

# Sinkhorn Distributionally Robust Optimization

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We study distributionally robust optimization (DRO) with Sinkhorn distance—a variant of Wasserstein distance based on entropic regularization. We provide convex programming dual reformulation for a general nominal distribution. Compared with Wasserstein DRO, it is computationally tractable for a larger class of loss functions, and its worst-case distribution is more reasonable. We propose an efficient first-order algorithm with bisection search to solve the dual reformulation. We demonstrate that our proposed algorithm finds  $\delta$ -optimal solution of the new DRO formulation with computation cost  $\tilde{O}(\delta^{-3})$  and memory cost  $\tilde{O}(\delta^{-2})$ , and the computation cost further improves to  $\tilde{O}(\delta^{-2})$  when the loss function is smooth. Finally, we provide various numerical examples using both synthetic and real data to demonstrate its competitive performance and light computational speed.

*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, and economics. When the data involves uncertainty due to measurement error, insufficient sample size, contamination, and anomalies, or model misspecification, 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 more promising out-of-sample performance than the traditional sample average approximation (SAA) method for stochastic programming [88]. We refer to [81] 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 literature. Among them, the ambiguity set based on Wasserstein distance has recently received much attention [108, 67, 19, 46]. 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 [46]. Nice statistical performance guarantees have been established for Wasserstein DRO both asymptotically [18, 21, 20], non-asymptotically [44, 24, 86], and empirically in a variety of applications in operations research [15, 29, 93, 73, 92, 105], machine learning [87, 25, 66, 16, 72, 98], stochastic control [110, 1, 96, 38, 111, 104], etc; see [60] and references therein for more discussions. We also provide a more detailed literature survey by the end of this section.

On the other hand, the current Wasserstein DRO framework is not without limitations. First, from the *computational efficiency* perspective, the tractability of Wasserstein DRO is usually available only under somewhat stringent conditions on the loss function, as its 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 [67] and efficient first-order algorithms are proposed only for special loss functions such as logistic loss [62]; 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 [94, 22]. 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 [46], 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 potentially 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 [35]. 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 (see Definition 1 in Section 2). 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) when the nominal distribution is any arbitrary distribution. 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 4). 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 5).
- (II) As a byproduct of our duality proof, we characterize the worst-case distribution of the Sinkhorn DRO (Remark 3), which is absolutely continuous with respect to some reference measure such as Lebesgue or counting measure. Compared with Wasserstein DRO, the worst-case distribution of Sinkhorn DRO is not necessarily finitely supported even 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 and analyze a computationally efficient stochastic mirror descent method using biased gradient oracles with bisection search for solving the Sinkhorn DRO problem (Section 4). By adequately balancing the trade-off between bias and variance of stochastic gradient estimators with low computation cost, we show the proposed algorithm achieves computation cost  $\tilde{O}(\delta^{-3})$  and memory cost  $\tilde{O}(\delta^{-2})$  for finding  $\delta$ -optimal solution for convex loss, and the computation cost improves to  $\tilde{O}(\delta^{-2})$  for convex and smooth loss.<sup>1</sup> Compared with Wasserstein DRO, the dual problem of Sinkhorn DRO is computationally tractable for broader class of loss functions, cost functions, nominal distributions, and probability support. See Table 1 for detailed comparison.
- (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 multi-class classification, using both synthetic and real data sets. Numerical results demonstrate its superior out-of-sample performances and light computational speed compared with several benchmarks including SAA, Wasserstein DRO, and KL-divergence DRO.

Finally, we remark that Blanchet and Kang [17, Section 3.2] solves the Wasserstein DRO formulation based on its log-sum-exp smooth approximation. This smoothed approximation can be viewed as a special case of the dual reformulation of our Sinkhorn DRO model. The main differences between

<sup>1</sup> In this paper, we say that  $f(\delta) = O(g(\delta))$  if there exists a real constant  $c > 0$  (which is independent of  $\delta$ ) and there exists  $\delta_0 > 0$  such that  $f(\delta) \leq cg(\delta)$  for every  $\delta \leq \delta_0$ . When  $f(\delta) = O(g(\delta) \cdot \text{polylog} \frac{1}{\delta})$ , we write  $f(\delta) = \tilde{O}(g(\delta))$  for simplicity.

**Table 1** Summarization on the tractability result of distributionally robust learning models. Here we aim to solve the minimax learning problem  $\min_{\theta \in \Theta} \max_{\mathbb{P} \in \mathcal{P}} \mathbb{E}_{z \sim \mathbb{P}}[f_{\theta}(z)]$ , where the set  $\Theta$  is closed and convex, the loss function  $f_{\theta}(z)$  is convex in  $\theta$ , and the ambiguity set  $\mathcal{P}$  is a probability ball centered around the nominal distribution  $\hat{\mathbb{P}}$  with respect to Wasserstein distance or Sinkhorn distance with support  $\mathcal{Z}$ .

