divergence. *IEEE Transactions on Information Theory*, 60(7):3797–3820, 2014.

[76] J. Wen, C.-N. Yu, and R. Greiner. Robust learning under uncertain test distributions: Relating covariate shift to model misspecification. In *Proceedings of the 31st International Conference on Machine Learning*, pages 631–639, 2014.
A Proofs

A.1 Proof of Lemma 2.1

We begin by deriving a likelihood ratio reformulation, where we use \( W := \mathbb{E}[\ell(\theta; (X,Y)) | X] \) to ease notation

\[
\sup_{Q_0 \in \mathcal{P}_{\alpha_0,X}} \mathbb{E}_{X \sim Q_0}[W] = \sup_{L} \left\{ \mathbb{E}_P[LW] \mid L : \Omega \to [0, 1/\alpha_0], \text{measurable}, \mathbb{E}_P[L] = 1 \right\}. \tag{30}
\]

To see that inequality \( \leq \) holds, let \( Q_0 \in \mathcal{P}_{\alpha_0,X} \) be a probability over \( X \). Note that \( Q_0 \) induces a distribution over \((\Omega, \sigma(X))\), which we denote by the same notation for simplicity. Since \( P_X = \alpha_0 Q_0 + (1 - \alpha_0) Q_1 \) for some probability \( Q_1 \), we have \( Q_0 \ll P_X \). Letting \( L := \frac{dQ_0}{dP_X} \), it belongs to the constraint set in the right hand side and we conclude \( \leq \) holds.

To see the reverse inequality \( \geq \), for any likelihood ratio \( L : \Omega \to [0, 1/\alpha_0] \), let \( Q_0 := P_X L \) so that \( Q_0(A) := \mathbb{E}_{P_X}[\{A\}L] \) for all \( A \in \sigma(X) \). Noting \( Q_1 := \frac{1}{1-\alpha_0} P_X - \frac{\alpha_0}{1-\alpha_0} Q_0 \) defines a probability measure and \( P_X = \alpha_0 Q_0 + (1 - \alpha_0) Q_1 \), we conclude that inequality \( \geq \) holds.

Next, the following lemma gives a variational form for conditional value-at-risk, which corresponds to the worst-case loss (2) under mixture covariate shifts.

**Lemma A.1** ([67, Example 6.19]). For any random variable \( W : X \to \mathbb{R} \) with \( \mathbb{E}|W| < \infty \),

\[
\inf_{\eta \in \mathbb{R}} \left\{ \frac{1}{\alpha_0} \mathbb{E}_{X \sim P_X} [(W - \eta)_+] + \eta \right\}.
\]

From the reformulation (30) and Lemma A.1, we obtain the first result.

We now show that when \( W \in [0, M] \),

\[
\inf_{\eta \in \mathbb{R}} \left\{ \frac{1}{\alpha_0} \mathbb{E}[(W - \eta)_+] + \eta \right\} = \inf_{\eta \in [0, M]} \left\{ \frac{1}{\alpha_0} \mathbb{E}[(W - \eta)_+] + \eta \right\}. \tag{31}
\]

Noting that \( \eta \mapsto g(\eta) := \frac{1}{\alpha_0} \mathbb{E}[(W - \eta)_+] + \eta \) is strictly increasing on \([M, \infty)\) since \( g(\eta) = \eta \) for \( \eta \in [M, \infty) \), we may assume w.l.o.g. that \( \eta \leq M \). Further, for \( \eta \leq 0 \), we have

\[
g(\eta) = \frac{1}{\alpha_0} \mathbb{E}[W] + \left( \frac{1}{\alpha_0} - 1 \right) |\eta| \geq \frac{1}{\alpha_0} \mathbb{E}[W] = g(0).
\]

We conclude that the equality (31) holds.

A.2 Proof of Proposition 1

Using the dual of Lemma 2.1, we show that with probability at least \( 1 - \gamma \),

\[
\sup_{\eta \in [0, M]} \left| \mathbb{E}_{X \sim P_X} \left[ (\mathbb{E}[\ell(\theta; (X,Y)) | X] - \eta)_+ \right] - \frac{1}{n} \sum_{i=1}^{n} \left( \frac{1}{m} \sum_{j=1}^{m} \ell(\theta_i; (X_i, Y_{i,j})) - \eta \right)_+ \right| \leq CM \sqrt{\frac{1 + |\log \delta|}{\min\{m,n\}}}. \tag{32}
\]
As the above gives a uniform approximation to the dual objective $\frac{1}{\alpha_0} \mathbb{E}[\mathbb{E}[\ell(\theta; (X, Y)) \mid X] - \eta] + \eta$, the proposition will then follow.

To show the result (32), we begin by noting that

$$
\sup_{\eta \in [0, M]} \left| \mathbb{E}_{X \sim P_X} \left[ \left( \mathbb{E}[\ell(\theta; (X, Y)) \mid X] - \eta \right)_+ \right] - \frac{1}{n} \sum_{i=1}^n \left( \frac{1}{m} \sum_{j=1}^m \ell(\theta; (X_i, Y_{i,j})) - \eta \right)_+ \right\|
\leq \sup_{\eta \in [0, M]} \left| \mathbb{E}_{X \sim P_X} \left[ \left( \mathbb{E}[\ell(\theta; (X, Y)) \mid X] - \eta \right)_+ \right] - \frac{1}{n} \sum_{i=1}^n \left( \mathbb{E}[\ell(\theta; (X, Y)) \mid X = X_i] - \eta \right)_+ \right| + \frac{1}{n} \sum_{i=1}^n \left( \frac{1}{m} \sum_{j=1}^m \ell(\theta; (X_i, Y_{i,j})) - \eta \right)_+. \quad (33)
$$

To bound the first term in the bound (33), note that since $\eta \mapsto (Z - \eta)_+$ is 1-Lipschitz, a standard symmetrization and Rademacher contraction argument [17, 7] yields

$$
\sup_{\eta \in [0, M]} \left| \mathbb{E} \left[ \left( \mathbb{E}[\ell(\theta; (X, Y)) \mid X] - \eta \right)_+ \right] - \frac{1}{n} \sum_{i=1}^n \left( \mathbb{E}[\ell(\theta; (X_i, Y)) \mid X = X_i] - \eta \right)_+ \right| \leq C \sqrt{\frac{M^2}{n}} (1 + t)
$$

with probability at least $1 - e^{-t}$. To bound the second term in the bound (33), we first note that

$$
\sup_{\eta \in [0, M]} \left| \mathbb{E}[\ell(\theta; (X, Y)) \mid X = X_i] - \eta \right)_+ - \frac{1}{m} \sum_{j=1}^m \ell(\theta; (X_i, Y_{i,j})) - \eta \right)_+ \right| \leq \left| \mathbb{E}[\ell(\theta; (X_i, Y_{i,j})) \mid X = X_i] - \frac{1}{m} \sum_{j=1}^m \ell(\theta; (X_i, Y_{i,j})) \right|
$$

since $| (x - \eta)_+ - (x' - \eta)_+ | \leq |x - x'|$. The preceding quantity has bound $M$, and using that its expectation is at most $M/\sqrt{m}$ the bounded differences inequality implies the uniform concentration result (32).

