Sinkhorn Distributionally Robust Optimization

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We study distributionally robust optimization with Sinkhorn distance—a variant of Wasserstein distance based on entropic regularization. We derive convex programming dual reformulations when the nominal distribution is an empirical distribution and a general distribution, respectively. Compared with Wasserstein DRO, it is computationally tractable for a larger class of loss functions, and its worst-case distribution is more reasonable. To solve the dual reformulation, we propose an efficient batch gradient descent with bisection search algorithm. Finally, we provide various numerical examples using both synthetic and real data to demonstrate its competitive performance.

Key words: Wasserstein distributionally robust optimization, Sinkhorn distance, Duality theory

1. Introduction

Decision-making problems under uncertainty have broad applications in operations research, machine learning, engineering, economics, etc. When the data involves uncertainty due to measurement error, insufficient sample size, contamination and anomalies, or model mis-specification, distributionally robust optimization (DRO) is a promising approach to data-driven optimization, by seeking a minimax robust optimal decision that minimizes the expected loss under the most adverse distribution within a given set of relevant distributions, called ambiguity set. It provides a principled framework to produce a solution with promising better out-of-sample performance than the traditional sample average approximation (SAA) method for stochastic programming [84]. We refer to [79] for a recent survey on DRO.

At the core of DRO is the choice of the ambiguity set. Ideally, a good ambiguity set should take account of the properties of practical applications while maintaining the computational tractability of resulted DRO formulation; and it should be rich enough to contain all distributions relevant to the decision-making but at the same time, should not include unnecessary distributions that lead to overly conservative decisions. Various DRO formulations have been proposed in the literature; see the last part of this section for a detailed review. Among them, the ambiguity set based on Wasserstein distance has recently received much attention [102, 65, 17, 45]. The Wasserstein distance incorporates the geometry of sample space, and thereby is suitable for comparing distributions with non-overlapping supports and hedging against data perturbations [45]. Nice statistical performance guarantees have been established for Wasserstein DRO both asymptotically [16, 19, 18], non-asymptotically [43, 23, 82], and empirically in a variety of applications in operations research [13, 29, 85, 71, 86, 98], machine learning [83, 24, 64, 14, 70, 91], stochastic control [104, 1, 89, 37, 105, 97], etc; see [60] and references therein for more discussions.

On the other hand, the current Wasserstein DRO framework is not without limitation. First, from the computational efficiency perspective, the tractability of Wasserstein DRO is usually available only under somewhat stringent conditions on the loss function, as the resulting dual formulation involves a subproblem that requires the global supremum of some regularized loss function over the sample space. In particular, for 1-Wasserstein DRO, a convex reformulation is only known when the loss
function can be expressed as a pointwise maximum of finitely many concave functions [65], and for 2-Wasserstein DRO, efficient first-order algorithms have been developed only for smooth loss functions and sufficiently small radius (or equivalently, sufficiently large Lagrangian multiplier) so that the involved subproblem becomes strongly convex [87, 20, 61, 25]. Second, from the modeling perspective, for data-driven Wasserstein DRO in which the nominal distribution is finitely supported (usually the empirical distribution), the worst-case distribution is shown to be a discrete distribution [45], despite that the underlying true distribution in many practical applications may well be continuous. This raises the concern of whether Wasserstein DRO hedges the right family of distribution and whether it causes potential over-conservative performance.

To address these potential issues while maintaining the advantages of Wasserstein DRO, in this paper, we propose Sinkhorn DRO, which hedges against distributions that are close to some nominal distribution in Sinkhorn distance [34]. The Sinkhorn distance can be viewed as a smoothed Wasserstein distance, defined as the cheapest transport cost between two distributions associated with an optimal transport problem with entropic regularization. As far as we know, this paper is the first to study the DRO formulation using the Sinkhorn distance. Our main contributions are summarized as follows.

(I) We derive a strong duality reformulation for Sinkhorn DRO (Theorem 1), both when the nominal distribution is a data-driven empirical distribution (Section 3.1) and when the nominal distribution is any arbitrary distribution (Section 3.2). The Sinkhorn dual objective smooths the maximization subproblem in the Wasserstein dual objective, and converges to Wasserstein dual objective as the entropic regularization parameter goes to zero (Remark 3). Moreover, the dual objective of Sinkhorn DRO is upper bounded by that of the KL-divergence DRO with the nominal distribution being a kernel density estimator (Remark 4).

(II) As a byproduct of our duality proof, we characterize the worst-case distribution of the Sinkhorn DRO (Remark 5), which is absolutely continuous with respect to some reference measure. Compared with Wasserstein DRO, the worst-case distribution of Sinkhorn DRO is not necessarily finitely supported when the nominal distribution is a finitely supported distribution. This indicates that Sinkhorn DRO is a more flexible modeling choice for many applications.

(III) On the algorithmic aspect, we propose a computationally efficient first-order method for solving the Sinkhorn DRO problem (Section 4), based on batch gradient descent and bisection search. Its convergence guarantees are also developed. Compared with Wasserstein DRO, the dual problem of Sinkhorn DRO is computationally tractable for any measurable loss functions.

(IV) We provide experiments (Section 5) to validate the performance of the proposed Sinkhorn DRO model in the context of newsvendor problem, mean-risk portfolio optimization, and semi-supervised learning, using both synthetic and real data sets. Numerical results demonstrate its superior out-of-sample performances compared with several benchmarks including SAA, Wasserstein DRO, and KL-divergence DRO.

Related Literature

On DRO Models Construction of ambiguity sets plays a key role in the performance of DRO models. Generally, there are two ways to construct ambiguity sets in literature. First, ambiguity sets can be defined using descriptive statistics, such as the support information [11], moment conditions [81, 35, 51, 110, 104, 28, 12], shape constraints [78, 92], marginal distributions [42, 67, 2, 38]. Second, a more recently popular approach makes full use of the available data to consider distributions within a pre-specified statistical distance from a nominal distribution, usually chosen as the empirical distribution of samples. Commonly used statistical distances used in literature include f-divergence [56, 10, 100, 9, 40], Wasserstein distance [76, 102, 65, 108, 17, 45, 27, 103], and maximum mean discrepancy [90, 109]. Our proposed Sinkhorn DRO can be viewed as a variant of Wasserstein DRO. In the literature on Wasserstein DRO, besides the computational tractability, its regularization effects and statistical inference have also be investigated. In particular, it has been shown that Wasserstein DRO is asymptotically equivalent
to a statistical learning problem with variation regularization [44, 16, 82], and when the radius is chosen properly, the worst-case loss of Wasserstein DRO serves as an upper confidence bound on the true loss [16, 19, 43, 18]. Other variants of Wasserstein DRO have been explored, by combining with other information such as moment information [47, 94] and marginal distribution [46, 41].

Finally, we remark that a recent work [41] on distributionally robust optimization with given marginals share a somewhat similar spirit as our work. They start from a dual formulation and propose to replace its supremum subproblem with a smooth penalization, and then dualize the dual problem to obtain a primal problem that penalizes the entropy of the distribution. The main differences between their formulation and ours are that: (i) we do not impose marginal distribution constraints in the primal formulation; (ii) our entropic regularization is on the transport plan (joint distribution) between the nominal distribution and a candidate distribution in the ambiguity set, but their entropic penalty is imposed only on the candidate distribution in the ambiguity set; (iii) our dual formulation smooths the supremum subproblem by log-exp-sum function, which is not covered in their considered family of penalizations.

On Sinkhorn Distance Sinkhorn distance [34] is proposed to improve the computational complexity of Wasserstein distance by regularizing the original mass transportation problem with relative entropy penalty on the transport mapping. In particular, this distance can be computed from its dual form by optimizing two blocks of decision variables alternatively, which only requires simple matrix-vector products and therefore significantly improves the computation speed [75]. Such an approach first aroused in the areas of economics and survey statistics [59, 107, 36, 7], and its convergence analysis is attributed to the mathematician Sinkhorn [88], which gives name of Sinkhorn distance. A recent work [3] further designs an accelerated algorithm to compute Sinkhorn distance in near-linear time. Using Sinkhorn distance other than Wasserstein distance has been demonstrated to be beneficial because of lower computational cost in various applications, including domain adaptations [31, 32, 30], generative modeling [49, 74, 63, 73], dimensionality reduction [62, 95, 96, 57], etc. To the best of our knowledge, the study of Sinkhorn distance for distributionally robust optimization is new in the literature.

The rest of the paper is organized as follows. In Section 2, we describe the main formulation for the Sinkhorn DRO model. In Section 3, we develop its strong dual reformulation. In Section 4, we propose a first-order optimization algorithm that solves the reformulation efficiently. We report several numerical results in Section 5, and conclude the paper in Section 6. All omitted proofs can be found in Appendix.

2. Model Setup

Notation. Assume that the logarithm function log is taken with base $e$. For a positive integer $N$, we write $[N]$ for $\{1, 2, \ldots, N\}$. For a measurable set $Z$, denote by $\mathcal{M}(Z)$ the set of measures on $Z$, and $\mathcal{P}(Z)$ the set of probability measures on $Z$. Given a probability distribution $P$ and a measure $\mu$, we denote $\text{supp}(P)$ the support of $P$, and write $P \ll \mu$ if $P$ is absolutely continuous with respect to $\mu$. For a given element $x$, denote by $\delta_x$ the one-point probability distribution supported on $\{x\}$. Denote $P \otimes Q$ as the product measure of two probability distributions $P$ and $Q$. Denote by $\text{Proj}_{\mathbb{R}^2}$ the first and the second marginal distributions of $\gamma$, respectively. For a given set $A$, define the characteristic function $\chi_A(x)$ such that $\chi_A(x) = 1$ when $x \in A$ and otherwise $\chi_A(x) = 0$, and define the indicator function $\tau_A(x)$ such that $\tau_A(x) = 0$ when $x \in A$ and otherwise $\tau_A(x) = \infty$. Define the distance between two sets $A$ and $B$ in the Euclidean space as $\text{Dist}(A, B) = \sup_{x \in A} \inf_{y \in B} \|x - y\|_2$.

We first review the definition of Sinkhorn distance.
Definition 1 (Sinkhorn Distance). Let \( Z \) be a measurable set. Consider distributions \( P, Q \in \mathcal{P}(Z) \), and let \( \mu, \nu \in \mathcal{M}(Z) \) be two reference measures such that \( P \ll \mu, Q \ll \nu \). For regularization parameter \( \epsilon \geq 0 \), the Sinkhorn distance between two distributions \( P \) and \( Q \) is defined as

\[
\mathcal{W}_\epsilon(P, Q) = \inf_{\gamma \in \Gamma(P, Q)} \left\{ E_{(X,Y) \sim \gamma} [c(X,Y)] + \epsilon H(\gamma | \mu \otimes \nu) \right\},
\]

where \( \Gamma(P, Q) \) denotes the set of joint distributions whose first and second marginal distributions are \( P \) and \( Q \) respectively, \( c(x, y) \) denotes the cost function, and \( H(\gamma | \mu \otimes \nu) \) denotes the relative entropy of \( \gamma \) with respect to the product measure \( \mu \otimes \nu \):

\[
H(\gamma | \mu \otimes \nu) = \int \log \left( \frac{d\gamma(x,y)}{d\mu(x) d\nu(y)} \right) d\gamma(x,y).
\]

Remark 1 (Variants of Wasserstein Distance). Sinkhorn distance in Definition 1 is based on general measures \( \mu \) and \( \nu \). The special form of the distance has been investigated in the literature, for instance [48, Section 2], when the reference measures \( \mu \) and \( \nu \) were chosen to be \( P, Q \), i.e., marginal distributions of \( \gamma \), respectively. The relative entropy regularization term can also be considered as a hard-constrained variant for the optimal transport problem, which has been discussed in [34, Definition 1] and [8]:

\[
\mathcal{W}_R^{\text{Info}}(P, Q) = \inf_{\gamma \in \Gamma(P, Q)} \left\{ E_{(X,Y) \sim \gamma} [c(X,Y)] : H(\gamma | P \otimes Q) \leq R \right\},
\]

where \( R \geq 0 \) quantifies the upper bound for the relative entropy between distributions \( \gamma \) and \( P \otimes Q \). Another variant of the optimal transport problem is to consider the negative entropy for regularization [34, Equation (2)]:

\[
\mathcal{W}_\epsilon^{\text{ent}}(P, Q) = \inf_{\gamma \in \Gamma(P, Q)} \left\{ E_{(X,Y) \sim \gamma} [c(X,Y)] + \epsilon H(\gamma) \right\},
\]

where \( H(\gamma) = \int \log \left( \frac{d\gamma(x,y)}{dx dy} \right) d\gamma(x,y) \) and \( dx, dy \) are Lebesgue measures if the corresponding marginal distributions are continuous, or counting measures if the marginal distributions are discrete. When probability distributions \( P \) and \( Q \) are known, these two regularized optimal transport distances are equivalent up to a constant.

In this paper, we study the Sinkhorn DRO model. Given the Sinkhorn radius \( \rho \) and the nominal distribution \( \widehat{P} \), the primal form of the worst-case expectation problem of Sinkhorn DRO is given by

\[
V := \sup_{P \in B_{\rho,\epsilon} (\widehat{P})} \mathbb{E}_{z \sim P} [f(z)],
\]

(Sinkhorn DRO)

where \( B_{\rho,\epsilon} (\widehat{P}) = \{ P : \mathcal{W}_\epsilon (\widehat{P}, P) \leq \rho \} \),

where \( B_{\rho,\epsilon} (\widehat{P}) \) is the Sinkhorn ball of the radius \( \rho \) centered at the nominal distribution \( \widehat{P} \).