(a) Wasserstein DRO

Reference(s)	Loss function $f_{\theta}(z)$	Cost function	Nominal distribution $\hat{\mathbb{P}}$	Support $\mathcal{Z}$
[114, 26, 64]	General	General	General	Discrete and finite set
[94]	$z \mapsto f_{\theta}(z) - \lambda^* c(x, z)$ is strongly concave <sup>i</sup>	General	General	General
[42, 46]	Piecewise concave in $z$	Norm function	Empirical distribution	Polytope
[87, 62, 112, 85]	Generalized linear model in $(z, \theta)$	Norm function	Empirical distribution	Whole Euclidean space <sup>ii</sup>
[22]	Generalized linear model in $(z, \theta)$	Squared norm function	General	Whole Euclidean space <sup>ii</sup>

<sup>i</sup> Sinha et al. [94] approximately solves the Wasserstein DRO by penalizing the Wasserstein ball constraint with fixed Lagrangian multiplier  $\lambda^*$ . Here the assumption of loss function holds for  $\hat{\mathbb{P}}$ -almost every  $x$ .

<sup>ii</sup> Here references therein essentially assume the numerical part of the probability vector is supported on the whole Euclidean space, such as the numerical features in logistic regression setup.

(b) Sinkhorn DRO

Reference(s)	Loss function $f_{\theta}(z)$	Cost function	Nominal distribution $\hat{\mathbb{P}}$	Support $\mathcal{Z}$
This paper	General	General	General	General

their formulation and ours are that: (i) we start with the primal form of the Sinkhorn DRO model and uncover it coincides with the smoothed approximation of the Wasserstein DRO dual formulation, while they focus on the dual formulation only. (ii) they focus on the data-driven DRO training for semi-supervised learning tasks only, while our DRO result applies to the general loss function, cost function, and nominal distribution. (iii) they optimize the smoothed objective function by simulating unbiased gradient estimators but with unbounded variance, and no convergence results are established.

Azizian et al. [6] (which is a contribution made public 234 days after we posted the first version of this paper in arXiv) present a very similar duality result shown in this paper. The main differences include the following: (i) their theoretical results rely on a Slater-like assumption which is more restrictive. (ii) they do not provide numerical algorithm to solve the Sinkhorn DRO formulation.

## 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 [12], moment conditions [84, 36, 52, 116, 107, 28, 13], shape constraints [79, 99], marginal distributions [43, 69, 2, 39]. Second, a more recently popular approach that makes full use of the available data is 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  $\phi$ -divergence [57, 10, 106, 9, 40], Wasserstein distance [77, 108, 67, 114, 19, 46, 27, 109], and maximum mean discrepancy [97, 115]. 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 been investigated. In particular, it has been shown that Wasserstein DRO is asymptotically equivalent to a statistical learning problem with variation regularization [45, 18, 86], and when the radius is chosen properly, the worst-case loss of Wasserstein DRO serves as an upper confidence bound on the true loss [18, 21, 44, 20]. Other variants of Wasserstein DRO have been explored, by combining with other information such as moment information [48, 101] and marginal distributions [47, 41].

**On Sinkhorn Distance** Sinkhorn distance [35] 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 [76]. Such an approach first aroused in the areas of economics and survey statistics [59, 113, 37, 7], and its convergence analysis is attributed to the mathematician Sinkhorn [95], which gives the name of Sinkhorn distance. Altschuler et al. [3] further design 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 [32, 33, 31], generative modeling [50, 75, 65, 74], dimensionality reduction [63, 102, 103, 58], etc. To the best of our knowledge, the study of Sinkhorn distance for distributionally robust optimization is new in literature.

**Solving DRO Models** In the introduction, we have elaborated on the literature that propose efficient optimization algorithms for solving the Wasserstein DRO formulation [114, 26, 64, 94, 42, 46, 87, 62, 112, 85, 22]. Unfortunately, the tractability of these literature is limited to the special loss function, cost function, nominal distribution, or probability support. In addition, the algorithmic framework for  $\phi$ -divergence DRO model is also exploited in recent literature. A natural optimization idea is to generate sample estimates of the dual formulation of  $\phi$ -divergence DRO and then optimize the approximated objective function [89, Section 7.5.4], called the *sample average approximation (SAA)* technique. It is worth noting that the SAA technique is not a computation- and storage- efficient choice, since it requires storing the input data for the approximated problem first, and then solving the new problem numerically. Recent literature [61, 68, 80] propose first-order methods to solve  $\phi$ -divergence DRO formulations. In comparison with the SAA technique, the complexity of first-order methods is usually independent of the sample size of the nominal distribution to obtain a near-optimal solution. Motivated by these literature, we propose to solve the Sinkhorn DRO model by simulating stochastic gradient estimators and then establish sample-size independent convergence results.