### A.3 Proof of Lemma 3.1

Let $\mathcal{L}_{\alpha_0} := \{ h : \mathcal{X} \to \mathbb{R}_+ \mid \mathbb{E}[h(X)] = \alpha_0 \}$. Since $\frac{dQ_0}{dP}$ is a likelihood ratio and $\mathbb{E}[dQ_0/dP] = 1$, we have the upper bound

$$
\mathbb{E}_{X \sim Q_0} \mathbb{E}[\ell(\theta; (X, Y)) \mid X] = \mathbb{E}_P \left[ \frac{dQ_0(X)}{dP(X)} \ell(\theta; (X, Y)) \right] \leq \sup_{h \in \mathcal{H}_{L,2} \cap \mathcal{L}_{\alpha_0}} \mathbb{E}_P \left[ \frac{h(X)}{\alpha_0} \ell(\theta; (X, Y)) \right].
$$

Then we use the sequence of inequalities, starting from our dual representation on $\mathcal{R}_{L,2}$, that

$$
\mathcal{R}_{L,2}(\theta) = \inf_{\eta} \sup_{h \in \mathcal{H}_{L,2}} \frac{1}{\alpha_0} \mathbb{E}_P \left[ h(X)(\ell(\theta; (X, Y)) - \eta) \right] + \eta
\geq \sup_{h \in \mathcal{H}_{L,2}} \inf_{\eta} \frac{1}{\alpha_0} \mathbb{E}_P \left[ h(X)(\ell(\theta; (X, Y)) - \eta) \right] + \eta
\geq \sup_{h \in \mathcal{H}_{L,2} \cap \mathcal{L}_{\alpha_0}} \frac{1}{\alpha_0} \mathbb{E}_P \left[ h(X)(\ell(\theta; (X, Y)) - \eta) \right] + \eta = \sup_{h \in \mathcal{H}_{L,2} \cap \mathcal{L}_{\alpha_0}} \mathbb{E}_P[h(X)\ell(\theta; (X, Y))].
$$

This gives the result.
A.4 Proof of Lemma 3.2

Since \( Z, \eta \in [0, M] \), we have

\[
\mathbb{E}_{X \sim P_X} \left[ (Z(X) - \eta)_+^p \right] \leq (M - \eta)^{p-1} \mathbb{E}_{X \sim P_X} \left[ (Z(X) - \eta)_+ \right]
\]

which gives the first bound. To get the second bound, note that for a \( L \)-Lipschitz function \( f \), we have \( \mathbb{E}[f(X)] \leq f(\mathbb{E}[X]) + L \mathbb{E}|X - \mathbb{E}[X]| \). Since \( f(x) = x^p \) is \( p(M - \eta)^{p-1} \)-Lipschitz on \([0, M - \eta] \), we get

\[
\mathbb{E}_{X \sim P_X} \left[ (Z(X) - \eta)_+^p \right] \leq (\mathbb{E}_{X \sim P_X} \left[ (Z(X) - \eta)_+ \right])^p + p(M - \eta)^{p-1} \mathbb{E} \left| (Z(X) - \eta)_+ - \mathbb{E}(Z(X) - \eta)_+ \right|.
\]

Taking \( 1/p \)-power on both sides, we obtain the second bound.

A.5 Proof of Lemma 4.1

First, we argue that

\[
\sup_h \left\{ \mathbb{E} \left[ h(X)(\ell(\theta; (X,Y)) - \eta) \right] \mid h : \mathcal{X} \to \mathbb{R}_+, \mathbb{E}[h^q(X)] \leq 1 \right\}
\]

\[
\leq \sup_{h \in \mathcal{H}_{L,p}} \left\{ \mathbb{E} \left[ \frac{h(X)}{\epsilon} (\ell(\theta; (X,Y)) - \eta) \right] \mid \epsilon > 0, \mathbb{E}[h^q(X)]^{1/q} \leq \epsilon \right\}
\]

and for any \( \epsilon > 0 \). We consider an arbitrary but fixed \( \theta \) and \( \eta \).

Suppose that \( \epsilon^{q-1} \geq (\mathbb{E}_{X \sim P_X} \left[ (\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)_+^p \right])^{1/p} \), then

\[
\epsilon^{q-1} \geq (\mathbb{E}_{X \sim P_X} \left[ (\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)_+^p \right])^{1/p}
\]

\[
= \sup_h \left\{ \mathbb{E} \left[ h(X)(\ell(\theta; (X,Y)) \mid X] - \eta) \right] \mid h : \mathcal{X} \to \mathbb{R} \text{ measurable, } h \geq 0, \mathbb{E}[h^q(X)] \leq 1 \right\}
\]

\[
\geq \sup_{h \in \mathcal{H}_{L,p}} \left\{ \mathbb{E} \left[ \frac{h(X)}{\epsilon} (\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta) \right] : h \geq 0, \mathbb{E}[h^q(X)]^{1/q} \leq \epsilon \right\},
\]

and we have the upper bound. On the other hand, assume \( \epsilon^{q-1} \leq (\mathbb{E}_{X \sim P_X} \left[ (\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)_+^p \right])^{1/p} \). The inner supremum in Eq. (12) is attained at \( h^* \) defined in expression (13), and from Assumption A2, for any \( x, x' \in \mathcal{X} \),

\[
|h^*(x) - h^*(x')| \leq \frac{1}{\epsilon} \left| (\mathbb{E}[\ell(\theta; (X,Y)) \mid X = x] - \eta)_+^p - (\mathbb{E}[\ell(\theta; (X,Y)) \mid X = x'] - \eta)_+^p \right|
\]

\[
\leq \frac{1}{\epsilon} \left| (\mathbb{E}[\ell(\theta; (X,Y)) \mid X = x] - \eta)_+ - (\mathbb{E}[\ell(\theta; (X,Y)) \mid X = x'] - \eta)_+ \right|^{p-1}
\]

\[
\leq \frac{1}{\epsilon} [\mathbb{E}[\ell(\theta; (X,Y)) \mid X = x] - \mathbb{E}[\ell(\theta; (X,Y)) \mid X = x']]|^{p-1}
\]

\[
\leq \frac{L^{p-1}}{\epsilon} \|x - x'\|^{p-1},
\]

where we used \( \epsilon \leq (\mathbb{E}_{X \sim P_X} \left[ (\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)_+^p \right])^{1/q} \) in the first inequality. Thus, we conclude that \( ch^* \) is in \( \mathcal{H}_{L,p} \), and obtain the equality

\[
(\mathbb{E}_{X \sim P_X} \left[ (\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)_+^p \right])^{1/p}
\]

\[
= \sup_h \left\{ \mathbb{E}_{X \sim P_X} \left[ (\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)h(X) \right] : h : \mathcal{X} \to \mathbb{R} \text{ measurable, } h \geq 0, \mathbb{E}[h^q(X)] \leq 1, \text{ and } eh \in \mathcal{H}_{L,p} \right\}
\]

\[
= \sup_{h \in \mathcal{H}_{L,p}} \left\{ \mathbb{E} \left[ \frac{h(X)}{\epsilon} (\ell(\theta; (X,Y)) - \eta) \right] : h \geq 0, \mathbb{E}[h^q(X)]^{1/q} \leq \epsilon \right\}
\]

31
where we did a change of variables $h$ to $h/\epsilon$ in the last equality. This yields the bound (34).