Remark 2 (Choice of Reference Measures). By definition of relative entropy and the law of probability, we can see that the regularization term in \( \mathcal{W}_\epsilon (\widehat{P}, P) \) can be written as

\[
H(\gamma | \mu \otimes \nu) = \int \log \left( \frac{d\gamma(x,y)}{d\mu(x) d\nu(y)} \right) d\gamma(x,y)
= \int \log \left( \frac{d\gamma(x,y)}{d\mu(x) d\nu(y)} \right) d\gamma(x,y) + \int \log \left( \frac{\widehat{P}(x)}{d\mu(x)} \right) d\widehat{P}(x).
\]
Therefore, any choice of the reference measure \( \mu \) satisfying \( \hat{\mathbb{P}} \ll \mu \) is equivalent up to a constant since the nominal distribution \( \hat{\mathbb{P}} \) is known. For simplicity, we take the reference measure \( \mu = \hat{\mathbb{P}} \). For a fixed reference measure \( \nu \), the optimal solution \( \mathbb{P} \) in \((\text{Sinkhorn DRO})\) should satisfy that \( \mathbb{P} \ll \nu \) since otherwise the entropic regularization in Definition 1 is undefined. As a consequence, the choice of the reference measure \( \nu \) will affect the tractable formulation of the DRO problem. To obtain a reliable DRO formulation, we need to pick measure \( \nu \) such that the underlying true distribution is absolutely continuous with respect to it. Typical choices include the Lebesgue measure, counting measure, or some probability measures. See [77, Section 3.6] for the construction of a general reference measure.

In the following sections, we first derive the tractable formulation of the Sinkhorn DRO model and then develop an efficient first-order method to solve it. Finally, we examine its performance by several numerical examples.

3. Strong Duality Reformulation

Problem \((\text{Sinkhorn DRO})\) is an infinite-dimensional optimization problem over probability distributions and appears to be intractable in general. In this section, we derive a strong duality result for \((\text{Sinkhorn DRO})\).

Our main goal is to derive the strong dual problem

\[
V_D := \inf_{\lambda \geq 0} \left\{ \lambda \hat{\rho} + \lambda \epsilon \int \log \left( \mathbb{E}_{Q_{x,\epsilon}} \left[ e^{f(z)/(\lambda \epsilon)} \right] \right) \mathrm{d}\hat{\mathbb{P}}(x) \right\},
\]

where the dual decision variable \( \lambda \) corresponds to the Sinkhorn distance constraint in \((\text{Sinkhorn DRO})\), and by convention we define the dual objective evaluated at \( \lambda = 0 \) as the limit of the objective values with \( \lambda \downarrow 0 \), which equals the essential supremum of the objective function with respect to the measure \( \nu \); and we define the constant

\[
\hat{\rho} := \rho + \epsilon \int \log \left( \int e^{-c(x,z)}/\epsilon \, \mathrm{d}\nu(z) \right) \mathrm{d}\hat{\mathbb{P}}(x),
\]

and the kernel probability distribution

\[
dQ_{x,\epsilon}(z) := \frac{e^{-c(x,z)}/\epsilon}{\int e^{-c(x,u)}/\epsilon \, \mathrm{d}\nu(u)} \, \mathrm{d}\nu(z).
\]

To make the above primal \((\text{Sinkhorn DRO})\) and dual \((\text{Dual})\) problems well-defined, we introduce the following assumptions on the cost function \( c \), the reference measure \( \nu \), and the loss function \( f \).

**Assumption 1.**

(I) \( \nu \{ z : 0 \leq c(x,z) < \infty \} = 1 \) for \( \hat{\mathbb{P}} \)-almost every \( x \);

(II) \( \int e^{-c(x,z)}/\epsilon \, \mathrm{d}\nu(z) < \infty \) for \( \hat{\mathbb{P}} \)-almost every \( x \);

(III) \( Z \) is a measurable space, and the function \( f : Z \to \mathbb{R} \cup \{ \infty \} \) is measurable.

Assumption 1(I) ensures that the Sinkhorn distance is well-defined. If Assumption 1(II) is not satisfied, then the Sinkhorn ball \( \mathbb{B}_{\rho,\epsilon}(\hat{\mathbb{P}}) = \mathcal{P}(Z) \) and the problem \((\text{Sinkhorn DRO})\) has a simple optimal value \( V = \sup_{z \in Z} f(z) \). Assumption 1(III) ensures the expected loss \( \mathbb{E}_{z \sim \hat{\mathbb{P}}} [f(z)] \) is well-defined and lower bounded for any distribution \( \hat{\mathbb{P}} \). In Appendix A, we present sufficient conditions for Assumption 1 that are easy to verify.

To distinguish the cases \( V_D < \infty \) and \( V_D = \infty \), we introduce the following light-tail condition on \( f \).

**Condition 1.** There exists \( \lambda > 0 \) such that \( \mathbb{E}_{Q_{x,\epsilon}} \left[ e^{f(z)/(\lambda \epsilon)} \right] < \infty \) for \( \hat{\mathbb{P}} \)-almost every \( x \).

Our main result in this section is as follows.
Theorem 1 (Strong Duality). Let $\hat{\mathbb{P}} \in \mathcal{P}(Z)$. Assume Assumption 1 is in force. Then the following holds:

(I) The primal problem (Sinkhorn DRO) is feasible if and only if $\bar{\rho} \geq 0$;

(II) Whenever $\bar{\rho} \geq 0$, it holds that $V = V_D$.

(III) If, in addition, Condition 1 holds, then $V = V_D < \infty$; otherwise $V = V_D = \infty$.

We remark that if $\bar{\rho} < 0$, by convention, $V = -\infty$ and $V_D = -\infty$ as well by Lemma 2 in Section 3.3 below. Therefore, we have $V = V_D$ as long as Assumption 1 holds.

In the following, we first show that $V = V_D$ when $\hat{\mathbb{P}}$ is an empirical distribution supported on $n$ points, as it is relatively straightforward to prove. Then we show that the same results hold when $\hat{\mathbb{P}}$ is a general distribution.

3.1. Empirical Nominal distributions

Given data points $\hat{x}_i$ for $i = 1, \ldots, n$, denote $\frac{1}{n} \sum_{i=1}^{n} \delta_{\hat{x}_i}$ as the corresponding empirical distribution. In this subsection, we discuss the dual reformulation provided that the nominal distribution $\hat{\mathbb{P}}$ is taken in this form. Although our strong duality result holds for arbitrary nominal distribution, this is still an interesting case, as the proof is relatively simple and $\hat{\mathbb{P}}$ is often chosen as the empirical distribution in practice.

The key to the proof is to write the primal problem in a Lagrangian form and then apply the minimax inequality to obtain a weak dual. Observe that the primal can be reformulated as a generalized KL-divergence DRO problem. Hence, by leveraging the strong duality result for the existing DRO model [56], the minimax inequality does not incur any duality gap.

Proof of Theorem 1 when $\hat{\mathbb{P}} = \frac{1}{n} \sum_{i=1}^{n} \delta_{\hat{x}_i}$. Based on Definition 1, we reformulate $V$ as

$$V = \sup_{\gamma \in \mathcal{P}(Z), \forall y = \hat{\mathbb{P}}} \left\{ \mathbb{E}_\gamma[f(z)] : \mathbb{E}_\gamma \left[ c(x, z) + \epsilon \log \left( \frac{d\gamma(x, z)}{d\hat{\mathbb{P}}(x, z)} \right) \right] \leq \bar{\rho} \right\}.$$ 

By the disintegration theorem [22] we represent the joint distribution $\gamma = \frac{1}{n} \sum_{i=1}^{n} \delta_{\hat{x}_i} \otimes \gamma_i$, where $\gamma_i$ is the conditional distribution of $\gamma$ given the first marginal of $\gamma$ equals $\hat{x}_i$. Thereby the constraint is equivalent to

$$\frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{\gamma_i} \left[ c(\hat{x}_i, z) + \epsilon \log \left( \frac{d\gamma_i(x, z)}{d\hat{\mathbb{P}}(x, z)} \right) \right] \leq \bar{\rho}, \quad \gamma_i \in \mathcal{P}(Z), i \in [n].$$

We remark that any feasible solution $\gamma$ satisfies that $\gamma \ll \hat{\mathbb{P}} \otimes \nu$ and hence $\gamma_i \ll \nu_i$. Consequently the term $\log \left( \frac{d\gamma_i(x, z)}{d\hat{\mathbb{P}}(x, z)} \right)$ is well-defined. For notational simplicity, we write $Q_i$ for $Q_{\hat{x}_i, \nu}$. Based on the change-of-measure identity $\log \left( \frac{d\gamma_i(x, z)}{d\hat{\mathbb{P}}(x, z)} \right) = \log \left( \frac{dQ_i(x, z)}{d\hat{\mathbb{P}}(x, z)} \right) + \log \left( \frac{d\gamma(x, z)}{dQ_i(x, z)} \right)$ and the expression of $Q_i$, the constraint can be reformulated as

$$\frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{\gamma_i} \left[ c(\hat{x}_i, z) + \epsilon \log \left( \frac{e^{-c(x, z)/\epsilon}}{\int e^{-c(x, u)/\epsilon} d\nu(u)} \right) \right] \leq \bar{\rho}, \quad \gamma_i \in \mathcal{P}(Z), i \in [n].$$

Combining the first two terms within the expectation term and substituting the expression of $\bar{\rho}$, it is equivalent to

$$\frac{\epsilon}{n} \sum_{i=1}^{n} \mathbb{E}_{\gamma_i} \left[ \log \left( \frac{d\gamma_i(x, z)}{dQ_i(x, z)} \right) \right] \leq \bar{\rho}, \quad \gamma_i \in \mathcal{P}(Z), i \in [n].$$

Similarly, the objective function of (Sinkhorn DRO) can be written as $\frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{\gamma_i}[f(z)]$. Consequently, the primal problem (Sinkhorn DRO) can be reformulated as a generalized KL-divergence DRO problem

$$V = \sup_{\gamma_i \in \mathcal{P}(Z), i \in [n]} \left\{ \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{\gamma_i}[f(z)] : \frac{\epsilon}{n} \sum_{i=1}^{n} D_{KL}(\gamma_i || Q_i) \leq \bar{\rho} \right\}.$$
Then Theorem 1(i) holds based on the non-negativity of KL-divergence.

Introducing the Lagrange multiplier $\lambda$ associated with the constraint, we reformulate (Sinkhorn DRO) as

$$ V = \sup_{y_i \in P(Z), i \in [n]} \inf_{\lambda \geq 0} \left\{ \lambda \bar{p} + \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{y_i} \left[ f(z) - \lambda \epsilon \log \left( \frac{d y_i(z)}{d Q_i(z)} \right) \right] \right\}. $$

Interchanging the supremum and infimum operators, we have that

$$ V \leq \inf_{\lambda \geq 0} \left\{ \lambda \bar{p} + \sup_{y_i \in P(Z), i \in [n]} \left\{ \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{y_i} \left[ f(z) - \lambda \epsilon \log \left( \frac{d y_i(z)}{d Q_i(z)} \right) \right] \right\} \right\}. $$

Since the optimization over $y_i, i \in [n]$ is separable, by defining for each $i$

$$ v_i(\lambda) := \sup_{y_i \in P(Z)} \left\{ \mathbb{E}_{y_i} \left[ f(z) - \lambda \epsilon \log \left( \frac{d y_i(z)}{d Q_i(z)} \right) \right] \right\}, $$

it holds that

$$ V \leq \inf_{\lambda \geq 0} \left\{ \lambda \bar{p} + \frac{1}{n} \sum_{i=1}^{n} v_i(\lambda) \right\}. $$

When Condition 1 holds, leveraging a well-known results on entropy regularized linear optimization (Lemma EC.1), we can see that

$$ v_i(\lambda) = \lambda \epsilon \log \left( \mathbb{E}_{Q_i} \left[ e^{f(z)/(\lambda \epsilon)} \right] \right) < \infty, $$

hence we obtain the weak duality $V \leq V_D < \infty$. Otherwise, for any $\lambda > 0$, there exists an index $i$ such that

$$ \mathbb{E}_{Q_i} \left[ e^{f(z)/(\lambda \epsilon)} \right] = \infty. $$

We also obtain that $V \leq V_D = \infty$, and the weak duality still holds.

Next we prove the strong duality. Recall that the primal problem is a generalized KL-divergence DRO problem. By leveraging the strong duality result from [56], the minimax inequality above does not incur any duality gap when $\bar{p} > 0$. When $\bar{p} = 0$, since $D_{KL}(y_i||Q_i) = 0$ if and only if $y_i = Q_i$, one can see that

$$ V = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{Q_i} [f(z)]. $$

On the other hand, denote by $h(\lambda)$ the objective function for the dual problem. Then we have the inequality

$$ V_D \leq \lim_{\lambda \to \infty} h(\lambda) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{Q_i} [f(z)] = V. $$

This, together with the weak duality result, completes the proof for Theorem 1(ii). Theorem 1(iii) also follows based on the discussion of the finiteness of $V_D$. $\Box$

When the sample space $Z$ is finite, the following result presents a conic programming reformulation.
Corollary 1 (Conic Reformulation for Finite Sample Space). Suppose that the sample space contains $L$ elements, i.e., $Z = \{z_t\}_{t=1}^L$. If Condition 1 holds and $\bar{p} \geq 0$, the dual problem \((\text{Dual})\) can be formulated as the following conic optimization:

$$
V_D = \min_{\lambda \geq 0, s \in \mathbb{R}^n, a \in \mathbb{R}^{n \times L}} \lambda \bar{p} + \frac{1}{n} \sum_{i=1}^n s_i
$$

s.t. \quad \lambda e \geq \sum_{t=1}^L q_{i,t} a_{i,t}, i \in [n],

$$(\lambda e, a_{i,t}, f(z_t) - s_i) \in K_{\exp}, i \in [n], t \in [L].$$

where $q_{i,t} := \Pr_{z \sim Q_{\hat{\delta},\bar{e}}}(z = z_t)$, with the distribution $Q_{\hat{\delta},\bar{e}}$ defined in (2), and $K_{\exp}$ denotes the exponential cone $K_{\exp} = \{(v, \lambda, \delta) \in \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{R} : \exp(\delta/v) \leq \lambda/v\}$.