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  $\{1, 2, \dots, N\}$ . For a measurable set  $\mathcal{Z}$ , denote by  $\mathcal{M}(\mathcal{Z})$  the set of measures (not necessarily probability measures) on  $\mathcal{Z}$ , and  $\mathcal{P}(\mathcal{Z})$  the set of probability measures on  $\mathcal{Z}$ . Given a probability distribution  $\mathbb{P}$  and a measure  $\mu$ , we denote  $\text{supp}(\mathbb{P})$  the support of  $\mathbb{P}$ , and write  $\mathbb{P} \ll \mu$  if  $\mathbb{P}$  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  $\mathbb{P} \otimes \mathbb{Q}$  as the product measure of two probability

distributions  $\mathbb{P}$  and  $\mathbb{Q}$ . Denote by  $\text{Proj}_{1\#}\gamma$  and  $\text{Proj}_{2\#}\gamma$  the first and the second marginal distributions of  $\gamma$ , respectively. For a given set  $A$ , define the characteristic function  $1_A(x)$  such that  $1_A(x) = 1$  when  $x \in A$  and otherwise  $1_A(x) = 0$ , 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  $\text{Dist}(A, B) = \sup_{x \in A} \inf_{y \in B} \|x - y\|_2$ . Define the sign function  $\text{sign}(\cdot)$  such that  $\text{sign}(x) = 1$  if  $x > 0$  and otherwise  $\text{sign}(x) = -1$ . For a given function  $\omega : \Theta \rightarrow \mathbb{R}$ , we say it is  $\kappa$ -strongly convex with respect to norm  $\|\cdot\|$  if  $\langle \theta' - \theta, \nabla\omega(\theta') - \nabla\omega(\theta) \rangle \geq \kappa\|\theta' - \theta\|^2, \forall \theta, \theta' \in \Theta$ .

We first review the definition of Sinkhorn distance.

**DEFINITION 1 (SINKHORN DISTANCE).** Let  $\mathcal{Z}$  be a measurable set. Consider distributions  $\mathbb{P}, \mathbb{Q} \in \mathcal{P}(\mathcal{Z})$ , and let  $\mu, \nu \in \mathcal{M}(\mathcal{Z})$  be two reference measures such that  $\mathbb{P} \ll \mu, \mathbb{Q} \ll \nu$ . For regularization parameter  $\epsilon \geq 0$ , the *Sinkhorn distance* between two distributions  $\mathbb{P}$  and  $\mathbb{Q}$  is defined as

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

where  $\Gamma(\mathbb{P}, \mathbb{Q})$  denotes the set of joint distributions whose first and second marginal distributions are  $\mathbb{P}$  and  $\mathbb{Q}$  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  $\mu \otimes \nu$ :

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

where  $\frac{d\gamma(x, y)}{d\mu(x) d\nu(y)}$  stands for the density ratio of  $\gamma$  with respect to  $\mu \otimes \nu$  evaluated at  $(x, y)$ .  $\diamond$

**REMARK 1 (VARIANTS OF SINKHORN DISTANCE).** Sinkhorn distance in Definition 1 is based on general reference measures  $\mu$  and  $\nu$ . Special forms of the distance has been investigated in literature, for instance, when the reference measures  $\mu$  and  $\nu$  were chosen to be  $\mathbb{P}, \mathbb{Q}$ , i.e., marginal distributions of  $\gamma$ , respectively [49, Section 2]. The relative entropy regularization term can also be considered as a hard-constrained variant for the optimal transport problem, which has been discussed in [35, Definition 1] and [8]:

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

where  $R \geq 0$  quantifies the upper bound for the relative entropy between distributions  $\gamma$  and  $\mathbb{P} \otimes \mathbb{Q}$ . Another variant of the optimal transport problem is to consider the negative entropy for regularization [35, Equation (2)]:

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

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. For given  $\mathbb{P}$  and  $\mathbb{Q}$ , one can check the two regularized optimal transport distances above are equivalent up to a constant:

$$\begin{aligned} \mathcal{W}_\epsilon^{\text{Ent}}(\mathbb{P}, \mathbb{Q}) &= \mathcal{W}_\epsilon(\mathbb{P}, \mathbb{Q}) + \int \log \left( \frac{d\mu(x) d\nu(y)}{dx dy} \right) d\gamma(x, y) \\ &= \mathcal{W}_\epsilon(\mathbb{P}, \mathbb{Q}) + \int \log \left( \frac{d\mu(x)}{dx} \right) d\mathbb{P}(x) + \int \log \left( \frac{d\nu(y)}{dy} \right) d\mathbb{Q}(y). \end{aligned}$$



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

$$V := \sup_{\mathbb{P} \in \mathbb{B}_{\rho, \epsilon}(\widehat{\mathbb{P}})} \mathbb{E}_{z \sim \mathbb{P}}[f(z)], \quad (\text{Sinkhorn DRO})$$