Now, for $\epsilon = (\mathbb{E}_{X \sim P_N} \left[ \left( \mathbb{E}[\ell(\theta; (X, Y)) | X] - \eta \right)_+^p \right])^{1/q}$, the bound (34) is actually an equality. This proves the first claim. To show the second claim, it remains to show that

$$\sup_{h \in H_{L,p}} \left\{ \mathbb{E} \left[ \frac{h(X)}{\epsilon} (\ell(\theta; (X, Y)) - \eta) \right] \vee \epsilon^{q-1} \bigg| h \geq 0, \ (\mathbb{E}[h^q(X)])^{1/q} \leq \epsilon \right\} - \epsilon^{q-1}$$

$$\leq \sup_{h} \left\{ \mathbb{E} [h(X) (\ell(\theta; (X, Y)) - \eta)] \bigg| h : \mathcal{X} \rightarrow \mathbb{R}, \text{ measurable, } h \geq 0, \mathbb{E}[h^q(X)] \leq 1 \right\}.$$

If $\epsilon^{q-1} \geq (\mathbb{E}_{X \sim P_N} \left[ \left( \mathbb{E}[\ell(\theta; (X, Y)) | X] - \eta \right)_+^p \right])^{1/p}$, then the left hand side is less than or equal to 0 by the same logic above. If $\epsilon^{q-1} \leq (\mathbb{E}_{X \sim P_N} \left[ \left( \mathbb{E}[\ell(\theta; (X, Y)) | X] - \eta \right)_+^p \right])^{1/p}$, then we have

$$\sup_{h \in H_{L,p}} \left\{ \mathbb{E} \left[ \frac{h(X)}{\epsilon} (\ell(\theta; (X, Y)) - \eta) \right] \vee \epsilon^{q-1} \bigg| h \geq 0, \ (\mathbb{E}[h^q(X)])^{1/q} \leq \epsilon \right\}$$

$$= \sup_{h} \left\{ \mathbb{E} [h(X) (\ell(\theta; (X, Y)) - \eta)] \bigg| h : \mathcal{X} \rightarrow \mathbb{R}, \text{ measurable, } h \geq 0, \mathbb{E}[h^q(X)] \leq 1 \right\},$$

so the result follows.

### A.6 Proof of Lemma 4.2

We take the dual of the following optimization problem

$$\text{maximize } \frac{1}{n} \sum_{i=1}^{n} h_i \frac{1}{\epsilon} (\ell(\theta; (X_i, Y_i)) - \eta)$$

subject to $h_i \geq 0$ for all $i \in [n]$, $\frac{1}{n} \sum_{i=1}^{n} h_i^q \leq \epsilon^q,

h_i - h_j \leq \frac{L^{p-1}}{\epsilon} \|X_i - X_j\|^{p-1}$ for all $i, j \in [n]$

where $h_i := h(X_i)$. To ease notation, we do a change of variables $h_i \leftarrow \frac{h_i}{\epsilon}$

$$\text{maximize } \frac{1}{n} \sum_{i=1}^{n} h_i (\ell(\theta; (X_i, Y_i)) - \eta)$$

subject to $h_i \geq 0$ for all $i \in [n]$, $\frac{1}{n} \sum_{i=1}^{n} h_i^q \leq 1,

h_i - h_j \leq \frac{L^{p-1}}{\epsilon} \|X_i - X_j\|^{p-1}$ for all $i, j \in [n]$.

For $\gamma \in \mathbb{R}_+^n$, $\lambda \geq 0$, $B \in \mathbb{R}_+^{n \times n}$, the associated Lagrangian is given by

$$\mathcal{L}(h, \gamma, \lambda, B) := \frac{1}{n} \sum_{i=1}^{n} h_i (\ell(\theta; (X_i, Y_i)) - \eta) + \gamma^\top h + \frac{\lambda}{q} \left( 1 - \frac{1}{n} \sum_{i=1}^{n} h_i^q \right)$$

$$+ \frac{1}{n^2} \left( \frac{L^{p-1}}{\epsilon} \text{tr}(B^\top D) - h^\top (B 1 - B^\top 1) \right).$$
where $D \in \mathbb{R}^{n \times n}$ is a matrix with entries $D_{ij} = \|X_i - X_j\|^{p-1}$. From strong duality, we have that the primal optimal value (35) is equal to $\inf_{\gamma \in \mathbb{R}_+^n} \sup_h \mathcal{L}(h, \gamma, \lambda, B)$.

Since $h \mapsto \mathcal{L}(h, \gamma, \lambda, B)$ is a quadratic, a bit of algebra shows that

$$\sup_h \mathcal{L}(h, \gamma, \lambda, B) = \frac{\lambda}{q} + \frac{L^{p-1}}{cn^2} \text{tr}(B^T D) + \frac{1}{q} \sum_{i=1}^n \left( \ell(\theta; (X_i, Y_i)) - \eta - \frac{1}{n} (B1 - B^T 1)_i + \gamma_i \right)^p.$$

From complementary slackness,

$$\inf_{\gamma \in \mathbb{R}_+^n} \sup_h \mathcal{L}(h, \gamma, \lambda, B) = \frac{\lambda}{q} + \frac{L^{p-1}}{cn^2} \text{tr}(B^T D) + \frac{1}{q} \sum_{i=1}^n \left( \ell(\theta; (X_i, Y_i)) - \eta - \frac{1}{n} (B1 - B^T 1)_i \right)^p.$$

Finally, taking infimum with respect to $\lambda \geq 0$, we obtain

$$\inf_{\lambda \geq 0, \gamma \in \mathbb{R}_+^n} \sup_h \mathcal{L}(h, \gamma, \lambda, B) = \frac{L^{p-1}}{cn^2} \text{tr}(B^T D) + \left( \frac{p-1}{n} \sum_{i=1}^n \left( \ell(\theta; (X_i, Y_i)) - \eta - \frac{1}{n} (B1 - B^T 1)_i \right)^p \right)^{1/p}.$$

Unpacking the matrix notation, we obtain the result.