Problem (3) is a convex program that minimizes a linear function with respect to linear and conic constraints, which can be solved using interior point algorithms [69, 93]. We also develop a customized first-order optimization algorithm in Section 4 that is able to solve (3) with large scale.

3.2. General Nominal Distributions

Before we present the proof of Theorem 1 in Section 3.3, we would like to make several remarks.

Remark 3 (Connection with Wasserstein DRO). As the regularization parameter $\epsilon \to 0$, the dual objective of the Sinkhorn DRO converges to the dual formulation of the Wasserstein DRO problem [45, Theorem 1]

$$
\lambda \bar{p} + \int_Z \sup_x \{f(z) - \lambda c(x, z)\} \, d\hat{P}(x).
$$

The proof is given in Appendix EC.3, which essentially follows from the fact that the log-sum-exp function is a smooth approximation of the supremum. There are several advantages of Sinkhorn DRO.

(I) As we will demonstrate in Section 4, Sinkhorn DRO is tractable for a large class of loss functions. For the empirical nominal distribution, the worst-case loss can be evaluated efficiently for any measurable loss function $f$. In contrast, the main computational difficulty in Wasserstein DRO is to solve the maximization problem inside the integration above. In fact, 1-Wasserstein DRO (i.e., $c(\cdot, \cdot) = ||\cdot - \cdot||$) is shown to be tractable only when the loss function can be expressed as a pointwise maximum of finitely many concave functions [65, Theorem 4.2], and 2-Wasserstein DRO $c(\cdot, \cdot) = ||\cdot - \cdot||^2$ is shown to be tractable only when the loss function is smooth and the radius of the ambiguity set is sufficiently small [20, Theorem 3].

(II) The strong duality of Sinkhorn DRO holds in an even more general setting. Essentially, the only requirements on the space $Z$ and the nominal distribution $\hat{P}$ are measurability. In contrast, the strong duality for Wasserstein DRO ([45, Theorem 1], [17, Theorem 1]) requires the nominal distribution $\hat{P}$ to be a Borel probability measure and the set $Z$ to be a Polish space.

We remark that Sinkhorn DRO and Wasserstein DRO result in different conditions for finite worst-case values. From Condition 1 we see that the Sinkhorn DRO is finite if and only if under a light-tail condition on $f$, while the Wasserstein DRO [45, Theorem 1] is finite iff and only if the loss function satisfies a growth condition $f(z) \leq Lc(z, z_0) + M, \forall z \in Z$ for some constants $L, M > 0$ and some $z_0 \in Z$.

Remark 4 (Connection with KL-DRO). Using Jensen’s inequality, we can see that the dual objective function of the Sinkhorn DRO model can be upper bounded as

$$
\lambda \bar{p} + \lambda e \log \left( \int_{\mathcal{Q}_{\hat{\delta},\bar{e}}} e^{f(z)/(\lambda e)} \, d\hat{P}(x) \right),
$$

which corresponds to the dual objective function [56] for the following KL-divergence DRO

$$
\sup_{\mathcal{P}} \{ E_{z \sim \mathcal{P}}[f(z)] : D_{\text{KL}}(\mathcal{P}||\mathcal{P}^0) \leq \bar{p}/\epsilon \}.
$$
where \( \mathbb{P}_0 \) satisfies \( d\mathbb{P}^0(z) = \int_x dQ_{x,\varepsilon}(z) d\hat{\mathbb{P}}(x) \), which can be viewed as a non-parametric kernel density estimation constructed from \( \hat{\mathbb{P}} \). Particularly, when \( \hat{\mathbb{P}} = \frac{1}{n} \sum_{i=1}^n \delta_{x_i}, Z = \mathbb{R}^d \) and \( c(x, y) = \|x - y\|_2^2 \), \( \mathbb{P}^0 \) is kernel density estimator with Gaussian kernel and bandwidth \( \varepsilon \):

\[
\frac{d\mathbb{P}^0(z)}{dz} = \frac{1}{n} \sum_{i=1}^n K_\varepsilon(z - x_i), \quad z \in \mathbb{R}^d,
\]

where \( K_\varepsilon(x) \propto \exp(-\|x\|_2^2/\varepsilon) \) represents the Gaussian kernel. Proceeding similarly as in the proof in Section 3.1 and decompose \( y(x, z) = \hat{\mathbb{P}}(x) \otimes y_x(z) \), (Sinkhorn DRO) can be reformulated as a generalized KL-divergence DRO problem:

\[
V = \sup_{y_x \in \mathcal{P}(Z), x \in \mathbb{R}^d} \left\{ \int E_{z \sim y_x} [f(z)] d\hat{\mathbb{P}}(x) : \int D_{KL}(y_x || Q_x) d\hat{\mathbb{P}}(x) \leq \overline{\mathbb{P}} / \varepsilon \right\}.
\]

Using Divergence inequality [33, Theorem 2.6.3], we can see the Sinkhorn DRO with \( \overline{\mathbb{P}} = 0 \) is reduced to the following SAA model based on the distribution \( \mathbb{P}^0 \):

\[
V = \mathbb{E}_{\mathbb{P}^0} [f(z)] = \int \mathbb{E}_{Q_{x,\varepsilon}} [f(z)] d\hat{\mathbb{P}}(x).
\]

In non-parametric statistics, the optimal bandwidth to minimize the mean-squared-error between the estimated distribution and the underlying true one is at rate \( \varepsilon = O(n^{-1/(d+4)}) \) [53, Theorem 4.2.1]. However, we remark that such an optimal choice for the kernel density estimator may not be the optimal choice for optimizing the out-of-sample performance of the Sinkhorn DRO. In our numerical experiments in Section 5, we select \( \varepsilon \) based on cross-validation.

Before closing this subsection, we illustrate our result for a linear loss function \( f \), which turns out to be equivalent to a simple optimization problem.

**Example 1.** Suppose that \( f(z) = a^Tz, Z = \mathbb{R}^d \) and \( \nu \) is the corresponding Lebesgue measure, and the cost function is the Mahalanobis distance, i.e., \( c(x, y) = \frac{1}{2} (x - y)^T \Omega (x - y) \). In this case, we have the reference measure

\[
Q_{x,\varepsilon} \sim \mathcal{N}(x, \varepsilon \Omega^{-1}).
\]

As a consequence, the dual problem can be written as

\[
V_D = \inf_{\lambda > 0} \left\{ \lambda \overline{\mathbb{P}} + \lambda \varepsilon \int \Lambda_x(\lambda) d\hat{\mathbb{P}}(x) \right\},
\]

where

\[
\Lambda_x(\lambda) = \log \left( \mathbb{E}_{(x,\varepsilon \Omega^{-1})} \left[ e^{a^T z/\lambda \varepsilon} \right] \right) = \frac{a^T x}{\lambda \varepsilon} + \frac{a^T \Sigma a}{2 \lambda^2 \varepsilon^2}.
\]

Therefore

\[
V_D = a^T \mathbb{E}_{\hat{\mathbb{P}}} [x] + \sqrt{2 \overline{\mathbb{P}}} \sqrt{a^T \Omega^{-1} a} := \mathbb{E}_{\hat{\mathbb{P}}} [a^T x] + \sqrt{2 \overline{\mathbb{P}}} \|a\|_{\Omega^{-1}}.
\]

This indicates that the Sinkhorn DRO is equivalent to an empirical risk minimization with norm regularization, and can be solved using efficiently using algorithms for the second-order cone program.

\[\square\]
3.3. Proof Sketch of Strong Duality

In this subsection, we outline the proof of Theorem 1 when \( \widehat{\mathbf{P}} \) is an arbitrary nominal distribution.

The feasibility result in Theorem 1(I) can be easily shown using the reformulation (4). To show \( V = V_D \), it is easy to show the weak duality result following a similar argument as in Section 3.1, by replacing the finite-sum with the integration with respect to \( \widehat{\mathbf{P}} \).

When Condition 1 holds, we prove the strong duality by constructing the worst-case distribution. We first show the existence of the dual minimizer (Lemma 2), and then build the corresponding first-order optimality condition (Lemma 3 and Lemma 4). Those results help us to construct a primal optimal solution for (Sinkhorn DRO) that shares the same optimal value as \( V_D \), which completes the first part of Theorem 1(III). When Condition 1 does not hold, we construct a sequence of DRO problems with finite optimal values converging into \( V \) and consequently \( V = V_D = \infty \), which completes the second part of Theorem 1(III). Putting these two parts together imply Theorem 1(II).

Lemma 1 (Weak Duality). Assume Assumption 1 holds. Then \( V \leq V_D \).

Below we provide the proof of the first part of Theorem 1(III) for the case \( \bar{p} > 0 \) under Condition 1, defer proofs of other degenerate cases to Appendix EC.4. To prove the strong duality, we will construct a feasible solution of (Sinkhorn DRO) whose loss coincides with \( V_D \). To this end, we first show that the dual minimizer exists.

Lemma 2 (Existence of Dual Minimizer). Suppose \( \bar{p} > 0 \) and Condition 1 is satisfied, then the dual minimizer \( \lambda^* \) exists, which either equals to 0 or satisfies Condition 1.

We separate two cases: \( \lambda^* > 0 \) and \( \lambda^* = 0 \), corresponding to whether the Sinkhorn distance constraint in (Sinkhorn DRO) is binding or not.

Lemma 3 below presents a necessary and sufficient condition for the dual minimizer \( \lambda^* = 0 \), corresponding to the case where the Sinkhorn distance constraint in (Sinkhorn DRO) is not binding.

Lemma 3 (Necessary and Sufficient Condition for \( \lambda^* = 0 \)). Suppose \( \bar{p} > 0 \) and Condition 1 is satisfied, then the dual minimizer \( \lambda^* = 0 \) if and only if all the following conditions hold:

(I) \( \text{ess sup } f \leq \inf \{ t : \nu \{ f(z) > t \} = 0 \} < \infty \).

(II) \( \bar{p} = \bar{p} + \epsilon \int \log (E_{Q_{x,e}} [1_A]) \, d\widehat{\mathbf{P}}(x) \geq 0 \), where \( A := \{ z : f(z) = \text{ess sup } f \} \).

Recall that we have the convention that the dual objective evaluated at \( \lambda = 0 \) equals \( \text{ess sup } f \). Thus Condition (I) ensures that the dual objective function evaluated at the minimizer is finite. When the minimizer \( \lambda^* = 0 \), the Sinkhorn ball should be large enough to contain at least one distribution with objective value \( \text{ess sup } f \), and the condition (II) characterizes the lower bound of \( \bar{p} \).

Lemma 4 below considers the optimality condition when the dual minimizer \( \lambda^* > 0 \), obtained by simply setting the derivative of the dual objective function to be zero.

Lemma 4 (First-order Optimality Condition when \( \lambda^* > 0 \)). Suppose \( \bar{p} > 0 \) and Condition 1 is satisfied, and assume further that the dual minimizer \( \lambda^* > 0 \), then \( \lambda^* \) satisfies

\[
\lambda^* \left[ \bar{p} + \epsilon \int \log (E_{Q_{x,e}} \left[ \frac{e^{f(z)/(\lambda^* e)}}{e} \right]) \, d\widehat{\mathbf{P}}(x) \right] = \int \frac{E_{Q_{x,e}} \left[ e^{f(z)/(\lambda^* e)} f(z) \right]}{E_{Q_{x,e}} \left[ e^{f(z)/(\lambda^* e)} \right]} \, d\widehat{\mathbf{P}}(x).
\]

Now we are ready to prove Theorem 1.

Proof of Theorem 1(III) under Condition 1 with \( \bar{p} > 0 \). The proof is separated for two cases: \( \lambda^* > 0 \) or \( \lambda^* = 0 \). For each case we prove by constructing a primal (approximate) optimal solution.