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

where  $\mathbb{B}_{\rho, \epsilon}(\widehat{\mathbb{P}})$  is the Sinkhorn ball of the radius  $\rho$  centered at the nominal distribution  $\widehat{\mathbb{P}}$ . Due to the convex entropic regularizer [34]  $\mathcal{W}_\epsilon(\widehat{\mathbb{P}}, \mathbb{P})$  with respect to  $\mathbb{P}$ , the Sinkhorn distance  $\mathcal{W}_\epsilon(\widehat{\mathbb{P}}, \mathbb{P})$  is convex in  $\mathbb{P}$ , i.e., when  $\mathbb{P}_1$  and  $\mathbb{P}_2$  are two probability distributions, it holds that

$$\mathcal{W}_\epsilon(\widehat{\mathbb{P}}, \lambda \mathbb{P}_1 + (1 - \lambda) \mathbb{P}_2) \leq \lambda \mathcal{W}_\epsilon(\widehat{\mathbb{P}}, \mathbb{P}_1) + (1 - \lambda) \mathcal{W}_\epsilon(\widehat{\mathbb{P}}, \mathbb{P}_2)$$

for all  $0 \leq \lambda \leq 1$ . Therefore, the Sinkhorn ball is a convex set, and the problem (Sinkhorn DRO) is an (infinite-dimensional) convex program. We refer to Remark 3 on the discussion of the existence of worst-case distribution.

**REMARK 2 (CHOICE OF REFERENCE MEASURES).** We discuss below the choices of the two reference measures  $\mu$  and  $\nu$  in Definition 1.

For the reference measure  $\mu$ , observe from the definition of relative entropy and the law of probability, we can see that the regularization term in  $\mathcal{W}_\epsilon(\widehat{\mathbb{P}}, \mathbb{P})$  can be written as

$$\begin{aligned} H(\gamma \mid \mu \otimes \nu) &= \int \log \left( \frac{d\gamma(x, y)}{d\widehat{\mathbb{P}}(x) d\nu(y)} \right) + \log \left( \frac{\widehat{\mathbb{P}}(x)}{d\mu(x)} \right) d\gamma(x, y) \\ &= \int \log \left( \frac{d\gamma(x, y)}{d\widehat{\mathbb{P}}(x) d\nu(y)} \right) d\gamma(x, y) + \int \log \left( \frac{\widehat{\mathbb{P}}(x)}{d\mu(x)} \right) d\widehat{\mathbb{P}}(x). \end{aligned}$$

Therefore, any choice of the reference measure  $\mu$  satisfying  $\widehat{\mathbb{P}} \ll \mu$  is equivalent up to a constant. For simplicity, in the sequel we will take  $\mu = \widehat{\mathbb{P}}$ .

For the reference measure  $\nu$ , observe that the worst-case solution  $\mathbb{P}$  in (Sinkhorn DRO) should satisfy that  $\mathbb{P} \ll \nu$  since otherwise the entropic regularization in Definition 1 is undefined. As a consequence, we can choose  $\nu$  such that the underlying true distribution is absolutely continuous with respect to it. Typical choices include the Lebesgue measure or Gaussian measure for continuous random variables, and counting measure for discrete measures. See [78, 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 (Sinkhorn DRO) is an infinite-dimensional optimization problem over probability distributions. To obtain a more tractable form, in this section, we derive a strong duality result for (Sinkhorn DRO). Our main goal is to derive the strong dual problem

$$V_D := \inf_{\lambda \geq 0} \left\{ \lambda \bar{\rho} + \lambda \epsilon \int \log \left( \mathbb{E}_{\mathbb{Q}_{x, \epsilon}} \left[ e^{f(z)/(\lambda \epsilon)} \right] \right) d\widehat{\mathbb{P}}(x) \right\}, \quad (\text{Dual})$$

where the dual decision variable  $\lambda$  corresponds to the Sinkhorn ball constraint in (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

$$\bar{\rho} := \rho + \epsilon \int \log \left( \int e^{-c(x,z)/\epsilon} d\nu(z) \right) d\hat{\mathbb{P}}(x), \quad (1)$$

and the kernel probability distribution

$$d\mathbb{Q}_{x,\epsilon}(z) := \frac{e^{-c(x,z)/\epsilon}}{\int e^{-c(x,u)/\epsilon} d\nu(u)} d\nu(z). \quad (2)$$

The rest of this section is organized as follows. In Section 3.1, we summarize our main results on the strong duality reformulation of Sinkhorn DRO. Next, we provide detailed discussions in Section 3.2. In Section 3.3, we provide a proof sketch of our main results.

### 3.1. Main Results

To make the above primal (Sinkhorn DRO) and dual (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)  $\int e^{-c(x,z)/\epsilon} d\nu(z) < \infty$  for  $\hat{\mathbb{P}}$ -almost every  $x$ ;  
 (III)  $\mathcal{Z}$  is a measurable space, and the function  $f : \mathcal{Z} \rightarrow \mathbb{R} \cup \{\infty\}$  is measurable.