### A.7 Proof of Lemma 4.3

From the extension theorem for Hölder continuous functions [54, Theorem 1], any $(p-1, 1)$-Hölder continuous function $h : \{X_1, \ldots, X_n\} \to \mathbb{R}$ extends to a $(p-1, 1)$-Hölder continuous $\hat{h} : \mathbb{R}^d \to \mathbb{R}$ with range($\hat{h}$) $\subseteq$ range($h$) so that $h = \hat{h}$ on $\{X_1, \ldots, X_n\}$. Since $\hat{h} \geq 0$ implies $h \geq 0$, we have

$$\hat{R}_{p,e,L}(\theta, \eta) = \sup_{h \in H_{L,p}} \left\{ \mathbb{E}_{\hat{P}_n} \left[ \frac{h(X)}{\epsilon} (\ell(\theta; (X,Y)) - \eta) \right] \mid h \geq 0, \left( \mathbb{E}_{\hat{P}_n} [h^q(X)] \right)^{1/q} \leq \epsilon \right\}.$$

To ease notation, for $c \in [0, \infty]$ define the function $R_{c,p,e,L} = R_{p,e,L} c$ so that $R_{p,e,L} = R_{1,p,e,L}$.

First, we establish the following claim, which relates $R_{p,e,L}$ and $R_{c,p,e,L}$.

**Claim A.2.**

$$R_{p,e,L}(\theta, \eta) \leq \left( \frac{\epsilon}{c} \right)^{q-1} \left\{ R_{c,p,e,L}(\theta, \eta) + (1 - c) \left( \mathbb{E} \left[ (\mathbb{E}[\ell(\theta; (X,Y)) | X] - \eta)^p \right] \right)^{1/p} \right\} \quad \text{if } c < 1$$

$$R_{c,p,e,L}(\theta, \eta) \leq c^{q-1} \left( \frac{\epsilon}{c} \right)^{q-1} \left\{ R_{p,e,L}(\theta, \eta) + (c - 1) \left( \mathbb{E} \left[ (\mathbb{E}[\ell(\theta; (X,Y)) | X] - \eta)^p \right] \right)^{1/p} \right\} \quad \text{if } c > 1.$$

**Proof of Claim**

We only prove the bound when $c < 1$ as the proof is similar when $c > 1$. In the case that

$$\left( \frac{\epsilon}{c} \right)^{q-1} \leq \left( \mathbb{E}_{X \sim P_X} \left[ (\mathbb{E}[\ell(\theta; (X,Y)) | X] - \eta)^p \right] \right)^{1/q},$$

the constraint sets that define $R_{p,e,L}$ and $R_{c,p,e,L}$ contain the maximizers $h^*$ and $c h^*$ (for $h^*$ defined in expression (13)), respectively. Hence,

$$R_{p,e,L}(\theta, \eta) = \left( \mathbb{E}_{X \sim P_X} \left[ (\mathbb{E}[\ell(\theta; (X,Y)) | X] - \eta)^p \right] \right)^{1/p} \quad \text{and}$$

$$R_{c,p,e,L}(\theta, \eta) = c \left( \mathbb{E}_{X \sim P_X} \left[ (\mathbb{E}[\ell(\theta; (X,Y)) | X] - \eta)^p \right] \right)^{1/p}.$$

and the desired bound holds. Otherwise, $R_{p,e,L}(\theta, \eta) \leq (\epsilon/c)^{q-1}$. \[\square\]
Using the two bounds in Claim A.2, we now bound $R_{p,\epsilon,L}$ by its empirical counterpart. To obtain an upper bound on $R_{p,\epsilon,L}$, let us first take $c_1 := (1 - \hat{n})^{1/q}$, where

$$
\hat{n} := \frac{q}{2} \land q \epsilon^{-q} L^{p-1} ((LR)^{p-1} + \epsilon)^{q-1} W_{p-1} (\tilde{P}_n, P).
$$

Noting that $(1 - \delta)^{-1/q} \leq 1 + \frac{4\delta}{q}$ for $\delta \in (0, \frac{1}{2}]$, and $1 - (1 - \delta)^{1/q} \leq \frac{2}{q} \delta$, the first bound in Claim A.2 yields for $\eta \geq 0$ that

$$
\epsilon^{q-1} \vee R_{p,\epsilon,L}(\theta, \eta) \leq \epsilon^{q-1} \vee R_{C_1,\epsilon,L}(\theta, \eta) + 2^{q-1} \epsilon + \frac{2M}{q} \delta_n.
$$

(36)

To bound $R_{C_1,\epsilon,L}(\theta, \eta)$ by $\tilde{R}_{p,\epsilon,L}(\theta, \eta)$, we first note

$$
R_{C_1,\epsilon,L}(\theta, \eta) \leq \sup_{h \in \mathcal{H}_{L,p}} \left\{ \mathbb{E} \left[ \frac{h(X)}{\epsilon} (\ell(\theta; (X, Y)) - \eta) \right] \mid h \geq 0, \mathbb{E}_{\tilde{P}_n}[h^q(X)] \leq \epsilon^q \right\}.
$$

(37)

Indeed, for $h \in \mathcal{H}_{L,p}$ satisfying $\mathbb{E}_Q[h(X)^q] \leq \epsilon^q$ for some probability measure $Q$, $h^q : \mathcal{X} \to \mathbb{R}$ is bounded by $((LR)^{p-1} + \epsilon)^{q-1}$. Hence, we have for all $x, x' \in \mathcal{X}$

$$
|h^q(x) - h^q(x')| \leq q \max \{ h(x), h(x') \}^{q-1} |h(x) - h(x')| \leq q L^{p-1} ((LR)^{p-1} + \epsilon)^{q-1} \|x - x'\|^{p-1}.
$$

From the definition of the Wasserstein distance $W_{p-1}$,

$$
\sup_{h \in \mathcal{H}_{L,p}} \left\| \mathbb{E}_{\tilde{P}_n}[h^q(X)] - \mathbb{E}[h^q(X)] \right\| \leq q L^{p-1} ((LR)^{p-1} + \epsilon)^{q-1} W_{p-1} (\tilde{P}_n, P),
$$

which implies that for any $h \in \mathcal{H}_{L,p}$ satisfying $\mathbb{E}[h^q(X)] \leq c'_1 \epsilon^q$

$$
\mathbb{E}_{\tilde{P}_n}[h^q(X)] \leq \mathbb{E}[h^q(X)] + q L^{p-1} ((LR)^{p-1} + \epsilon)^{q-1} W_{p-1} (\tilde{P}_n, P) \leq \epsilon^q.
$$