When \( \lambda^* > 0 \), we take a probability measure \( \gamma \), such that

\[
d\gamma(x, z) = \frac{\exp \left( \frac{\phi(\lambda^*; x, z)}{\lambda^* e} \right)}{\int \exp \left( \frac{\phi(\lambda^*; x, u)}{\lambda^* e} \right) \, dv(u)} \, dv(z) \, d\widehat{\mathbf{P}}(x), \quad \text{where } \phi(\lambda; x, z) = f(z) - \lambda c(x, z).
\]
Also define the primal (approximate) optimal distribution
\[ \mathbb{P}_* := \text{Proj}_{2\gamma_\ast}. \]

Recall the expression of the Sinkhorn distance in Definition 1, one can verify that
\[
\mathcal{W}_\varepsilon(\mathbb{P}, \mathbb{P}_*) = \inf_{y \in \Gamma(\mathbb{P}, \mathbb{P}_*)} \left\{ \mathbb{E}_y \left[ c(x, z) + \varepsilon \log \left( \frac{d\gamma_\ast(x, z)}{d\mathbb{P}(x) d\nu(z)} \right) \right] \right\} 
\]
\[
\leq \mathbb{E}_{\gamma_\ast} \left[ c(x, z) + \varepsilon \log \left( \frac{d\gamma_\ast(x, z)}{d\mathbb{P}(x) d\nu(z)} \right) \right] 
\]
\[
= \mathbb{E}_{\gamma_\ast} \left[ c(x, z) + \varepsilon \log \left( \frac{\exp \left( \frac{\phi(\lambda_\ast; x, x)}{\lambda_\ast} \right)}{\exp \left( \frac{\phi(\lambda_\ast; u, u)}{\lambda_\ast} \right) d\nu(u)} \right) \right] 
\]
\[
= \frac{1}{\lambda_\ast} \left\{ \iiint f(z) \exp \left( \frac{\phi(\lambda_\ast; x, z)}{\lambda_\ast} \right) d\nu(z) d\mathbb{P}(x) - \lambda_\ast \varepsilon \int \log \left( \int \exp \left( \frac{\phi(\lambda_\ast; x, u)}{\lambda_\ast} \right) d\nu(u) \right) d\mathbb{P}(x) \right\},
\]
where the second relation is because \( \gamma_\ast \) is a feasible solution in \( \Gamma(\mathbb{P}, \mathbb{P}_*) \), the third and the fourth relation is by substituting the expression of \( \gamma_\ast \). Since \( \mathbb{P} > 0 \) and the dual minimizer \( \lambda_\ast > 0 \), the optimality condition in (6) holds, which implies that \( \mathcal{W}_\varepsilon(\mathbb{P}, \mathbb{P}_*) \leq \rho \), i.e., the distribution \( \mathbb{P}_* \) is primal feasible for the problem (Sinkhorn DRO). Moreover, we can see that the primal optimal value is lower bounded by the dual optimal value:
\[
V \geq \mathbb{E}_\mathbb{P} \left[ f(z) \right] = \int f(z) d\gamma_\ast(x, z) 
\]
\[
= \iiint f(z) \left( \frac{d\gamma_\ast(x, z)}{d\mathbb{P}(x) d\nu(z)} \right) d\nu(z) d\mathbb{P}(x) 
\]
\[
= \iiint f(z) \exp \left( \frac{\phi(\lambda_\ast; x, z)}{\lambda_\ast} \right) \frac{d\nu(z) d\mathbb{P}(x)}{\int \exp \left( \frac{\phi(\lambda_\ast; u, u)}{\lambda_\ast} \right) d\nu(u)} 
\]
\[
= \lambda_\ast \left[ \rho + \varepsilon \int \log \left( \int \exp \left( \frac{\phi(\lambda_\ast; x, z)}{\lambda_\ast} \right) d\nu(z) \right) d\mathbb{P}(x) \right] 
\]
\[
= V_D,
\]
where the third equality is based on the optimality condition in Lemma 4. This, together with the weak duality result, completes the proof for \( \lambda_\ast > 0 \).

When \( \lambda_\ast = 0 \), the optimality condition in Lemma 3 holds. We construct the primal (approximate) solution \( \mathbb{P}_* = \text{Proj}_{2\gamma_\ast} \), where \( \gamma_\ast \) satisfies
\[
d\gamma_\ast(x, z) = d\gamma_\ast^\varepsilon(z) d\mathbb{P}(x), \quad \text{where} \quad d\gamma_\ast^\varepsilon(y) = \begin{cases} \frac{d\gamma_\ast^\varepsilon}{d\mathbb{P}(x) d\nu(z)} d\mathbb{P}(x), & \text{if } z \notin A, \\ e^{-\varepsilon(c(x, z))} \frac{d\gamma_\ast^\varepsilon}{d\mathbb{P}(x) d\nu(z)} d\mathbb{P}(x), & \text{if } z \in A. \end{cases}
\]

We can verify easily that the primal solution is feasible based on the optimality condition \( \mathbb{P}_* \geq 0 \) in Lemma 3. Moreover, we can check that the primal optimal value is lower bounded by the dual optimal value:
\[
V \geq \int f(z) d\gamma_\ast(x, z) = \iiint f(z) d\gamma_\ast^\varepsilon(z) d\mathbb{P}(x) = \iiint \text{ess sup} f d\gamma_\ast^\varepsilon(z) d\mathbb{P}(x) = \text{ess sup} \int f = V_D,
\]
where the second equality is because that \( z \in A \) so that \( f(z) = \text{ess sup}_v f \). This, together with the weak duality result, completes the proof for \( \lambda^* = 0 \). \( \square \)

**Remark 5 (Worst-case Distribution).** From the proof presented above we observe that when \( \lambda^* > 0 \), the worse-case distribution for (Sinkhorn DRO) can be expressed as

\[
d\hat{P}_\ast(z) = \int \left( \frac{e^{f(z)/(\lambda^* \epsilon)}}{\mathbb{E}_{Q_{\delta_i,\epsilon}}[e^{f(z)/(\lambda^* \epsilon)}]} \right) d\hat{P}(x),
\]

from which we can see that the worst-case distribution shares the same support as the measure \( \nu \). Particularly, when \( \hat{P} \) is the empirical distribution \( \frac{1}{n} \sum_{i=1}^n \delta_{\hat{x}_i} \) and \( \nu \) is any continuous distribution on \( \mathbb{R}^d \), the worst-case distribution \( P_\ast \), is supported on the entire \( \mathbb{R}^d \). In contrast, the worst-case distribution for Wasserstein DRO is supported on at most \( n + 1 \) points [45]. This is another difference, or advantage possibly, of Sinkhorn DRO compared with Wasserstein DRO. Indeed, for many practical problems, the underlying distribution can be modeled as a continuous distribution. The worst-case distribution for Wasserstein DRO is often finitely supported, raising the concern of whether it hedges against the wrong family of distributions and thus results in suboptimal solutions. The numerical results in Section 5 demonstrate some empirical advantages of Sinkhorn DRO. \( \blacktriangle \)

### 4. Efficient First-order Algorithm for Data-driven Sinkhorn Robust Learning

In this section, we consider the data-driven Sinkhorn robust learning problem, where we seek an optimal decision to minimize the worst-case risk

\[
\inf_{\theta \in \Theta} \sup_{P \in B_{\rho,\epsilon}(\hat{P})} \mathbb{E}_{z \sim P}[f_\theta(z)],
\]

where the feasible set \( \Theta \) contains all possible candidates of decision vector \( \theta \), and we take \( \hat{P} \) as the empirical distribution corresponding to sample points \( \hat{x}_i, i = 1, \ldots, n \). Based on our strong dual (dual), we reformulate (7) as

\[
\inf_{\theta \in \Theta, \lambda \geq 0} \left\{ \frac{F(\lambda, \theta)}{\lambda \bar{p}} + \frac{1}{n} \lambda \epsilon \log \left( \mathbb{E}_{Q_{\delta_i,\epsilon}} \left[ \exp \left( \frac{f_\theta(z)}{\lambda \epsilon} \right) \right] \right) \right\},
\]

where the constant \( \bar{p} \) and the distribution \( Q_{\delta_i,\epsilon} \) are defined in (1) and (2), respectively.

In Example 1 we have seen an instance of (8) where we can get a closed-form expression for the above integration. In general, when a closed-form expression is not available, in the following we present a first-order algorithm to solve this problem, and discuss some alternatives in Section 4.1. Observe that the objective function of (8) involves a nonlinear transformation of the expectation, thus an unbiased gradient estimate could be challenging when \( Q_{\delta_i,\epsilon} \) is a general probability distribution. We propose to solve the following approximation

\[
\inf_{\theta \in \Theta, \lambda \geq 0} \left\{ \hat{F}(\lambda, \theta) := \frac{1}{n} \lambda \epsilon \log \left( \mathbb{E}_{\hat{Q}_{\delta_i,\epsilon}} \left[ \exp \left( \frac{f_\theta(z)}{\lambda \epsilon} \right) \right] \right) \right\},
\]

where \( \hat{Q}_{\delta_i,\epsilon} := \frac{1}{m} \sum_{i=1}^m \delta_{\hat{x}_i,\epsilon} \) denotes the empirical distribution constructed from \( \{\hat{x}_i,\epsilon\}_{i=1}^m \), independent and identically distributed samples from \( Q_{\delta_i,\epsilon} \). In many cases, generating samples from \( Q_{\delta_i,\epsilon} \) is easy. For instance, choosing the cost function \( c(\cdot, \cdot) = \frac{1}{2} \|\cdot - \cdot\|_2^2 \) and \( Z = \mathbb{R}^d \), then the distribution \( Q_{\delta_i,\epsilon} \) becomes a Gaussian distribution \( \mathcal{N}(\hat{x}_i, \sigma^2 I_d) \). Otherwise we can generate samples by, for example, the acceptance-rejection method [5]. As a brief summary of our proposed method, we first simulate a batch of samples to approximate the original Sinkhorn DRO dual objective function, and then use projected
Algorithm 1 A batch gradient descent with bisection search for solving (9)

Require: An interval $[\lambda_l, \lambda_u]$ so that $0 < \lambda_l \leq \lambda^* \leq \lambda_u$, where $\lambda^*$ is an optimal dual variable for (9).

Terminating tolerance $\Delta > 0$.
1: for $t = 0, 1, \ldots, T - 1$ do
2: \hspace{1em} $\lambda_0 \leftarrow (\lambda_l + \lambda_u)/2$.
3: \hspace{1em} Solve the subproblem (10) at $\lambda_0$ to get $\theta_0$.
4: \hspace{1em} Compute $a \in \partial \hat{f}(m)(\lambda_0, \theta_0)$.
5: \hspace{1em} Terminate the iteration if $a = 0$ or $\lambda_u - \lambda_l < \Delta$.
6: \hspace{1em} Let $t_u \leftarrow t_0$ when $a > 0$. Let $t_i \leftarrow t_0$ when $a < 0$.
7: end for

Return $\lambda_0$ and $\theta_0$.

gradient descent with bisection search to solve the approximated problem. Hence our method is named the batch gradient descent with bisection search.

When the function $f_\theta(z)$ is convex in $\theta$, problem (9) is a finite convex programming because the second term of the objective function $\hat{f}(m)(\lambda, \theta)$ in (9) is a perspective transformation [21, Section 2.3.3] of the log-sum-exp function in composition of a convex function. We develop a customized batch gradient descent with bisection search method to solve problem (9) efficiently. The gradient of the objective function of (9) can be calculated as

$$\nabla_\theta \hat{f}(m)(\lambda, \theta) = \frac{1}{n} \sum_{i=1}^{n} \frac{E_{\hat{Q}^m_{\hat{x}_i}}[e^{f_\theta(z)/(\lambda \epsilon)} \nabla_\theta f_\theta(z)]}{E_{\hat{Q}^m_{\hat{x}_i}}[e^{f_\theta(z)/(\lambda \epsilon)}]}$$

$$\frac{\partial}{\partial \lambda} \hat{f}(m)(\lambda, \theta) = \bar{\nu} + \frac{c}{n} \sum_{i=1}^{n} \log \left( \frac{E_{\hat{Q}^m_{\hat{x}_i}}[e^{f_\theta(z)/(\lambda \epsilon)}]}{E_{\hat{Q}^m_{\hat{x}_i}}[e^{f_\theta(z)/(\lambda \epsilon)}]} \right) - \frac{1}{n} \sum_{i=1}^{n} \frac{E_{\hat{Q}^m_{\hat{x}_i}}[e^{f_\theta(z)/(\lambda \epsilon)}]}{\lambda E_{\hat{Q}^m_{\hat{x}_i}}[e^{f_\theta(z)/(\lambda \epsilon)}]}.$$

For fixed $\lambda > 0$, denote $\hat{F}^{(m)}_\lambda$ as the optimal value of the following problem

$$\hat{F}^{(m)}_\lambda = \lambda \bar{\nu} + \inf_{\theta \in \Theta} \left\{ \frac{1}{n} \sum_{i=1}^{n} \lambda \epsilon \log \left( E_{\hat{Q}^m_{\hat{x}_i}}[e^{f_\theta(z)/(\lambda \epsilon)}] \right) \right\}.$$  \hspace{1em} (10)

By the convexity of $f^{(m)}(\lambda, \theta)$, the function $\hat{F}^{(m)}_\lambda$ is convex in $\lambda$. This, together with the fact that $\hat{F}^{(m)}_\lambda$ is sub-differentiable with respect to $\lambda$, motivates us to use the bisection search method in Algorithm 1 to solve problem (9). In particular, in each iteration we first find the optimal solution to problem (10) for a fixed $\lambda$, and then use the bisection method to search for the optimal $\lambda$. When the gradient $\nabla_\theta f_\theta(z)$ is bounded for any $\theta$ and $z$, the sub-problem (10) can be solved using the projected gradient method with convergence rate $O(1/\sqrt{M})$, where $M$ denotes the number of inner iterations [58, Theorem 2.5]. We also argue that the iteration points of Algorithm 1 converge to the optimal solution of $\inf_{\lambda \geq 0} \hat{F}^{(m)}_\lambda$ with linear rate.

Proposition 1. Suppose the function $f_\theta(z)$ is convex in $\theta$. Then the iteration points $\{\lambda^t\}_t$ of Algorithm 1 converge into $\lambda$, linearly, i.e., $|\lambda^t - \lambda^*| = O(2^{-t})$, where $\lambda^*$ is the optimal solution of $\inf_{\lambda \geq 0} \hat{F}^{(m)}_\lambda$.

Our last result in this section establishes the consistency for the Monte Carlo approximation (9).

Proposition 2. Let $S^*$ and $V^*$ be the set of optimal solutions and the corresponding optimal value of problem (8), respectively. And let $S^{(m)}$ and $V^{(m)}$ be the set of optimal solutions and the optimal value to problem (9), respectively. Assume that

1. The function $f_\theta(z)$ is random lower semi-continuous, and convex in $\theta$. The set $\Theta$ is closed, convex, and contains a non-empty interior.
The value function $F(\lambda, \theta)$ defined in (8) is lower semi-continuous, and there exists a point $(\bar{\lambda}, \bar{\theta}) \in \Xi$ such that $F(\lambda, \theta) < \infty$ for all $(\lambda, \theta)$ in a neighborhood of $(\bar{\lambda}, \bar{\theta})$.

(III) The set $S^*$ is non-empty and bounded.

Then as $m \to \infty$, $V^{(m)} \to V^*$ almost surely and $\text{Dist}(S^{(m)}, S^*) \to 0$ almost surely.