By reference [76, Proposition 4.1], the Sinkhorn distance has the equivalent formulation:

$$\mathcal{W}_\epsilon(\hat{\mathbb{P}}, \mathbb{P}) = \min_{\gamma \in \Gamma(\hat{\mathbb{P}}, \mathbb{P})} \int \log \left( \frac{d\gamma}{d\mathcal{K}}(x, y) \right) d\gamma(x, y), \quad \text{where } d\mathcal{K}(x, y) = e^{-c(x,y)/\epsilon} d\hat{\mathbb{P}}(x) d\nu(y).$$

Assumption 1(I) implies that  $0 \leq c(x, y) < \infty$  for  $\hat{\mathbb{P}} \otimes \nu$ -almost every  $(x, y)$ , and therefore the reference measure  $\mathcal{K}$  is well-defined. Assumption 1(II) ensures the optimal transport mapping  $\gamma^*$  for Sinkhorn distance  $\mathcal{W}_\epsilon(\hat{\mathbb{P}}, \mathbb{P})$  exists with density value  $\frac{d\gamma^*(x,y)}{d\hat{\mathbb{P}}(x) d\nu(y)} \propto e^{-c(x,y)/\epsilon}$ . Hence, Assumption 1(I) and 1(II) together ensure the Sinkhorn distance is well-defined. Assumption 1(III) ensures the expected loss  $\mathbb{E}_{z \sim \mathbb{P}}[f(z)]$  to be well-defined and lower bounded for any distribution  $\mathbb{P}$ .

To distinguish the cases  $V_D < \infty$  and  $V_D = \infty$ , we introduce the light-tail condition on  $f$  in Condition 1. In Appendix A, we present sufficient conditions for Condition 1 that are easy to verify.

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

In the following, we provide main results on the strong duality reformulation.

**THEOREM 1 (Strong Duality).** *Let  $\hat{\mathbb{P}} \in \mathcal{P}(\mathcal{Z})$ , and assume Assumption 1 holds. 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 3 in Section 3.3 below. Therefore, we have  $V = V_D$  as long as Assumption 1 holds. Along the proof we also obtain the dual reformulation on the soft distributionally robust formulation of (Sinkhorn DRO).

**COROLLARY 1.** *Let  $\hat{\mathbb{P}} \in \mathcal{P}(\mathcal{Z})$  and  $\lambda > 0$ , and assume Assumption 1 holds. Then the primal problem*

$$V_\lambda = \sup_{\mathbb{P}} \left\{ \mathbb{E}_{z \sim \mathbb{P}}[f(z)] - \lambda \mathcal{W}_\epsilon(\hat{\mathbb{P}}, \mathbb{P}) \right\}. \quad (\text{SDRO}(\lambda))$$

has the equivalent dual reformulation:

$$V_\lambda^{\text{Dual}} = \lambda\epsilon \int \log \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [e^{f(z)/(\lambda\epsilon)}] \right) d\widehat{\mathbb{P}}(x) + C, \quad (\text{SDRO}(\lambda)\text{-Dual})$$

where the constant

$$C = \lambda\epsilon \int \log \left( \int e^{-c(x,u)/\epsilon} d\nu(u) \right) d\widehat{\mathbb{P}}(x).$$

### 3.2. Discussions

In the following, we make several remarks regarding the strong duality result.

**REMARK 3 (WORST-CASE DISTRIBUTION).** Assume the optimal Lagrangian multiplier in (Dual)  $\lambda^* > 0$ . As we will demonstrate in the proof of Theorem 1, the worst-case distribution for (Sinkhorn DRO) maps every  $x \in \text{supp } \widehat{\mathbb{P}}$  to a (conditional) distribution whose density function (with respect to  $\nu$ ) at  $z$  is

$$\alpha_x \cdot \exp \left( \left( f(z) - \lambda^* c(x, z) \right) / (\lambda^* \epsilon) \right),$$

where  $\alpha_x := \left[ \int \exp \left( \left( f(z) - \lambda^* c(x, z) \right) / (\lambda^* \epsilon) \right) d\nu(z) \right]^{-1}$  is a normalizing constant to ensure the conditional distribution well-defined. As such, the density of the worst-case distribution can be expressed as

$$d\mathbb{P}_*(z) = \int \alpha_x \cdot \exp \left( \left( f(z) - \lambda^* c(x, z) \right) / (\lambda^* \epsilon) \right) d\widehat{\mathbb{P}}(x),$$

from which we can see that the worst-case distribution shares the same support as the measure  $\nu$ . For the case where  $\lambda^* = 0$ , the worst-case distribution will ensure the corresponding objective function equal the essential supremum of the loss function  $f$ . Particularly, when  $\widehat{\mathbb{P}}$  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  $\mathbb{P}_*$  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 [46]. 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. ♣