To further bound the expression (37), we check that for any $\theta \in \Theta$ and $\eta \in [0, M]$, the map $(x, y) \mapsto \frac{h(x)}{\epsilon} (\ell(\theta; (x, y)) - \eta)$ is Hölder continuous. By Assumption A2, we observe

$$
\left| \frac{h(x)}{\epsilon} (\ell(\theta; (x, y)) - \eta) - \frac{h(x')}{\epsilon} (\ell(\theta; (x', y')) - \eta) \right|
\leq \frac{h(x)}{\epsilon} \left| \ell(\theta; (x, y)) - \ell(\theta; (x', y')) \right| + \left| \ell(\theta; (x', y')) - \eta \right| \frac{|h(x) - h(x')|}{\epsilon}
\leq \frac{(LR)^{p-1} + \epsilon}{\epsilon} L \left\| (x, y) - (x', y') \right\| + \frac{ML^{p-1}}{\epsilon} \left\| x - x' \right\|^{p-1}
= \frac{(LR)^{p-1} + \epsilon}{\epsilon} LR \left\| (x, y) - (x', y') \right\| + \frac{ML^{p-1}}{\epsilon} \left\| x - x' \right\|^{p-1}
\leq \frac{(LR)^{p-1} + \epsilon}{\epsilon} LR \left\| (x, y) - (x', y') \right\|^{p-1} + \frac{ML^{p-1}}{\epsilon} \left\| x - x' \right\|^{p-1}
\leq \frac{1}{\epsilon} \left\{ LR^{2-p} ((LR)^{p-1} + \epsilon) + ML^{p-1} \right\} \left\| (x, y) - (x', y') \right\|^{p-1}
$$

for all $(x, y), (x', y') \in \mathcal{X} \times \mathcal{Y}$. Using the definition of the Wasserstein distance to bound right hand side of (37),

$$
R_{C_1,\epsilon,L}(\theta, \eta) \leq \tilde{R}_{p,\epsilon,L}(\theta, \eta) + \frac{1}{\epsilon} \left\{ LR^{2-p} ((LR)^{p-1} + \epsilon) + ML^{p-1} \right\} W_{p-1} (\tilde{P}_n, P).
$$

34
Plugging in the preceding display in the bound (36), we get

\[
\epsilon^q - 1 \vee R_{p, \epsilon, L}(\theta, \eta) \leq \epsilon^q - 1 \vee \tilde{R}_{p, \epsilon, L}(\theta, \eta) + 2^{q - 1}\epsilon
\]

\[+ M \left(1 \land 2\epsilon^{-q}L^{p - 1}((LR)^{p - 1} + \epsilon)^{q - 1}W_{p - 1}(\tilde{P}_n, P)\right)\]

\[+ \frac{1}{\epsilon} \left\{LR^{2 - p}((LR)^{p - 1} + \epsilon) + ML^{p - 1}\right\} W_{p - 1}(\tilde{P}_n, P).\]

To obtain the lower bound on the empirical risk Lemma 4.3 claims, let \(c_2 := (1 + \tilde{c}_0)^{1/q}\) where

\[
\tilde{c}_0 = q\epsilon^{-q}L^{p - 1}((LR)^{p - 1} + \epsilon)^{q - 1}W_{p - 1}(\tilde{P}_n, P).
\]

From the second bound in Claim A.2,

\[
\epsilon^q - 1 \vee R_{c_2, p, \epsilon, L}(\theta, \eta) \leq \epsilon^q - 1 \vee R_{p, \epsilon, L}(\theta, \eta) + \left(\frac{\epsilon^q - 1}{p} + \frac{M}{q}\right) \tilde{c}_0
\]

holds, and from a similar argument as before, we have

\[
R_{c_2, p, \epsilon, L}(\theta, \eta) \geq \sup_{h \in \mathcal{H}_{L, p}} \left\{ \mathbb{E} \left[ \frac{h(X)}{\epsilon} (\ell(\theta; (X, Y)) - \eta) \right] \bigg| h \geq 0, \mathbb{E}_{\tilde{P}_n}[h^\theta](X) \leq \epsilon^q \right\}
\]

\[
\geq \tilde{R}_{p, \epsilon, L}(\theta, \eta) - \frac{1}{\epsilon} \left\{LR^{2 - p}((LR)^{p - 1} + \epsilon) + ML^{p - 1}\right\} W_{p - 1}(\tilde{P}_n, P).
\]

We conclude that

\[
\epsilon^q - 1 \vee \tilde{R}_{p, \epsilon, L}(\theta, \eta) \leq \epsilon^q - 1 \vee R_{p, \epsilon, L}(\theta, \eta)
\]

\[+ ((q - 1)L^{p - 1}\epsilon^{-1} + M\epsilon^{-q}L^{p - 1})((LR)^{p - 1} + \epsilon)^{q - 1}W_{p - 1}(\tilde{P}_n, P)
\]

\[+ \frac{1}{\epsilon} (LR^{2 - p}((LR)^{p - 1} + \epsilon) + ML^{p - 1}) W_{p - 1}(\tilde{P}_n, P).
\]

### A.8 Proof of Theorem 2

We use the following concentration result for the Wasserstein distance between an empirical distribution and its population counterpart.

**Lemma A.3** (Fournier and Guillin [29], Theorem 2). Let \(p \in (1, 2]\), and \(d > 1\). Then for any \(t > 0\),

\[
\mathbb{P} \left( W_{p - 1}(P, \tilde{P}_n) \geq t \right) \leq c_1 \exp \left( -c_1 n(t^{\frac{d + 1}{p - 1}} \wedge t^2) \right)
\]

where \(c_1\) and \(c_2\) are positive constants that depend on \(M, d, p\).

See Fournier and Guillin [29] and Lei [49] for general concentration results.

Let \(B_k := LR + \epsilon^{-1}2^kL(2M + (q - 1)LR) + \epsilon^{-q}2^{q - 1}RM^{2q - 1} + \epsilon^{q - 2}(q - 1)2^{q - 2}L\) to ease notation. From Lemmas 4.3 and A.3, for any fixed \(\epsilon > 0\), with probability at least \(1 - c_1 \exp \left( -c_2 n(t^{\frac{d + 1}{p - 1}} \wedge t^2) \right)\)

\[
\sup_{Q_0(x) \in \mathcal{P}_{a_0} \times X} \mathbb{E}_{X \sim Q_0} \left[ \mathbb{E}[\hat{\theta}_{n, \epsilon}^{\text{rob}}(\theta; (X, Y)) \mid X] \right] \leq \inf_{\eta \in [0, M]} \left\{ \frac{1}{\alpha_0} \left( R_{p, \epsilon, L}(\tilde{\theta}_{n, \epsilon}^{\text{rob}}, \eta) \vee \epsilon^{-1} \right) + \eta \right\}
\]

\[
\leq \inf_{\eta \in [0, M]} \left\{ \frac{1}{\alpha_0} \left( \tilde{R}_{p, \epsilon, L}(\tilde{\theta}_{n, \epsilon}^{\text{rob}}, \eta) \vee \epsilon^{-1} \right) + \eta \right\} + \frac{B_{k} t}{\alpha_0}
\]

\[
\leq \inf_{\eta \in [0, M]} \left\{ \frac{1}{\alpha_0} \left( \tilde{R}_{p, \epsilon, L}(\tilde{\theta}_{n, \epsilon}, \eta) \vee \epsilon^{-1} \right) + \eta \right\} + \frac{B_{k} t}{\alpha_0}
\]
for any $\theta \in \Theta$, where we used the fact that $\widehat{\theta}_{n,\eta}^{\text{rob}}$ is an empirical minimizer.