This indicates that we can obtain a near-optimal solution of (Sinkhorn DRO) with an arbitrarily small sub-optimality gap as long as we increase the number of simulation times for Monte Carlo approximation. The proof leverages results from [84], while the key difference is that the objective function studied in this paper involves the nonlinear transform of the expectation such that the existing result in [84] cannot be applied directly. A detailed proof can be found in Appendix EC.5.

4.1. Alternative Algorithmic Choices

In this subsection, we discuss some other possibilities for designing an algorithm to solve (8).

As the objective in (8) involves the composition of two expectations, a natural idea to solve this problem is to design algorithms leveraging techniques from stochastic compositional optimization problem [99, 50, 106], but they cannot be applied directly here because they assume that the inner expected-value is independent of the randomness in the outer expectation, while the inner expectation of our objective in (8) depends on samples $\tilde{x}_i, i = 1, \ldots, n$. The recent conditional stochastic compositional (CSCO) optimization [54, 55], which aims to minimize a composition of two expected-value functions with the inner expectation taken with respect to a conditional distribution, also opens the door for designing efficient algorithms for solving (8). Although the objective in (8) cannot be written as a CSCO problem, it naturally fits the structure when the dual variable $\lambda > 0$ is fixed. However, we find that it takes relatively long time to obtain an optimal variable $\theta$ when $\lambda$ is fixed, as the lack of strong-convexity and smoothness structure of the objective makes the state-of-the-art CSCO algorithm (BSGD in [54]) difficult to converge empirically. Since we need to optimize variables $(\lambda, \theta)$ jointly, the global convergence of CSCO for the problem (8) is even more challenging. In extensive simulations that we omit, we find that our proposed method solves the Sinkhorn DRO problem more efficiently than the state-of-the-art CSCO algorithm and standard projected gradient descent without bisection search.

In our algorithm, we optimize $\theta$ for a fixed $\lambda$. An alternative would be to optimize $(\lambda, \theta)$ jointly. However, as pointed out in [66], for $\lambda$ of a small value, the variance of the gradient estimate of the objective function with respect to $\lambda$ is unstable. Hence, we develop a bisection method to update $\lambda$ in outer iterations in Algorithm 1.

Moreover, we observe that in each inner iteration for solving the sub-problem (10), the most computationally expensive step is to obtain the gradient of $\hat{F}_\lambda^{(m)}$, the complexity of which is of $O(nm)$. For large-scale statistical learning problems, it is therefore promising to use the projected stochastic gradient method instead of projected gradient descent to solve the sub-problem (10), but the condition that guarantees convergence is more restrictive, which can be a topic for future study. For small-scale problems, one can also write the problem in standard conic optimization form and use the interior point method [68, 52] to solve it.

We use the Monte Carlo samples problem (9) to approximat (8). It is promising to use other numerical integration techniques such as Quasi-Monte Carlo method [72] and Wavelet method [6] to approximate the objective (8) efficiently, which is of research interest for future study.

5. Applications

In this section, we apply our methodology on three applications: the newsvendor model, mean-risk portfolio optimization, and semi-supervised learning. We examine the performance of the (Sinkhorn DRO) model by comparing it with three benchmarks: (i) the classical sample average approximation (SAA) model; (ii) the Wasserstein DRO model; and (iii) the KL-divergence DRO model. Unless otherwise specified, the cost function is chosen to be $c(\cdot, \cdot) = \frac{1}{2} \| \cdot - \cdot \|$, and the reference measure $\nu$ for the Sinkhorn distance is chosen to be the Lebesgue measure.
For each of the three applications, with \( n \) training samples, we select the pair of hyper-parameters \( (\epsilon, \overline{\rho}) \) using the \( K \)-fold cross-validation method with \( K = 10 \). Since the grid search for an optimal pair of hyper-parameters is more costly than the search for a single hyper-parameter, we first tune the hyper-parameter \( \epsilon \) while fixing \( \overline{\rho} = 0 \), which corresponds to the SAA problem in (5). Then for the chosen \( \epsilon \), we tune the Sinkhorn radius \( \overline{\rho} \). We run the repeated experiments for 200 times.

In Section 5.1 and Section 5.2, we measure the out-of-sample performance of a solution \( \theta \) by its relative performance gap \( \frac{f(\theta) - f^*}{1 + f^*} \), where \( f^* \) denotes the true optimal value when the true distribution is known exactly, and \( f(\theta) \) the expected loss of the solution \( \theta \) under the true distribution, estimated through an SAA objective value with \( 10^5 \) testing samples. Thus, the smaller the relative performance gap is, the better out-of-sample performance the solution has.

Further details are included in Appendix EC.1.

### 5.1. Newsvendor Model

We consider the following distributionally robust newsvendor model:

\[
\min_{\theta} \max_{\mathbb{P} \in B_{\rho,\sigma}(\mathbb{P}_s)} \left\{ \mathbb{E}_\mathbb{P}[k\theta - u \min\{\theta,z\}] \right\},
\]

where the random variable \( z \) stands for the random demand; its empirical distribution \( \mathbb{P}_s \) consists of \( n = 20 \) independent samples from an exponential distribution \( \mathbb{P}_s \), with the density \( f(x; s) = \frac{1}{s} \exp\left(-\frac{x}{s}\right) \), where \( s \in \{0.25, 0.5, 0.75, 1, 2, 4\} \); the decision variable \( \theta \) represents the inventory level; and \( k = 5, u = 7 \) are constants corresponding to overage and underage costs, respectively.

Values of hyper-parameters are recorded in Table 1, from which we can see that the optimal entropic regularization parameter \( \epsilon \) increases when the distribution scale parameter \( s \) increases. This is because a distribution \( \mathbb{P}_s \) with larger value of \( s \) has larger variance, and to achieve better out-of-sample performance, a larger entropic regularization parameter \( \epsilon \) is needed to encourage larger spread of probability mass.

| Parameter \( s \) | Regularization \( \epsilon \) | Sinkhorn Radius \( \overline{\rho} \) | Wasserstein Radius \( \rho \) | KL-DRO Radius \( \eta \) |
|------------------|-------------------|-----------------|-----------------|-----------------|
| 0.25             | 2e-2              | 1e-2            | 1e-3            | 2e-3            |
| 0.5              | 5e-2              | 6e-3            | 2e-3            | 7e-3            |
| 0.75             | 8e-2              | 1e-3            | 1e-2            | 2e-2            |
| 1                | 2e-1              | 6e-3            | 3e-1            | 1e-2            |
| 2                | 4e-1              | 1e-2            | 3e-1            | 4e-2            |
| 4                | 1e-0              | 6e-2            | 4e-1            | 5e-3            |

We report the violin plots, i.e., box plots with shapes formed by kernel density estimation, for the relative performance gap across different approaches in Fig. 1. We find that Sinkhorn DRO has the best out-of-sample mean/median performance in all figures, and has the most stable performance as indicated by the most concentrated violin plot. Wasserstein DRO, on the other hand, has a comparable performance as SAA when \( s \) is small (and small radius \( \rho \), as indicated in Table 1), but is even worse than SAA for large \( s \) (and large \( \rho \), as indicated in Table 1). This is because for small \( \rho \), the Wasserstein robust solution coincides with the SAA solution and thus does not regularizer the problem, similar to the observation made in [65, Remark 6.7] when the support of \( \mathbb{P}_s \) is \( \mathbb{R} \); whereas for large \( \rho \), it hedges distributions that are too extreme (which puts positive probability mass on zero demand), leading to an overly conservative solution. Moreover, the KL-divergence DRO does not have much improvement compared with the SAA model, likely because the induced worst-case distribution shares the same support as the empirical distribution.
5.2. Mean-risk Portfolio Optimization

We consider the following distributionally robust mean-risk portfolio optimization problem

$$\min_{\theta} \max_{P \in B(U, \bar{\theta})} \mathbb{E}_P [\theta^T z] + \rho \cdot \mathbb{P} \text{-CVaR}_\alpha (\theta^T z)$$

subject to \( \theta \in \Theta = \{ \theta \in \mathbb{R}_+^d : \theta^T 1 = 1 \} \),

where the random vector \( z \in \mathbb{R}^d \) stands for the returns of assets; the decision variable \( \theta \in \Theta \) represents the portfolio strategy that invests a certain percentage \( \theta_i \) of the available capital in the \( i \)-th asset; and the term \( \mathbb{P} \text{-CVaR}_\alpha (\theta^T z) \) quantifies conditional value-at-risk [80], i.e., the average of the \( \alpha \times 100\% \) worst portfolio losses under the distribution \( P \). We follow a similar setup as in [65]. Specifically, we set \( \alpha = 0.2, \rho = 10 \). The random asset \( z \sim P \) can be decomposed into a systematic risk factor \( \psi \in \mathbb{R} \) and idiosyncratic risk factors \( \epsilon \in \mathbb{R}_+^d \):

$$z_i = \psi + \epsilon_i, \quad i = 1, 2, \ldots, D,$$

where \( \psi \sim \mathcal{N}(0, 0.02) \) and \( \epsilon_i \sim \mathcal{N}(i \times 0.03, i \times 0.025) \). We fixed the training sample size \( n = 20 \) and vary the number of assets \( D \in \{10, 20, 50\} \). We solve this problem using Algorithm 1, in which the projected gradient descent step to update \( \theta \) follows the implementation in [26] to project onto the probability simplex \( \Theta \).

The violin plots for the relative performance gap across different approaches are reported in Fig. 2. Similar as the finding in Section 5.1, both the Wasserstein DRO and KL-divergence DRO models do not outperform the SAA method too much, while Sinkhorn DRO has the best out-of-sample performance for all plots as indicated by the smallest mean/median as well as the most concentrated violin plots, and the contrast is more apparent when the dimension \( D \) is large.

5.3. Semi-supervised Learning

Our last example is a semi-supervised learning task following a similar setup as in [15]. Suppose we have a training data set \( D_n = \{(X_i, Y_i)\}_{i=1}^n \), where \( Y_i \in \{-1, 1\} \) denotes the label of the \( i \)-th observation.
Additionally, we have a set of unlabeled observations \( \{X_i\}_{i=1}^N \). We build the set \( \mathcal{E}_{N-n} = \{(X_i, 1)\}_{i=1}^N \cup \{(X_i, -1)\}_{i=1}^N \), which means we replicate each unlabeled data point twice, recognizing that the missing label can be any of the two available alternatives. Then we formulate an empirical distribution consisting of samples from the set \( \mathcal{X}_N = \mathcal{D}_n \cup \mathcal{E}_{N-n} \), which is denoted as \( \hat{\mathbb{P}} \). Considering the following distributionally robust formulation:

\[
\min_{\theta} \max_{P \in \mathbb{B}(\hat{\mathbb{P}})} \mathbb{E}_P[\ell(\theta; (X, Y))]
\]

where \( \ell(\theta; (X, Y)) = \log(1 + \exp(-Y \cdot \theta^T X)) \).

We also solve this task using the other three benchmark models. The cost function over this subsection is set to be

\[
c((x, y), (x', y')) = \frac{1}{2} ||x - x'||^2 1\{y = y'\} + \kappa 1\{y \neq y'\},
\]

where the parameter \( \kappa = \infty \) means that there is no labeling error. In this case, in the duality result for the Sinkhorn DRO, we only need to robustify the feature vectors \( X \).

We consider three performance measures for the obtained classifiers: (i) the training error of samples with known labels; (ii) the training error of samples with unknown labels; and (iii) the testing error for new observations. The experiment is conducted using 4 binary classification real data sets from UCI machine learning data base [39]. In each of the repeated experiments for each data set, we randomly partition the collected samples into training and testing data sets.

Classification results for these different approaches are reported in Table 2, where the first number of each entry represents the average classification error, and the second number of entry represents the half-length of the 95% confidence interval. Detailed parameters for the settings of this task and the choices of hyper-parameters are reported in Appendix EC.1. We observe that though the Sinkhorn DRO does not have the best in-sample performance (as indicated by the training error of samples with known labels), it has the best out-of-sample performance for all data sets (as indicated by the smallest training error of samples with unknown labels and the smallest testing error).

6. Concluding Remarks

In this paper, we investigated a new distributionally robust optimization framework based on the Sinkhorn distance. By developing a strong dual reformulation and a customized batch gradient descent with bisection search algorithm, we have shown that the resulting DRO problem is tractable under mild assumptions, greatly spans the tractability of Wasserstein DRO. Analysis on the worst-case distribution indicates that Sinkhorn DRO hedges a more reasonable set of adverse scenarios and thus less conservative compared with Wasserstein DRO, which is then demonstrated via extensive numerical experiments. Based on theoretical and numerical findings, we conclude that the Sinkhorn
distance is a promising candidate for modeling distributional ambiguities in decision-making under uncertainty from the perspective of computational tractability, modeling rationality and out-of-sample performance.

In the meantime, several topics worth in-depth investigating are left for future works. First, it is interesting to design efficient first-order algorithms for Sinkhorn DRO when the nominal distribution is arbitrary or when the loss function is non-convex in the decision variable. Second, it is important to study the optimal selection of hyper-parameters in Sinkhorn DRO, including the radius of the ambiguity set \( \tilde{\rho} \), the entropic regularization parameters \( \epsilon \), and reference measures \( \nu \). Third, regularization of Wasserstein distance beyond the entropic regularization as in Sinkhorn distance is worth exploring. Last, we are enthusiastic to explore applications of the Sinkhorn DRO for other problems in operations research and machine learning.