**REMARK 4 (CONNECTION WITH WASSERSTEIN DRO).** As the regularization parameter  $\epsilon \rightarrow 0$ , the dual objective of the Sinkhorn DRO converges to

$$\lambda\rho + \int \text{ess sup}_\nu \{ f(\cdot) - \lambda c(x, \cdot) \} d\widehat{\mathbb{P}}(x).$$

The proof is provided in Appendix EC.3, which essentially follows from the fact that the log-sum-exp function is a smooth approximation of the supremum. Particularly, when  $\text{supp}(\nu) = \mathcal{Z}$ , the dual objective of the Sinkhorn DRO converges to the dual formulation of the Wasserstein DRO problem [46, Theorem 1]. 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 is shown to be tractable only when the loss function can be expressed as a pointwise maximum of finitely many concave functions [67, Theorem 4.2], and 2-Wasserstein DRO is shown to be tractable only when the loss function is smooth and the radius of the ambiguity set is sufficiently small [22, Theorem 3].



- (II) The strong duality of Sinkhorn DRO holds in an even more general setting. Essentially, the only requirements on the space  $\mathcal{Z}$  and the nominal distribution  $\mathbb{P}$  are measurability. In contrast, the strong duality for Wasserstein DRO ([46, Theorem 1], [19, Theorem 1]) requires the nominal distribution  $\mathbb{P}$  to be a Borel probability measure and the set  $\mathcal{Z}$  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 based on [46, Theorem 1 and Proposition 2], the Wasserstein DRO is finite if and only if the loss function satisfies a growth condition  $f(z) \leq L_f c(z, z_0) + M, \forall z \in \mathcal{Z}$  for some constants  $L_f, M > 0$  and some  $z_0 \in \mathcal{Z}$ . ♣

REMARK 5 (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

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

which corresponds to the dual objective function [57] for the following KL-divergence DRO

$$\sup_{\mathbb{P}} \left\{ \mathbb{E}_{z \sim \mathbb{P}} [f(z)] : D_{\text{KL}}(\mathbb{P} \parallel \mathbb{P}^0) \leq \bar{\rho} / \epsilon \right\},$$

where  $\mathbb{P}^0$  satisfies  $d\mathbb{P}^0(z) = \int_x d\mathbb{Q}_{x,\epsilon}(z) d\widehat{\mathbb{P}}(x)$ , which can be viewed as a non-parametric kernel density estimation constructed from  $\widehat{\mathbb{P}}$ . Particularly, when  $\widehat{\mathbb{P}} = \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$ ,  $\mathcal{Z} = \mathbb{R}^d$  and  $c(x, y) = \|x - y\|_2^2$ ,  $\mathbb{P}^0$  is kernel density estimator with Gaussian kernel and bandwidth  $\epsilon$ :

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

where  $K_\epsilon(x) \propto \exp(-\|x\|_2^2/\epsilon)$  represents the Gaussian kernel. By Lemma 1 and divergence inequality [34, Theorem 2.6.3], we can see the Sinkhorn DRO with  $\bar{\rho} = 0$  is reduced to the following SAA model based on the distribution  $\mathbb{P}^0$ :

$$V = \mathbb{E}_{\mathbb{P}^0} [f(z)] = \int \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [f(z)] d\widehat{\mathbb{P}}(x). \quad (3)$$

In non-parametric statistics, the optimal bandwidth to minimize the mean-squared-error between the estimated distribution  $\mathbb{P}_0$  and the underlying true one is at rate  $\epsilon = O(n^{-1/(d+4)})$  [53, Theorem 4.2.1]. However, 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  $\epsilon$  based on cross-validation. ♣

REMARK 6 (CONNECTION WITH BAYESIAN DRO). Recently, the Bayesian DRO [90] framework proposed to solve

$$R(Z) := \mathbb{E}_{x \sim \widehat{\mathbb{P}}} \left[ \sup_{\mathbb{P}} \left\{ \mathbb{E}_{z \sim \mathbb{P}} [f(z)] : \mathbb{P} \in \mathcal{P}_x \right\} \right],$$

where  $\widehat{\mathbb{P}}$  is a special posterior distribution constructed from collected observations, and the ambiguity set  $\mathcal{P}_x$  is typically constructed as a KL-divergence ball, i.e.,  $\mathcal{P}_x := \{\mathbb{P} : D_{\text{KL}}(\mathbb{P} \parallel \mathbb{Q}_x) \leq \eta\}$ , with  $\mathbb{Q}_x$  being the parametric distribution conditioned on  $x$ . According to [90, Section 2.1.3], a relaxation of the Bayesian DRO dual formulation given by

$$\inf_{\lambda \geq 0} \left\{ \lambda \eta + \lambda \int \log \left( \mathbb{E}_{\mathbb{Q}_x} [e^{f(z)/\lambda}] \right) d\widehat{\mathbb{P}}(x) \right\}.$$

When specifying the parametric distribution  $\mathbb{Q}_x$  as the kernel probability distribution in (2) and applying the change-of-variable technique such that  $\lambda$  is replaced with  $\lambda\epsilon$ , this relaxed formulation becomes

$$\inf_{\lambda \geq 0} \left\{ \lambda(\eta\epsilon) + \lambda\epsilon \int \log \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} \left[ e^{f(z)/(\lambda\epsilon)} \right] \right) d\widehat{\mathbb{P}}(x) \right\}.$$

In comparison with (Dual), we find the Sinkhorn DRO model can be viewed as a special relaxation formulation of the Bayesian DRO model.  $\clubsuit$

Let us illustrate our result for a linear or quadratic loss function  $f$ , which turns out to be equivalent to a simple optimization problem.