Applying uniform convergence of $\widehat{R}_{p,\epsilon,L}(\theta, \eta)$ to $R_{p,\epsilon,L}$ again (Lemmas 4.3 and A.3), we get

$$\sup_{Q_0(x) \in \mathcal{P}_{n,0}} \mathbb{E}_{X \sim Q_0}[\mathbb{E}[\ell(\widehat{\theta}_{n,\epsilon}^{\text{rob}}; (X,Y)) \mid X]]$$

$$\leq \inf_{\eta \in [0,M]} \left\{ \frac{1}{\alpha_0} (R_{p,\epsilon,L}(\theta, \eta) \vee \epsilon) + \frac{2Bt}{\alpha_0} + \frac{e^{\epsilon - 1}}{\alpha_0} + \frac{2Bt}{\alpha_0} \right\}$$

with probability at least $1 - 2c_1 \exp \left( -c_2n(\frac{d+1}{p} + t^2) \right)$, where we used the second bound of Lemma 4.1. Taking infimum over $\theta \in \Theta$, we obtain the result.

### A.9 Proof of Proposition 3

Since our desired bound holds trivially if $(\mathbb{E}(\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)_{+}^{p})^{1/p} \leq \epsilon^{-1}$, we assume $(\mathbb{E}(\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)_{+}^{p})^{1/p} \geq \epsilon^{-1}$. First, we rewrite the left hand side as

$$(\mathbb{E}(\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)_{+}^{p})^{1/p} = \frac{\mathbb{E}(\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)_{+}^{p}}{(\mathbb{E}(\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)_{+}^{p})^{1/q}}$$

where for convenience we defined

$$Z(\theta, \eta; (X,Y)) := (\ell(\theta; (X,Y)) - \eta) (\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)_{+}^{p}.$$ 

Now, note that $\eta \mapsto Z(\theta, \eta; (X,Y))$ is $pM$-Lipschitz. Applying a standard bracketing number argument for uniform concentration of Lipschitz functions [74, Theorem 2.7.11]

$$\sup_{\eta \in [0,M]} \mathbb{E}[(\mathbb{E}[Z(\theta, \eta; (X,Y))] - \mathbb{E}_{\hat{P}_n}[Z(\theta, \eta; (X,Y))]) \leq c_1 M^2 \sqrt{\frac{\log \frac{1}{\gamma}}{n}}$$

with probability at least $1 - \gamma$, where $c_1$ is some universal constant. We conclude that with probability at least $1 - \gamma$, for all $\eta \in [0,M]$

$$(\mathbb{E}(\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)_{+}^{p})^{1/p} \leq (\mathbb{E}(\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)_{+}^{p})^{-1/q} \mathbb{E}_{\hat{P}_n}[Z(\theta, \eta; (X,Y))]$$

$$+ (\mathbb{E}(\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)_{+}^{p})^{-1/q} c_1 M^2 \sqrt{\frac{\log \frac{1}{\gamma}}{n}}. \quad (38)$$

Next, we upper bound the first term by our empirical objective $\widehat{R}_{p,\epsilon,L}(\theta, \eta)$

$$\left( \mathbb{E}(\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)_{+}^{p} \right)^{-1/q} \mathbb{E}_{\hat{P}_n}[Z(\theta, \eta; (X,Y))]$$

$$= (1 + \tau_n(\gamma, \epsilon))^{1/q} \mathbb{E}_{\hat{P}_n} \left[ \frac{h_n(\theta; (X,Y))}{\tau_n(1 + \tau_n(\gamma, \epsilon))^{1/q}}(\ell(\theta; (X,Y)) - \eta) \right].$$

Uniform concentration of Lipschitz functions [74, Theorem 2.7.11] implies that there exists a universal constant $c_2 > 0$ such that with probability at least $1 - \gamma$

$$\mathbb{E}_{\hat{P}_n}[\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)_{+}^{p}] \leq \mathbb{E}(\mathbb{E}[\ell(\theta; (X,Y)) \mid X] - \eta)_{+}^{p} + c_2 M^2 \sqrt{\frac{1}{n} \log \frac{1}{\gamma}}$$

36
for all $\eta \in [0, M]$. Recalling the definition (13) of $h_\eta^*(x)$ (where we now make the dependence on $\eta$ explicit), we have

$$\mathbb{E}_{\hat{P}_n} [h_\eta^*(X)|^p] \leq 1 + c_2 M^2 \left( \mathbb{E} \left( \mathbb{E}[\ell(\theta; (X, Y)) \mid X] - \eta \right)_+^{p} \right)^{-1} \frac{1}{n} \log \frac{1}{\gamma}. \tag{39}$$

with probability at least $1 - \gamma$.

Recalling the definition (17) of $\hat{H}_{L,p}$, since $x \mapsto h_\eta^*(x)$ is $\frac{L}{\epsilon}$-Lipschitz, we get

$$\left( \mathbb{E} \left( \mathbb{E}[\ell(\theta; (X, Y)) \mid X] - \eta \right)_+^{p} \right)^{-1} \mathbb{P}_{\hat{P}_n} [Z(\theta; \eta; (X, Y))] \leq (1 + \tau_n(\gamma, \epsilon))^{1/q} \sup_{h \in \mathcal{H}_{L_n(\gamma), n}} \left\{ \mathbb{E}_{\hat{P}_n} \left[ \frac{h(X)}{\epsilon} (\ell(\theta; (X, Y)) - \eta) \right] : \mathbb{E}_{\hat{P}_n} [h^q(X)] \leq \epsilon^q \right\}$$

with probability at least $1 - \gamma$, where we used the bound (39) in the second inequality. Combining the preceding display with the bound (38), with probability at least $1 - 2\gamma$,

$$\left( \mathbb{E} \left( \mathbb{E}[\ell(\theta; (X, Y)) \mid X] - \eta \right)_+^{p} \right)^{1/p} \leq (1 + \tau_n(\gamma, \epsilon))^{1/q} \left( \frac{c_1 M^2}{\epsilon^{q-1}} \right) \frac{1}{n} \log \frac{1}{\gamma}$$

for all $\eta \in [0, M]$.

## A.10 Proof of Lemma 5.1

First, note that variational form for the $L^p(P)$-norm gives

$$\left( \mathbb{E}_{(X, C) \sim P_{X,C}} \left[ (\mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta \right)_+^{p} \right)^{1/p} \tag{40}$$

$$= \sup_{h \in \mathcal{H}} \{ \mathbb{E}[\bar{h}(X, C)(\ell(\theta; (X, Y)) - \eta)] : \bar{h} : \mathcal{X} \times \mathcal{C} \to \mathbb{R} \text{ measurable}, \bar{h} \geq 0, \mathbb{E}[\bar{h}(X, C)^q] \leq 1 \}.$$  

For ease of notation, let

$$e(x) := \mathbb{E}[\ell(\theta; (X, Y)) \mid X = x], \quad e(x, c) := \mathbb{E}[\ell(\theta; (X, Y)) \mid X = x, C = c].$$

We first show the equality (25). To see that “≥” direction holds, let $\epsilon := (\mathbb{E} (e(X, C) - \eta)_+^{p})^{1/q}$. Then, we have

$$R_{p,c,L,\delta}(\theta, \eta) \leq \sup_{h, f \text{ measurable}} \left\{ \mathbb{E} [(h(X) + f(X, C))(\ell(\theta; (X, Y)) - \eta)] : h + f \geq 0, \mathbb{E}[(h(X) + f(X, C))^q] \leq 1 \right\}$$

$$= \left( \mathbb{E} (\mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta)_+^{p} \right)^{1/p} \tag{41}$$

where we used the variational form (40) in the last inequality.