### Table 2

Classification results on real datasets for the semi-supervised learning task. Each experiment is repeated for 200 independent trials, and 95% confidence intervals of classification errors are reported for different approaches.

| Dataset     | SAA       | Sinkhorn | Wasserstein | KL-divergence |
|-------------|-----------|----------|-------------|---------------|
| Breast Cancer | Train (Labeled) | .058 ± .061 | .051 ± .065 | .051 ± .063 | .057 ± .060 |
|             | Test Error | .19 ± .073 | .11 ± .067 | .17 ± .075 | .19 ± .073 |
| Magic       | Train (Labeled) | .17 ± .12 | .18 ± .11 | .17 ± .11 | .15 ± .12 |
|             | Test Error | .28 ± .064 | .25 ± .074 | .27 ± .077 | .26 ± .078 |
| QSAR Bio    | Train (Labeled) | .12 ± .067 | .15 ± .076 | .16 ± .073 | .11 ± .066 |
|             | Test Error | .25 ± .057 | .22 ± .063 | .23 ± .073 | .25 ± .037 |
| Spambase    | Train (Labeled) | .10 ± .046 | .10 ± .048 | .096 ± .045 | .10 ± .043 |
|             | Test Error | .19 ± .038 | .14 ± .046 | .16 ± .036 | .18 ± .034 |
Appendix A: Sufficient condition for Assumption 1

Proposition 3. Assumption 1 holds if there exists \( p \geq 1 \) so that the following conditions are satisfied:

(I) For any \( x, y, z \in \mathcal{Z} \), \( c(x, y) \geq 0 \), and

\[
(c(x, y))^{1/p} \leq (c(x, z))^{1/p} + (c(z, y))^{1/p}.
\]

(II) The nominal distribution \( \hat{\mathbb{P}} \) has a finite mean, denoted as \( \bar{x} \). Moreover, \( \nu\{z : 0 \leq c(\bar{x}, z) < \infty\} = 1 \) and

\[
\Pr_{x \sim \mathbb{P}} \{c(x, \bar{x}) < \infty\} = 1.
\]

(III) There exists \( \lambda > 0 \) such that

\[
\int e^{(z)(\lambda e)} e^{-2^p c(\bar{x}, z)/\epsilon} d\nu(z) < \infty.
\]

We make some remarks for the sufficient conditions listed above. The first condition can be satisfied by taking the cost function as the \( p \)-th power of the metric defined on \( \mathcal{Z} \) for any \( p \geq 1 \). The second condition requires the nominal distribution \( \hat{\mathbb{P}} \) is finite almost surely, e.g., it can be a subgaussian distribution with respect to the cost function \( c \). Combining three conditions together and leveraging concentration arguments completes the proof of Proposition 3.
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Proofs of Statements

Appendix EC.1: Detailed Experiment Setup

All the experiments are performed on a MacBook Pro laptop with 32GB of memory running Python 3.7. Candidates of hyper-parameters for DRO models are listed as follows. In each experiment we pick the regularization term $\epsilon$ spaced from $1e-3$ to $9e-1$ in exponentially increasing steps. The Sinkhorn radius $\rho$ and KL-DRO radius $\eta$ are chosen spaced from $1e-3$ to $9e-1$ in exponentially increasing steps. Hyper-parameters for the second and third experiments are reported in Table EC.1 and Table EC.2, respectively. To obtain the Monte Carlo approximated objective function for the Sinkhorn DRO model, we take the nominal distribution $\hat{P}$ as the empirical distribution based on collected samples, and the inner batch size $m = 20$. We use the projected gradient descent method to solve the subproblem in (10). For portfolio optimization problems we try the step size $\eta_{\ell} = \frac{1}{\sqrt{\ell+1}}$ for the $\ell$-th inner iteration. Otherwise we try the step size $\eta_{\ell} = \frac{1}{\ell+1}$ during the $\ell$-th inner iteration. Denote by $\text{obj}_{\ell}$ the objective function obtained at the $\ell$-th iteration. The inner iteration is terminated when $\|\text{obj}_{\ell+1} - \text{obj}_{\ell}\| \leq 1e-3$.

The SAA, Wasserstein DRO, and KL-divergence DRO models are solved exactly based on the interior point method-based solver Mosek [4]. In particular, based on [65, Corollary 5.1], the Wasserstein DRO formulation for the newsvendor problem in Section 5.1 becomes

$$
\min_{\theta, \lambda, s, y} \lambda \rho + \frac{1}{n} \sum_{i=1}^{n} s_i
$$

s.t. $(k-u)\theta + y_{i,1}\hat{z}_i \leq s_i, i \in [n],$

$k\theta - u\hat{z}_i + y_{i,1}\hat{z}_i \leq s_i, i \in [n],$

$y_{i,1} \leq \lambda, i \in [n],$

$| - y_{i,2} + u | \leq \lambda, i \in [n],$

$y \geq 0,$

where $\{\hat{z}_1, \ldots, \hat{z}_n\}$ denotes collected samples from $\hat{P}_\pi$. From [65, Eq. (27)] we can see that the Wasserstein DRO formulation for the portfolio optimization problem becomes

$$
\min_{\theta, r, s, \lambda} \lambda \rho + \frac{1}{n} \sum_{i=1}^{n} s_i
$$

s.t. $\theta \in \Theta,$

$b_j \tau + a_j(\theta, \hat{z}_i) \leq s_i, i \in [n], j \in [H],$

$\|a_j\theta\|_2 \leq \lambda, j \in [H].$

Recall that the KL-divergence DRO problem with radius $\eta \geq 0$ has the following tractable formulation:

$$
\min_{\theta \in \Theta, \lambda \geq 0} \left\{ \lambda \eta + \lambda \log \left( \mathbb{E}_{\hat{P}} \left[ e^{\theta(x)/\lambda} \right] \right) \right\} .
$$
Table EC.1  Values of selected hyper-parameters by cross-validation for the portfolio optimization problem.

| Dimension $D$ | Regularization $\epsilon$ | Sinkhorn Radius $\bar{\rho}$ | Wasserstein Radius $\rho$ | KL-DRO Radius $\eta$ |
|---------------|-----------------------------|-------------------------------|---------------------------|----------------------|
| 10            | 5e-2                        | 2e-4                          | 6e-3                      | 1e-3                 |
| 20            | 7e-1                        | 3e-4                          | 5e-2                      | 2e-3                 |
| 50            | 4e-1                        | 2e-4                          | 1e-3                      | 2e-3                 |

Table EC.2  Values of classification parameters and hyper-parameters for DRO models.

|                    | Breast Cancer | Magic | QSAR Bio | Spambase |
|--------------------|---------------|-------|----------|----------|
| Number of Predictors | 30            | 10    | 30       | 56       |
| Train Size (Labeled) | 40            | 30    | 80       | 150      |
| Train Size (Unlabeled) | 200          | 300   | 500      | 600      |
| Test Size          | 329           | 18690 | 475      | 3850     |
| Sinkhorn Para. $(\bar{\rho}, \epsilon)$ | (2e-1,2e-5)   | (5e-1,6e-2) | (8e-1,2e-3) | (9e-3,2e-5) |
| Wasserstein Para. $\rho$ | 1e-3          | 3e-3  | 3e-1     | 1e-2     |
| KL-DRO Para. $\eta$ | 2e-3          | 5e-3  | 3e-2     | 4e-2     |
Appendix EC.2: Proofs of Technical Results in Section 3.1

In order to show the strong duality result in Theorem 1 when $\widehat{P}$ is an empirical distribution, we present the following technical lemma.

**Lemma EC.1.** For fixed $\tau$ and a reference probability distribution $Q \in \mathcal{P}(Z)$, consider the optimization problem

$$
\nu(\tau) = \sup_{P \in \mathcal{P}(Z)} \left\{ E_P \left[ f(z) - \tau \log \left( \frac{dP(z)}{dQ(z)} \right) \right] \right\}.
$$

(I) When $\tau = 0$,

$$
\nu(0) = \underset{Q}{\text{ess sup}}(f) \triangleq \inf \{ t \in \mathbb{R} : \Pr_{z \sim Q} \{ f(z) > t \} = 0 \}.
$$

(II) When $\tau > 0$ and

$$
\mathbb{E}_Q \left[ e^{f(z)/\tau} \right] < \infty,
$$

it holds that

$$
\nu(\tau) = \tau \log \left( \mathbb{E}_Q \left[ e^{f(z)/\tau} \right] \right),
$$

and $\lim_{\tau \to 0} \nu(\tau) = \nu(0)$. The optimal solution in (EC.1) has the expression

$$
dP(z) = \frac{e^{f(z)/\tau}}{\int e^{f(u)/\tau} dQ(u)} dQ(z).
$$

(III) When $\tau > 0$ and

$$
\mathbb{E}_Q \left[ e^{f(z)/\tau} \right] = \infty,
$$

we have that $\nu(\tau) = \infty$.

*Proof of Lemma EC.1* We reformulate $\nu(\tau)$ based on the importance sampling trick:

$$
\nu(\tau) = \sup_{L : L \geq 0} \left\{ \int \left[ f(z) L(z) - \tau L(z) \log L(z) \right] dQ(z) : \int L(z) dQ(z) = 1 \right\}.
$$

Then the remaining part follows the discussion in [56, Section 2.1].

*Proof of Corollary 1* We now introduce the epigraphical variables $s_i, i = 1, \ldots, n$ to reformulate $V_D$ as

$$
V_D = \left\{ \begin{array}{l}
\inf_{\lambda \geq 0, s_i} \lambda \overline{p} + \frac{1}{n} \sum_{i=1}^{n} s_i \\
\text{s.t. } \lambda \epsilon \log \left( \mathbb{E}_{Q_{i,\epsilon}} \left[ e^{f(z)/(\lambda \epsilon)} \right] \right) \leq s_i, \forall i
\end{array} \right\}
$$

For fixed $i$, the $i$-th constraint can be reformulated as

$$
\begin{align*}
\left\{ \exp \left( \frac{s_i}{\lambda \epsilon} \right) & \geq \mathbb{E}_{Q_{i,\epsilon}} \left[ e^{f(z)/(\lambda \epsilon)} \right] \right\} \\
= \left\{ 1 \geq \mathbb{E}_{Q_{i,\epsilon}} \left[ e^{f(z)-s_i}/(\lambda \epsilon) \right] \right\} \\
= \left\{ \lambda \epsilon \geq \mathbb{E}_{Q_{i,\epsilon}} \left[ e^{f(z)-s_i}/(\lambda \epsilon) \right] \right\} \\
= \left\{ \lambda \epsilon \geq \sum_{r=1}^{n} Q_{i,\epsilon} (z_r) a_{i,r} \right\} \cap \left\{ a_{i,r} \geq \lambda \epsilon \exp \left( \frac{f(z_r) - s_i}{\lambda \epsilon} \right), \forall r \right\},
\end{align*}
$$

where the second constraint set can be formulated as

$$
(\lambda \epsilon, a_{i,r}, f(z_r) - s_i) \in K_{\exp}.
$$

Substituting this expression into $V_D$ completes the proof. \hfill \Box
Appendix EC.3: Proof of the Technical Result in Section 3.2

Proof of Remark 3  We can reformulate the dual objective function as
\[
v(\lambda; \epsilon) = \lambda \rho + \lambda \epsilon \int \log \left( \int \exp \left( \frac{f(z) - \lambda c(x, z)}{\lambda \epsilon} \right) \, d\nu(z) \right) \, d\widehat{\mathbb{P}}(x).
\]
We take \( \lim_{\epsilon \to 0} \lambda \epsilon \) for the second term in \( v(\lambda; \epsilon) \) to obtain:
\[
\begin{align*}
\lim_{\epsilon \to 0} \lambda \epsilon \int \log \left( \int \exp \left( \frac{f(z) - \lambda c(x, z)}{\lambda \epsilon} \right) \, d\nu(z) \right) \, d\widehat{\mathbb{P}}(x) & \\
= \int \lim_{\beta \to \infty} \frac{\lambda}{\beta} \log \left( \int \exp \left( \frac{[f(z) - \lambda c(x, z)] \beta}{\lambda} \right) \, d\nu(z) \right) \, d\widehat{\mathbb{P}}(x) & \\
= \int \lim_{\beta \to \infty} \lambda \nabla \log \left( \int \exp \left( \frac{[f(z) - \lambda c(x, z)] \beta}{\lambda} \right) \, d\nu(z) \right) \, d\widehat{\mathbb{P}}(x) & \\
= \int \left[ \lim_{\beta \to \infty} \frac{\int \exp \left( \frac{[f(z) - \lambda c(x, z)] \beta}{\lambda} \right) [f(z) - \lambda c(x, z)] \, d\nu(y)}{\int \exp \left( \frac{[f(z) - \lambda c(x, z)] \beta}{\lambda} \right) \, d\nu(y)} \right] \, d\widehat{\mathbb{P}}(x) & \\
= \int \sup_z \left[ f(z) - \lambda c(x, z) \right] \, d\widehat{\mathbb{P}}(x).
\end{align*}
\]

Hence, we conclude that the dual objective function of the Sinkhorn DRO problem converges into that of the Wasserstein DRO problem.  \( \square \)
Appendix EC.4: Proofs of Technical Results in Section 3.3

Proof of Lemma 1  Recall from Remark 4 that the primal problem $V$ can be reformulated as

$$V = \sup_{y_x \in \mathcal{P}(Z), \forall x \in Z} \left\{ \int \mathbb{E}_{y_x} \left[ f(z) \right] \, d\bar{P}(x) : \epsilon \int \mathbb{E}_{y_x} \left[ \log \left( \frac{d y_x(z)}{d Q_{x,\epsilon}(z)} \right) \right] \, d\bar{P}(x) \leq \bar{P} \right\}.$$  

Introducing the Lagrange multiplier $\lambda$ associated to the constraint, we reformulate $V$ as

$$V = \sup_{y_x \in \mathcal{P}(Z), \forall x \in Z} \left\{ \inf_{\lambda \geq 0} \left\{ \lambda \bar{P} + \epsilon \int \mathbb{E}_{y_x} \left[ f(z) - \lambda \epsilon \log \left( \frac{d y_x(z)}{d Q_{x,\epsilon}(z)} \right) \right] \, d\bar{P}(x) \right\} \right\}.$$  