**EXAMPLE 1 (DISTRIBUTIONALLY ROBUST OPTIMIZATION WITH LINEAR LOSS).** Suppose that the loss function  $f(z) = a^\top z$ , support  $\mathcal{Z} = \mathbb{R}^d$ ,  $\nu$  is the corresponding Lebesgue measure, and the cost function is the Mahalanobis distance, i.e.,  $c(x, y) = \frac{1}{2}(x - y)^\top \Omega (x - y)$ , where  $\Omega$  is a positive definite matrix. In this case, we have the reference measure

$$\mathbb{Q}_{x,\epsilon} \sim \mathcal{N}(x, \epsilon\Omega^{-1}).$$

As a consequence, the dual problem can be written as

$$V_D = \inf_{\lambda > 0} \left\{ \lambda\bar{\rho} + \lambda\epsilon \int \Lambda_x(\lambda) d\widehat{\mathbb{P}}(x) \right\},$$

where

$$\Lambda_x(\lambda) = \log \left( \mathbb{E}_{z \sim \mathcal{N}(x, \epsilon\Omega^{-1})} \left[ e^{a^\top z / (\lambda\epsilon)} \right] \right) = \frac{a^\top x}{\lambda\epsilon} + \frac{a^\top \Omega^{-1} a}{2\lambda^2 \epsilon^2}.$$

Therefore

$$V_D = a^\top \mathbb{E}_{\widehat{\mathbb{P}}}[x] + \sqrt{2\bar{\rho}} \sqrt{a^\top \Omega^{-1} a} := \mathbb{E}_{\widehat{\mathbb{P}}}[a^\top x] + \sqrt{2\bar{\rho}} \cdot \|a\|_{\Omega^{-1}}.$$

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.  $\clubsuit$

**EXAMPLE 2 (DISTRIBUTIONALLY ROBUST OPTIMIZATION WITH QUADRATIC LOSS).** Consider the example of performing linear regression with quadratic loss  $f(z) = (a^\top \theta - b)^2$ , where  $z := (a, b)$  denotes the predictor-response pair,  $\theta \in \mathbb{R}^d$  denotes the fixed parameter choice, and  $\mathcal{Z} = \mathbb{R}^{d+1}$ . Taking  $\nu$  as the Lebesgue measure and the cost function as  $c((a, b), (a', b')) = \|a - a'\|_2^2 + \infty|b - b'|$ . In this case, the dual problem becomes

$$V_D = \mathbb{E}_{\widehat{\mathbb{P}}}[(a^\top \theta - b)^2] + \inf_{\lambda > 2\|\theta\|_2^2} \left\{ \lambda\bar{\rho} + \frac{\mathbb{E}_{\widehat{\mathbb{P}}}[(a^\top \theta - b)^2]}{\frac{1}{2}\lambda\|\theta\|_2^{-2} - 1} - \frac{\lambda\epsilon}{2} \log \det \left( I - \frac{\theta\theta^\top}{\frac{1}{2}\lambda} \right) \right\}.$$

In comparison with the corresponding Wasserstein DRO formulation with radius  $\rho$  (see, e.g., [20, Example 4])

$$V_D^{\text{Wasserstein}} = \mathbb{E}_{\widehat{\mathbb{P}}}[(a^\top \theta - b)^2] + \inf_{\lambda > 2\|\theta\|_2^2} \left\{ \lambda\rho + \frac{\mathbb{E}_{\widehat{\mathbb{P}}}[(a^\top \theta - b)^2]}{\frac{1}{2}\lambda\|\theta\|_2^{-2} - 1} \right\},$$

one can check in this case the Sinkhorn DRO formulation is equivalent to the Wasserstein DRO formulation with log-determinant regularization.  $\clubsuit$

When the support  $\mathcal{Z}$  is finite, the following result presents a conic programming reformulation.