For the “≤” inequality, fix an arbitrary $\epsilon > 0$. If $(\mathbb{E} (e(X, C) - \eta)_+^{p})^{1/q} \leq \epsilon$, then the bound follows. Otherwise, consider $(\mathbb{E} (e(X, C) - \eta)_+^{p})^{1/q} > \epsilon > 0$. Note that the supremum in the variational form (40) is attained by

$$\bar{h}^*(x, c) := \frac{(e(x, c) - \eta)_+^{p-1}}{(\mathbb{E} (e(X, C) - \eta)_+^{p})^{1/q}}.$$
Now, define

\[ h^*(x) := \frac{(e(x) - \eta)^{p-1}_+}{(\mathbb{E}(e(X,C) - \eta)^{p}_+)^{1/q}}, \]

\[ f^*(x, c) := \frac{1}{(\mathbb{E}(e(X,C) - \eta)^{p}_+)^{1/q}} \left((e(x, c) - \eta)^{p-1}_+ - (e(x) - \eta)^{p-1}_+\right) \]

so that \( \bar{h}^* = h^* + f^* \). Since \( \epsilon h^* \in \mathcal{H}_{L,p} \) and \( \|f^*(X,C)\|_{L^\infty(P)} \leq \frac{\delta^{p-1}}{\epsilon} \), \( h^* \) and \( f^* \) are in the feasible region of the maximization problem that defines \( R_{p,\epsilon,L,\delta}(\theta, \eta) \). We conclude that

\[ \left(\mathbb{E}(\mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta)^{p}_+\right)^{1/p} \leq \inf_{\epsilon \geq 0} \left\{ \epsilon \vee \sup_{h,f \text{ meas.}} \left\{ \mathbb{E}[(h(X) + f(X,C))(<\ell(\theta; (X, Y)) - \eta)] : h + f \geq 0, \mathbb{E}[(h(X) + f(X,C))^q] \leq 1, \epsilon h \in \mathcal{H}_{L,p}, \|f(X,C)\|_{L^\infty(P)} \leq \frac{\delta^{p-1}}{\epsilon}\right\}\right. \]

Rescaling the supremum problem by \( 1/\epsilon \), we obtain the first result (25).

To show the second result, fix an arbitrary \( \epsilon > 0 \). If \( \left(\mathbb{E}(e(X,C) - \eta)^{p}_+\right)^{1/q} \leq \epsilon \), then from our upper bound (41)

\[ (R_{p,\epsilon,L,\delta}(\theta, \eta) \vee \epsilon^{q-1}) - \epsilon^{q-1} \leq 0 \]

so that our desired result trivially holds. On the other hand, if \( \left(\mathbb{E}(e(X,C) - \eta)^{p}_+\right)^{1/q} \geq \epsilon \), then

\[ R_{p,\epsilon,L,\delta}(\theta, \eta) = \left(\mathbb{E}(X,C) \sim_{pX,C} [\mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta]^p_{+}\right)^{1/p} \]

from our argument above, so the desired result again holds.

**A.11 Proof of Proposition 4**

We proceed similarly as in the proof of Proposition 3. Letting

\[ Z(\theta, \eta; (X, C, Y)) : = (\ell(\theta; (X, Y)) - \eta) (\mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta)^{p-1}_+, \]

rewrite the \( L^p \)-norm as

\[ \left(\mathbb{E}(\mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta)^{p}_+\right)^{1/p} = \frac{\mathbb{E}(\mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta)^{p}_+}{\left(\mathbb{E}(\mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta)^{p}_+\right)^{1/q}} = \frac{\mathbb{E}[Z(\theta, \eta; (X, C, Y))]}{\left(\mathbb{E}(\mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta)^{p}_+\right)^{1/q}}. \]

Since \( (\theta, \eta) \mapsto Z(\theta, \eta; (X, C, Y)) \) is \( pM \)-Lipschitz, we again get from a standard bracketing number argument for uniform concentration of Lipschitz functions [74, Theorem 2.7.11]

\[ \sup_{\eta \in [0, M]} \left| \mathbb{E}[Z(\theta, \eta; (X, C, Y))] - \mathbb{E}_{\tilde{F}_n}[Z(\theta, \eta; (X, C, Y))] \right| \leq c_1 M^2 \sqrt{\frac{\log 1/\gamma}{n}} \quad (42) \]
with probability at least $1 - \gamma$, where $c_1$ is some universal constant. Hence, with probability at least $1 - \gamma$, for all $\theta \in \Theta, \eta \in [0, M]$

$$(\mathbb{E} \mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta)_{+}^{p} \leq (\mathbb{E} \mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta)_{+}^{p} + \mathbb{E}_{\tilde{P}_n}[Z(\theta, \eta; (X, C, Y))]$$

$$+ (\mathbb{E} \mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta)_{+}^{p} - 1/q \frac{c_1 M^2 \sqrt{\frac{\log \frac{1}{\gamma}}{n}}}{n}.$$ (43)

Next, we upper bound $\mathbb{E}_{\tilde{P}_n}[Z(\theta, \eta; (X, C, Y))]$ by our empirical objective $\hat{R}_{p, \epsilon, L, \delta}(\theta, \eta)$. To this end, uniform concentration of Lipschitz functions [74, Theorem 2.7.11] again yields

$$\mathbb{E}_{\tilde{P}_n}(\mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta)_{+}^{p-1} \leq \mathbb{E} \mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta)_{+}^{p-1} + c_2 M^2 \log \frac{1}{\gamma}$$

$$\sqrt{\frac{n}{q}}.$$ (44)

for all $\theta \in \Theta, \eta \in [0, M]$, with probability at least $1 - \gamma$. Define the functions

$$h_{\eta}^{*}(x) := \frac{(e(x) - \eta)_{+}^{p-1}}{(e(e(X, C) - \eta)_{+}^{p})^{1/q}},$$

$$f^{*}(x, c) := \frac{1}{(e(e(X, C) - \eta)_{+}^{p})^{1/q}} \left( (e(x, c) - \eta)_{+}^{p-1} - (e(x) - \eta)_{+}^{p-1} \right),$$

and note that

$$\mathbb{E}_{\tilde{P}_n}[(h_{\eta}^{*}(X) + f^{*}(X, C))^{q}] \leq 1 + c_2 M^2 \left( \mathbb{E} \mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta)_{+}^{p} \right)^{-1/q} \sqrt{\frac{\log \frac{1}{\gamma}}{n}}.$$ (45)

with probability at least $1 - \gamma$.