Interchanging the order of the supremum and infimum operators, we have that

$$V \leq \inf_{\lambda \geq 0} \left\{ \lambda \bar{P} + \epsilon \int \mathbb{E}_{y_x} \left[ f(z) - \lambda \epsilon \log \left( \frac{d y_x(z)}{d Q_{x,\epsilon}(z)} \right) \right] \, d\bar{P}(x) \right\}.$$  

Since the optimization over $y_x, \forall x$ is separable for each $x$, by defining

$$v_x(\lambda) = \sup_{y_x \in \mathcal{P}(Z)} \left\{ \mathbb{E}_{y_x} \left[ f(z) - \lambda \epsilon \log \left( \frac{d y_x(z)}{d Q_{x,\epsilon}(z)} \right) \right] \right\}, \forall x,$$

and swap the supremum and the integration, we obtain

$$V \leq \inf_{\lambda \geq 0} \left\{ \lambda \bar{P} + \epsilon \int v_x(\lambda) \, d\bar{P}(x) \right\}. \quad \text{(EC.2)}$$

When there exists $\lambda > 0$ such that Condition 1 holds, by leveraging a well-known reformulation on entropy regularized linear optimization in Lemma EC.1, we can see that almost surely,

$$v_x(\lambda) = \lambda \epsilon \log \left( \mathbb{E}_{Q_{x,\epsilon}} \left[ e^{f(z)/(\lambda \epsilon)} \right] \right) < \infty.$$  

Substituting this expression into (EC.2) implies that $V \leq V_0 < \infty$. Suppose on the contrary that for any $\lambda > 0$,

$$\text{Pr}_{x \sim \mathbb{P}} \left\{ x : \mathbb{E}_{Q_{x,\epsilon}} \left[ e^{f(z)/(\lambda \epsilon)} \right] = \infty \right\} > 0,$$

then intermediately we obtain $V \leq V_0 = \infty$, and the weak duality still holds. □

Proof of Lemma 2  We first show that $\lambda^* < \infty$. Denote by $v(\lambda)$ the objective function for the dual problem, then

$$v(\lambda) = \lambda \bar{P} + \epsilon \int \log \left( \mathbb{E}_{Q_{x,\epsilon}} \left[ e^{f(z)/(\lambda \epsilon)} \right] \right) \, d\bar{P}(x).$$

The integrability condition for the dominated convergence theorem is satisfied, which implies

$$\lim_{\lambda \to \infty} \lambda \epsilon \int \log \left( \mathbb{E}_{Q_{x,\epsilon}} \left[ e^{f(z)/(\lambda \epsilon)} \right] \right) \, d\bar{P}(x)$$

$$= \int \lim_{\beta \to 0} \frac{\epsilon}{\beta} \log \left( \mathbb{E}_{Q_{x,\epsilon}} \left[ e^{\beta f(z)/\epsilon} \right] \right) \, d\bar{P}(x)$$

$$= \int \lim_{\beta \to 0} \epsilon \nabla \beta \log \left( \mathbb{E}_{Q_{x,\epsilon}} \left[ e^{\beta f(z)/\epsilon} \right] \right) \, d\bar{P}(x)$$

$$= \int \lim_{\beta \to 0} \epsilon \frac{1}{\mathbb{E}_{Q_{x,\epsilon}} \left[ e^{\beta f(z)/\epsilon} \right]} \left( \mathbb{E}_{Q_{x,\epsilon}} \left[ \frac{f(z)}{\epsilon} e^{(\beta f(z))/\epsilon} \right] \right) \, d\bar{P}(x)$$

$$= \int \mathbb{E}_{Q_{x,\epsilon}} \left[ f(z) \right] \, d\bar{P}(x),$$
where the first equality follows from the change-of-variable technique with \( \beta = 1/\lambda \), the second equality follows from the L'Hospital rule the third and the last equality follows from the dominated convergence theorem. As a consequence, as long as \( \rho > 0 \), we have

\[
\lim_{\lambda \to \infty} v(\lambda) = \infty.
\]

We can take \( \lambda \) satisfying Condition 1 and then \( v(\lambda) < \infty \), which guarantees the existence of the dual minimizer. Hence \( \lambda^* < \infty \), which implies that either \( \lambda^* = 0 \) or \( \lambda^* \) satisfies Condition 1. \( \Box \)

Proof of Lemma 3  Suppose the dual minimizer \( \lambda^* = 0 \), then taking the limit of the dual objective function gives

\[
\lim_{\lambda \to 0} v(\lambda) = \int H^\mu(x) \, d\tilde{P}(x) < \infty,
\]

where

\[
H^\mu(x) := \inf \{ t : Q_{x,\epsilon} \{ f(z) > t \} = 0 \} \triangleq \text{ess sup } f.
\]

For notational simplicity we take \( H^\mu = \text{ess sup } f \). One can check that \( H^\mu(x) \equiv H^\mu \) for any \( x \in \text{supp}(\tilde{P}) \):

for any \( t \) so that \( Q_{x,\epsilon} \{ f(z) > t \} = 0 \), we have that

\[
\int 1\{f(z) > t\} e^{-c(x,z)/\epsilon} \, dv(z) = 0,
\]

which, together with the fact that \( v\{c(x,z) < \infty\} = 1 \) for fixed \( x \), implies

\[
\int 1\{f(z) > t\} \, dv(z) = 0.
\]

On the contrary, for any \( t \) so that \( v\{f(z) > t\} = 0 \), we have that

\[
0 \leq \int 1\{f(z) > t\} e^{-c(x,z)/\epsilon} \, dv(z) \leq \int 1\{f(z) > t\} \, dv(z) = 0,
\]

where the second inequality is because that \( v\{c(x,z) \geq 0\} = 1 \). As a consequence, \( Q_{x,\epsilon} \{ f(z) > t \} = 0 \). Hence we can assert that \( H^\mu(x) = H^\mu \) for all \( x \in \text{supp}(\tilde{P}) \), which implies

\[
\lim_{\lambda \to 0} v(\lambda) = H^\mu < \infty.
\]

Then we show that almost surely for all \( x \),

\[
E_{Q_{x,\epsilon}} [1_A] > 0, \quad \text{where } A = \{ z : f(z) = H^\mu \}.
\]

Denote by \( D \) the collection of samples \( x \) so that \( E_{Q_{x,\epsilon}} [1_A] = 0 \). Assume the condition above does not hold, which means that \( \tilde{P}\{D\} > 0 \). For any \( \tau > 0 \) and \( x \in D \), there exists \( H^I(x) < H^\mu \) such that

\[
0 < \beta_x := E_{Q_{x,\epsilon}} [1_{B(x)}] \leq \tau, \quad \text{where } B(x) = \{ z : H^I(x) \leq f(z) \leq H^\mu \}.
\]

Define \( H^{\text{gap}}(x) = H^\mu - H^I(x) \), \( \beta_x^c = 1 - \beta_x \). Then we find that for \( x \in D \),

\[
v_x(\lambda) = \lambda \epsilon \log \left( E_{Q_{x,\epsilon}} \left[ e^{f(z)/(\lambda \epsilon)} 1_{B(x)} \right] + E_{Q_{x,\epsilon}} \left[ e^{f(z)/(\lambda \epsilon)} 1_{B(x)^c} \right] \right)
\]

\[
\leq H^\mu + \lambda \epsilon \log \left( \beta_x + e^{-H^{\text{gap}}(x)/(\lambda \epsilon)} \beta_x^c \right).
\]
Since \( \hat{P}\{D\} > 0 \), the dual objective function for \( \lambda > 0 \) is upper bounded as

\[
v(\lambda) = \lambda \hat{\rho} + \int_D v(\lambda) \, d\hat{P}(x) \leq H^u + \lambda \hat{\rho} + \lambda \epsilon \int_D \log \left( \hat{b}_x + e^{-H^{upp}(x)/(\lambda \epsilon)} \hat{b}_x^c \right) \, d\hat{P}(x).
\]

We can see that

\[
\lim_{\lambda \to 0} \lambda \hat{\rho} + \lambda \epsilon \int_D \log \left( \hat{b}_x + e^{-H^{upp}(x)/(\lambda \epsilon)} \hat{b}_x^c \right) \, d\hat{P}(x) = 0,
\]

and

\[
\lim_{\lambda \to 0} \nabla \left[ \lambda \hat{\rho} + \lambda \epsilon \int_D \log \left( \hat{b}_x + e^{-H^{upp}(x)/(\lambda \epsilon)} \hat{b}_x^c \right) \, d\hat{P}(x) \right] = \hat{\rho} + \epsilon \int_D \log (\hat{b}_x) \, d\hat{P}(x)
\]

\[
\leq \hat{\rho} + \epsilon \log (\tau) \hat{P}(D) \leq -\hat{\rho} < 0,
\]

where the second inequality is by taking the constant \( \tau = \exp \left( -\frac{2\pi}{e\hat{P}(D)} \right) \). Hence, there exists \( \lambda > 0 \) such that

\[
v(\lambda) \leq H^u + \lambda \hat{\rho} + \lambda \epsilon \int_D \log \left( \hat{b}_x + e^{-H^{upp}(x)/(\lambda \epsilon)} \hat{b}_x^c \right) \, d\hat{P}(x) < v(0),
\]

which contradicts to the optimality of \( \lambda^* = 0 \). As a result, almost surely for all \( x \), we have that

\[
\mathbb{E}_{Q_{x,\epsilon}}[1_{A}] > 0.
\]

To show the second condition, we re-write the dual objective function for \( \lambda > 0 \) as

\[
v(\lambda) = \lambda \hat{\rho} + \lambda \epsilon \int \left[ \log \left( \mathbb{E}_{Q_{x,\epsilon}}[1_{A}] + \mathbb{E}_{Q_{x,\epsilon}} \left[ e^{[f(z) - H^u]/(\lambda \epsilon)} 1_{A^c} \right] \right) \right] \, d\hat{P}(x) + H^u.
\]

The gradient of \( v(\lambda) \) becomes

\[
\nabla v(\lambda) = \hat{\rho} + \epsilon \int \left[ \log \left( \mathbb{E}_{Q_{x,\epsilon}}[1_{A}] + \mathbb{E}_{Q_{x,\epsilon}} \left[ e^{[f(z) - H^u]/(\lambda \epsilon)} 1_{A^c} \right] \right) \right] \, d\hat{P}(x)
\]

\[
+ \int \frac{\mathbb{E}_{Q_{x,\epsilon}} \left[ e^{[f(z) - H^u]/(\lambda \epsilon)} 1_{A^c} (H^u - f(z))/\epsilon \right]}{\mathbb{E}_{Q_{x,\epsilon}}[1_{A}] + \mathbb{E}_{Q_{x,\epsilon}} \left[ e^{[f(z) - H^u]/(\lambda \epsilon)} 1_{A^c} \right]} \, d\hat{P}(x).
\]

We can see that \( \lim_{\lambda \to 0} \nabla v(\lambda) = \hat{\rho} \). Take

\[
v_{1,\lambda}(\lambda) = \mathbb{E}_{Q_{x,\epsilon}} \left[ e^{[f(z) - H^u]/(\lambda \epsilon)} 1_{A^c} \right].
\]

Then \( \lim_{\lambda \to 0} v_{1,\lambda}(\lambda) = 0 \) and \( v_{1,\lambda}(\lambda) \geq 0 \). Take

\[
v_{2,\lambda}(\lambda) = \frac{\mathbb{E}_{Q_{x,\epsilon}} \left[ e^{[f(z) - H^u]/(\lambda \epsilon)} 1_{A^c} (H^u - f(z))/\epsilon \right]}{\mathbb{E}_{Q_{x,\epsilon}}[1_{A}] + \mathbb{E}_{Q_{x,\epsilon}} \left[ e^{[f(z) - H^u]/(\lambda \epsilon)} 1_{A^c} \right]}.
\]

Then \( \lim_{\lambda \to 0} v_{2,\lambda}(\lambda) = 0 \) and \( v_{2,\lambda}(\lambda) \geq 0 \). It follows that

\[
\lim_{\lambda \to 0} \nabla v(\lambda) = \hat{\rho} + \epsilon \int \log \left( \mathbb{E}_{Q_{x,\epsilon}}[1_{A}] \right) \, d\hat{P}(x) = \hat{\rho}'.
\]
Hence, if the last condition is violated, based on the mean value theorem, we can find \( \overline{\lambda} > 0 \) so that \( \nabla v(\lambda) = 0 \), which contradicts to the optimality of \( \lambda^* = 0 \).

Now we show the converse direction. For any \( \lambda > 0 \), we find that
\[
\nabla v(\lambda) = \overline{\rho} + \epsilon \int \left[ \log (E_{Q_{x,\epsilon}}[1_A] + v_{1,x}(\lambda)) \right] d\widehat{P}(x) + \int v_{2,x}(\lambda) d\widehat{P}(x).
\]
For fixed \( x \), when \( E_{Q_{x,\epsilon}}[1_A] = 1 \), we can see that \( v_{1,x}(\lambda) = v_{2,x}(\lambda) = 0 \), then
\[
\overline{\rho} + \epsilon \left[ \log (E_{Q_{x,\epsilon}}[1_A] + v_{1,x}(\lambda)) \right] + v_{2,x}(\lambda) = \overline{\rho} > 0.
\]
When \( E_{Q_{x,\epsilon}}[1_A] \in (0, 1) \), we can see that \( v_{1,x}(\lambda) > 0, v_{2,x}(\lambda) > 0 \). Then
\[
\overline{\rho} + \epsilon \left[ \log (E_{Q_{x,\epsilon}}[1_A] + v_{1,x}(\lambda)) \right] + v_{2,x}(\lambda) = \overline{\rho} + \epsilon \log (E_{Q_{x,\epsilon}}[1_A]) = \overline{\rho}' \geq 0.
\]
Therefore, \( \nabla v(\lambda) > 0 \) for any \( \lambda > 0 \). By the convexity of \( v(\lambda) \), we conclude that the dual minimizer \( \lambda^* = 0 \).