Since our desired bound holds trivially if $(\mathbb{E} \mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta)_{+}^{p} \leq \epsilon$, we now assume that $(\mathbb{E} \mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta)_{+}^{p} \geq \epsilon$. Since $eh_{\eta}^{*}(x) \in H_{L, p}$, we have

$$(\mathbb{E} \mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta)_{+}^{p} \leq (1 + \tau_n(\gamma, \epsilon))^{1/q} \mathbb{E}_{\tilde{P}_n}[Z(\theta, \eta; (X, C, Y))]$$

$$= (1 + \tau_n(\gamma, \epsilon))^{1/q} \mathbb{E}_{\tilde{P}_n} \left[ \frac{h_{\eta}^{*}(X) + f^{*}(X, C)}{(1 + \tau_n(\gamma, \epsilon))^{1/q}} \ell(\theta; (X, Y)) - \eta \right]$$

$$\leq (1 + \tau_n(\gamma, \epsilon))^{1/q} \sup_{h \in H_{L, p}, f \in F_{\delta_n(\gamma), p, n}} \left\{ \mathbb{E}_{\tilde{P}_n} \left[ \frac{h(X) + f(X, C)}{\epsilon} (\ell(\theta; (X, Y)) - \eta) \right] \right\}$$

with probability at least $1 - \gamma$, where we used the bound (45) in the second inequality. Combining the preceding display with the bound (43), with probability at least $1 - 2\gamma$,

$$(\mathbb{E} \mathbb{E}[\ell(\theta; (X, Y)) \mid X, C] - \eta)_{+}^{p} \leq (1 + \tau_n(\gamma, \epsilon))^{1/q} \hat{R}_{p, \epsilon, L, \delta}(\theta, \eta) + c_1 M^2 \epsilon q^{-1} \sqrt{\frac{\log \frac{1}{\gamma}}{n}},$$

for all $\theta \in \Theta, \eta \in [0, M]$. 39
We take the dual of the optimization problem
\[
\begin{align*}
\text{maximize} & \quad \frac{1}{n} \sum_{i=1}^{n} \frac{h_i + f_i}{\epsilon} (\ell(\theta; (X_i, Y_i)) - \eta) \\
\text{subject to} & \quad h_i + f_i \geq 0 \quad \text{for all } i \in [n], \quad \frac{1}{n} \sum_{i=1}^{n} (h_i + f_i)^q \leq \epsilon^q, \\
& \quad h_i - h_j \leq L^{p-1} \|X_i - X_j\|^{p-1} \quad \text{for all } i, j \in [n], \\
& \quad |f_i| \leq \delta^{p-1} \quad \text{for all } i \in [n]
\end{align*}
\]
where \( h_i := h(X_i) \) and \( f_i = f(X_i, C_i) \). To ease notation, we do a change of variables \( h_i \leftarrow \frac{h_i}{\epsilon} \), \( f_i \leftarrow \frac{f_i}{\epsilon} \) and \( q_i \leftarrow h_i + f_i \) which gives
\[
\begin{align*}
\text{maximize} & \quad \frac{1}{n} \sum_{i=1}^{n} q_i (\ell(\theta; (X_i, Y_i)) - \eta) \\
\text{subject to} & \quad q_i \geq 0 \quad \text{for all } i \in [n], \quad \frac{1}{n} \sum_{i=1}^{n} q_i^q \leq 1, \\
& \quad h_i - h_j \leq \frac{L^{p-1}}{\epsilon} \|X_i - X_j\|^{p-1} \quad \text{for all } i, j \in [n], \\
& \quad |q_i - h_i| \leq \frac{\delta^{p-1}}{\epsilon} \quad \text{for all } i \in [n].
\end{align*}
\]

For \( \gamma \in \mathbb{R}^n_+ \), \( \lambda \geq 0 \), \( B \in \mathbb{R}^{n \times n}_+ \), \( \alpha^+, \alpha^- \in \mathbb{R}^n_+ \), the associated Lagrangian is
\[
\mathcal{L}(q, h, \gamma, \lambda, B, \alpha^+, \alpha^-) := \frac{1}{n} \sum_{i=1}^{n} q_i (\ell(\theta; (X_i, Y_i)) - \eta) + \frac{1}{n^2} \gamma^T q + \frac{\lambda}{2} \left( 1 - \frac{1}{n} \sum_{i=1}^{n} q_i^q \right) + \frac{1}{n^2} \left( \frac{L^{p-1}}{\epsilon} \text{tr}(B^T D) - h^T (B \mathbf{1} - B^\top \mathbf{1}) \right) + \frac{\alpha^+}{n} \left( \frac{\delta^{p-1}}{\epsilon} \mathbf{1} - (q - h) \right) + \frac{\alpha^-}{n} \left( \frac{\delta^{p-1}}{\epsilon} \mathbf{1} + (q - h) \right)
\]
where \( D \in \mathbb{R}^{n \times n} \) is a matrix with entries \( D_{ij} = \|X_i - X_j\|^{p-1} \). From strong duality, the primal optimal value (46) is
\[
\inf_{\gamma \in \mathbb{R}^n_+, \lambda \geq 0, B \in \mathbb{R}^{n \times n}_+} \sup_{q, h} \mathcal{L}(q, h, \gamma, \lambda, B, \alpha^+, \alpha^-).
\]

The first order conditions for the inner supremum give
\[
q^*_i := \frac{1}{n \lambda} \left( \ell(\theta; (X_i, Y_i)) - \eta + n \gamma - \alpha_i^+ + \alpha_i^- \right), \quad \frac{1}{n} (B \mathbf{1} - B^\top \mathbf{1}) = (\alpha^+ - \alpha^-).
\]
By nonnegativity of \( B \) and \( \alpha^+, \alpha^- \), the second equality implies that \( \alpha^+ = \frac{1}{n} B \mathbf{1} \) and \( \alpha^- = \frac{1}{n} B^\top \mathbf{1} \). Substituting these values and infimizing out \( \lambda, \gamma \geq 0 \) as in Lemma 4.2, we obtain
\[
\inf_{\lambda \geq 0, \gamma \in \mathbb{R}^n_+} \sup_{q, h} \mathcal{L}(q^*_i, h, \gamma, \lambda, B, \alpha^+, \alpha^-) = \left( \frac{p-1}{p} \right)^{1/p} \left( \frac{\delta^{p-1}}{p} \sum_{i=1}^{n} \|X_i - X_j\| B_{ij} + \frac{2\delta^{p-1}}{pen^2} \sum_{i,j=1}^{n} |B_{ij}| \right)^{1/p}.
\]
Taking the infimum with respect to \( B \in \mathbb{R}^{n \times n}_+ \) gives the lemma.