\( \square \)

Proof of Lemma 4. Since \( \lambda^* > 0 \), based on the optimality condition of the dual problem, we have that
\[
0 = \nabla_{\lambda} \left[ \lambda \overline{\rho} + \lambda \epsilon \int \log \left( E_{Q_{x,\epsilon}} \left( e^{f(z)/(\lambda \epsilon)} \right) \right) d\widehat{P}(x) \right]_{\lambda = \lambda^*}.
\]
Or equivalently, we have that
\[
\overline{\rho} + \epsilon \int \log \left( E_{Q_{x,\epsilon}} \left( e^{f(z)/(\lambda^* \epsilon)} \right) \right) d\widehat{P}(x) - \int E_{Q_{x,\epsilon}} \left( e^{f(z)/(\lambda^* \epsilon)} f(z) \right) d\widehat{P}(x) = 0.
\]
Re-arranging the term completes the proof.

\( \square \)

Proof of Theorem 1. The feasibility result in Theorem 1(I) can be easily shown by considering the reformulation of \( V \) in (4) and the non-negativity of KL-divergence. When \( \overline{\rho} = 0 \), one can see that
\[
V_D \leq \lim_{\lambda \to \infty} \lambda \epsilon \int \log \left( E_{Q_{x,\epsilon}} \left( e^{f(z)/(\lambda \epsilon)} \right) \right) d\widehat{P}(x) = E_{z \sim \hat{P}} [f(z)] = V.
\]
Therefore, the strong duality result holds in this case. The proof for \( \overline{\rho} > 0 \) can be found in the main context. It remains to show the second part of Theorem 1(III). We consider a sequence of real numbers \( \{R_j\} \) such that \( R_j \to \infty \) and take the objective function \( f_j(z) = f(z)1\{z \leq R_j\} \). Hence, there exists \( \lambda > 0 \) satisfying \( \Pr_x : E_{Q_{x,\epsilon}} \left( e^{f_j(z)/(\lambda \epsilon)} \right) = \infty \) = 0. According to the necessary condition in Lemma 3, the corresponding dual minimizer \( \lambda_j^* > 0 \) for sufficiently large index \( j \). Then we can apply the duality result in the first part of Theorem 1(III) to show that for sufficiently large \( j \), it holds that
\[
\sup_{P \in \mathbb{P}_{R_j}(\hat{P})} \left\{ E_{z \sim \hat{P}} [f_j(z)] \right\} \geq \lambda_j^* \overline{\rho} + \lambda_j^* \epsilon \int \log \left( E_{Q_{x,\epsilon}} \left( e^{f_j(z)/(\lambda \epsilon)} \right) \right) d\widehat{P}(x).
\]
Taking \( j \to \infty \) both sides implies that \( V = \infty \), which completes the proof.

\( \square \)
Appendix EC.5: Proofs of Technical Results in Section 4

Proof of Proposition 1. For any fixed $\lambda_0 > 0$, denote by $\theta_0$ the optimal solution to problem (10). We can argue that for any $a \in \frac{\partial}{\partial \lambda} \hat{F}^{(m)}(\lambda_0, \theta_0)$, $a$ is a subgradient of $\hat{F}^{(m)}_\lambda$ at $\lambda = \lambda_0$. For any $\lambda > 0$, let $\theta(\lambda)$ be the optimal solution for $\hat{F}^{(m)}_\lambda$. Then we can see

$$\hat{F}^{(m)}_\lambda = \hat{F}^{(m)}(\lambda, \theta(\lambda)) \geq \hat{F}^{(m)}(\lambda_0, \theta_0) + a(\lambda - \lambda_0) + \langle \nabla \hat{F}^{(m)}(\lambda_0, \theta_0), \theta(\lambda) - \theta_0 \rangle \geq \hat{F}^{(m)}(\lambda_0, \theta_0) + a(\lambda - \lambda_0),$$

where $\nabla \hat{F}^{(m)}(\lambda_0, \theta_0)$ denotes the subdifferential of $\hat{F}^{(m)}$ with respect to $\theta = \theta_0$, the first inequality is by the convexity of $\hat{F}^{(m)}(\lambda, \theta)$ with respect to $(\lambda, \theta)$, and the second inequality is by the optimality condition for $\theta_0$.

When $a = 0$, we immediately obtain that $0 \in \partial \hat{F}^{(m)}_\lambda$, which means that $\lambda_0$ is the minimizer of $\hat{F}^{(m)}_\lambda$. Otherwise, the algorithm will update the interval so that $a(\lambda - \lambda_0) \leq 0$ for any $\lambda$ within it. We claim that this interval will contain $\lambda_*$. Suppose on the contrary that $a(\lambda_* - \lambda_0) > 0$. By the convexity of $\hat{F}^{(m)}_\lambda$,

$$\hat{F}^{(m)}_\lambda = \hat{F}^{(m)}(\lambda_0, \theta_0) + a(\lambda_* - \lambda_0) > \hat{F}^{(m)}_\lambda,$$

which contradicts to the optimality of $\lambda_*$. As a result, the interval length $l_t = \lambda_* - \lambda_t$ at the $t$-th iteration in Algorithm 1 vanishes at the rate $l_t = (1/2)^t l_0$, which indicates that the algorithm will converge into the optimal solution of $\inf_{\lambda \geq 0} \hat{F}^{(m)}_\lambda$ linearly. \hfill $\square$

Proof of Proposition 2. For notational simplicity, we write $s = (\lambda, \theta)$ and $\Xi = \mathbb{R}_+ \times \Theta$. We first show the second part of this theorem. To begin with, we introduce the following functions:

$$\hat{F}_m(s) = \hat{F}^{(m)}(s) + \tau_\Xi(s), \quad \hat{F}(s) = F(s) + \tau_\Xi(s).$$

We build the pointwise law of large numbers (LLN) for $\hat{F}_m$. By the strong law of large numbers (LLN), for each $i$ and every $(\lambda, \theta) \in \Xi$,

$$E_{\hat{Q}_m} \left[ e^{{f_0}(z)/(\lambda \epsilon)} \right] \overset{a.s.}{\longrightarrow} E_{Q_{\lambda \epsilon}} \left[ e^{{f_0}(z)/(\lambda \epsilon)} \right].$$

Then by the continuous mapping theorem, for each $i$ and every $(\lambda, \theta) \in \Xi$,

$$\lambda \epsilon \log \left( E_{\hat{Q}_m} \left[ e^{{f_0}(z)/(\lambda \epsilon)} \right] \right) \overset{a.s.}{\longrightarrow} \lambda \epsilon \log \left( E_{Q_{\lambda \epsilon}} \left[ e^{{f_0}(z)/(\lambda \epsilon)} \right] \right).$$

Therefore, using the addition and scalar multiplication rule of almost sure convergence, for every $(\lambda, \theta) \in \Xi$, it holds that

$$\frac{1}{n} \sum_{i=1}^{n} \lambda \epsilon \log \left( E_{\hat{Q}_m} \left[ e^{{f_0}(z)/(\lambda \epsilon)} \right] \right) \overset{a.s.}{\longrightarrow} \frac{1}{n} \sum_{i=1}^{n} \lambda \epsilon \log \left( E_{Q_{\lambda \epsilon}} \left[ e^{{f_0}(z)/(\lambda \epsilon)} \right] \right),$$

which reveals that $\hat{F}^{(m)}(s) \overset{a.s.}{\longrightarrow} F(s)$ for each $s \in \Xi$. This further implies the corresponding LLN for $\hat{F}_m(s)$.

Now take a compact subset $C$ so that $S^*$ is contained in the interior of $C$. Such a set exists because $S^*$ is bounded. Denote by $\bar{S}_m$ the set of minimizers of $\hat{F}_m$ over $C$. By the lower semi-continuity, together with the pointwise LLN of $\hat{F}_m$, we find $\bar{S}_m$ is finite-valued on $S^*$ for large $m$, which implies that the set $\bar{S}_m$ is non-empty for large $m$. We show that $\text{Dist}(\bar{S}_m, S^*) \rightarrow 0$ almost surely. Let $\omega = \{z_{i,j}\}_{i,j}$ be such that $\hat{F}_m(\cdot, \omega) \overset{\epsilon}{\longrightarrow} \hat{F}(\cdot)$. This event holds almost surely for all $\omega$. Suppose on the contrary that for any $m$, there exists a minimizer $\bar{s}_m(\omega)$ of $\hat{F}_m$ over $C$ such that $\text{Dist}(\bar{s}_m, S^*) \geq \epsilon$. Due to the compactness of $C$, there
exists a sub-sequence \( \{\tilde{s}_m\}_J \) that converges into a point \( s^* \in C \), but \( s^* \notin S^* \). On the other hand, we can argue that \( s^* \in \arg\min_{s \in S} \tilde{F}(s) = S^* \) by applying [84, Proposition 7.26]. Then we obtain a contradiction.

Then we show that \( \bar{S}_m = S^{(m)} \) for large \( m \). Because of the convexity assumption, any minimizer of \( \bar{F}_m \) over \( C \) which lies inside of the interior of \( C \), is also an optimal solution to the problem \( 9 \). Hence, for large \( m \) we have that \( \bar{S}_m = S^{(m)} \). This, together with the fact that \( \text{Dist}(\bar{S}_m, S^*) \to 0 \) implies \( \text{Dist}(S^{(m)}, S^*) \to 0 \). Moreover, it suffices to restrict the feasible set into the compact set \( C \cap \Xi \). By the convexity of \( F(s) \) in \( s \), \( \hat{F}^{(m)} \xrightarrow{a.s.} F \) holds uniformly on \( C \cap \Xi \). As a consequence, the first part of this proposition can be proved by applying [84, Proposition 5.2]. \( \square \)
Appendix EC.6: Proof of the Technical Result in Appendix A

We first present an useful technical lemma before showing Proposition 3.

**Lemma EC.2.** Under the first condition of Proposition 3, for any \( x \in \mathcal{Z} \), it holds that

\[
\int e^{-c(x,z)/\epsilon} \, dv(z) \geq e^{-2^{p-1}c(x,\overline{x})/\epsilon} \int e^{-2^{p-1}c(\overline{x},z)/\epsilon} \, dv(z).
\]

**Proof of Lemma EC.2** Based on the inequality \((a+b)^p \leq 2^{p-1}(a^p + b^p)\), we can see that

\[
c(x, z) \leq (c(y, z)^{1/p} + c(z, y)^{1/p})^p \leq 2^{p-1}(c(y, z) + c(z, y)), \quad \forall x, y, z \in \mathcal{Z}.
\]

Since \( c(x, z) \leq 2^{p-1}(c(\overline{x}, z) + c(x, \overline{x})) \), we can see that

\[
\int e^{-c(x,z)/\epsilon} \, dv(z) \geq \exp\left(-2^{p-1}c(x, \overline{x})/\epsilon\right) \int e^{-2^{p-1}c(\overline{x},z)/\epsilon} \, dv(z).
\]

The proof is completed.

**Proof of Proposition 3** One can see that for any \( x \in \text{supp}(\hat{P}) \), it holds that

\[
\mathbb{E}_{Q_{x\epsilon}} \left[ e^{f(z)/(\lambda \epsilon)} \right] \\
= \int e^{f(z)/(\lambda \epsilon)} \frac{e^{-c(x,z)/\epsilon}}{\int e^{-c(x,u)/\epsilon} \, dv(u)} \, dv(z) \\
\leq \int e^{f(z)/(\lambda \epsilon)} \frac{e^{-c(x,z)/\epsilon}}{\int e^{-2^{p-1}c(\overline{x},z)/\epsilon} \, dv(z)} \, dv(z) \\
\leq \int e^{f(z)/(\lambda \epsilon)} \frac{e^{-2^{p-1}c(\overline{x},z)/\epsilon}}{\int e^{-2^{p-1}c(\overline{x},z)/\epsilon} \, dv(z)} \, dv(z) \\
= \frac{e^{c(x,\overline{x})(1+2^{p-1})/\epsilon}}{\int e^{-2^{p-1}c(\overline{x},z)/\epsilon} \, dv(z)} \int e^{f(z)/(\lambda \epsilon)} e^{-2^{p-1}c(\overline{x},z)/\epsilon} \, dv(z),
\]

where the first inequality is based on the lower bound in Lemma EC.2, the second inequality is based on the triangular inequality \( c(x, z) \geq 2^{1-p}c(\overline{x}, z) - c(x, \overline{x}) \). Note that almost surely for all \( x \in \text{supp}(\hat{P}) \), \( c(x, \overline{x}) < \infty \). Moreover,

\[
0 < \int e^{-2^{p-1}c(\overline{x},z)/\epsilon} \, dv(z) \leq \int e^{-c(\overline{x},z)/\epsilon} \, dv(z) < \infty,
\]

where the lower bound is because \( c(\overline{x}, z) < \infty \) almost surely for all \( z \), the upper bound is because \( c(\overline{x}, z) \geq 0 \) almost surely for all \( z \). Based on these observations, we have that

\[
\mathbb{E}_{Q_{x\epsilon}} \left[ e^{f(z)/(\lambda \epsilon)} \right] \leq \frac{e^{c(x, \overline{x})(1+2^{p-1})/\epsilon}}{\int e^{-2^{p-1}c(\overline{x},z)/\epsilon} \, dv(z)} \int e^{f(z)/(\lambda \epsilon)} e^{-2^{p-1}c(\overline{x},z)/\epsilon} \, dv(z) < \infty
\]

almost surely for all \( x \sim \hat{P} \).