**COROLLARY 2 (Conic Reformulation for Finite Support).** *Suppose that the support contains  $L$  elements, i.e.,  $\mathcal{Z} = \{z_\ell\}_{\ell=1}^L$ , and the nominal distribution  $\widehat{\mathbb{P}} = \frac{1}{n} \sum_{i=1}^n \delta_{\hat{x}_i}$ . If Condition 1 holds and  $\bar{\rho} \geq 0$ , the dual problem (Dual) can be formulated as the following conic optimization:*

$$\begin{aligned} V_D = \min_{\substack{\lambda \geq 0, s \in \mathbb{R}^n, \\ a \in \mathbb{R}^{n \times L}}} & \lambda \bar{\rho} + \frac{1}{n} \sum_{i=1}^n s_i \\ \text{s.t.} & \lambda \epsilon \geq \sum_{\ell=1}^L q_{i,\ell} a_{i,\ell}, i \in [n], \\ & (\lambda \epsilon, a_{i,\ell}, f(z_\ell) - s_i) \in \mathcal{K}_{\text{exp}}, i \in [n], \ell \in [L]. \end{aligned} \quad (4)$$

where  $q_{i,\ell} := \Pr_{z \sim \mathbb{Q}_{\hat{x}_i, \epsilon}} \{z = z_\ell\}$ , with the distribution  $\mathbb{Q}_{\hat{x}_i, \epsilon}$  defined in (2), and  $\mathcal{K}_{\text{exp}}$  denotes the exponential cone  $\mathcal{K}_{\text{exp}} = \{(\nu, \lambda, \delta) \in \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{R} : \exp(\delta/\nu) \leq \lambda/\nu\}$ .

Problem (4) is a convex program that minimizes a linear function with respect to linear and conic constraints, which can be solved using interior point algorithms [71, 100]. We will develop an efficient first-order optimization algorithm in Section 4 that is able to solve a more general problem (without a finite support).

### 3.3. Proof of Theorem 1

In this subsection, we present a sketch of the proof for Theorem 1. We first show the feasibility result in Theorem 1(I). The key is based on the observation that the primal problem (Sinkhorn DRO) can be reformulated as a generalized KL-divergence DRO problem.

**LEMMA 1 (Reformulation of (Sinkhorn DRO)).** *Under Assumption 1, it holds that*

$$V = \sup_{\gamma_x \in \mathcal{P}(\mathcal{Z}), x \in \text{supp}(\widehat{\mathbb{P}})} \left\{ \int \mathbb{E}_{\gamma_x} [f(z)] d\widehat{\mathbb{P}}(x) : \epsilon \int \mathbb{E}_{\gamma_x} \left[ \log \left( \frac{d\gamma_x(z)}{d\mathbb{Q}_{x,\epsilon}(z)} \right) \right] d\widehat{\mathbb{P}}(x) \leq \bar{\rho} \right\}.$$

Due to Lemma 1, Theorem 1(I) holds based on the non-negativity of KL-divergence.

Next, we develop the duality result for the primal problem  $V$ . We begin with the weak duality result in Lemma 2, which can be shown by the application of Lagrangian weak duality theorem.

**LEMMA 2 (Weak Duality).** *Assume Assumption 1 holds. Then  $V \leq V_D$ .*

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 3), and then build the corresponding first-order optimality condition (Lemma 4 and Lemma 5). 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).

Below we provide the proof of the first part of Theorem 1(III) for the case  $\bar{\rho} > 0$  under Condition 1, and 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 3 (Existence of Dual Minimizer).** *Suppose  $\bar{\rho} > 0$  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 DR0) is binding or not.

Lemma 4 below presents a necessary and sufficient condition for the dual minimizer  $\lambda^* = 0$ , corresponding to the case where the Sinkhorn distance constraint in (Sinkhorn DR0) is not binding.

**LEMMA 4 (Necessary and Sufficient Condition for  $\lambda^* = 0$ ).** *Suppose  $\bar{\rho} > 0$  and Condition 1 is satisfied, then the dual minimizer  $\lambda^* = 0$  if and only if all the following conditions hold:*

$$(I) \operatorname{ess\,sup} f \stackrel{\nu}{\triangleq} \inf\{t : \nu\{f(z) > t\} = 0\} < \infty.$$

$$(II) \bar{\rho}' = \bar{\rho} + \epsilon \int \log \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [1_A] \right) d\widehat{\mathbb{P}}(x) \geq 0, \text{ where } A := \{z : f(z) = \operatorname{ess\,sup}_{\nu} f\}.$$

Recall that we have the convention that the dual objective evaluated at  $\lambda = 0$  equals  $\operatorname{ess\,sup}_{\nu} f$ . 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  $\operatorname{ess\,sup}_{\nu} f$ , and Condition (II) characterizes the lower bound of  $\bar{\rho}$ .

Lemma 5 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 5 (First-order Optimality Condition when  $\lambda^* > 0$ ).** *Suppose  $\bar{\rho} > 0$  and Condition 1 is satisfied, and assume further that the dual minimizer  $\lambda^* > 0$ , then  $\lambda^*$  satisfies*

$$\lambda^* \left[ \bar{\rho} + \epsilon \int \log \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} \left[ e^{f(z)/(\lambda^*\epsilon)} \right] \right) d\widehat{\mathbb{P}}(x) \right] = \int \frac{\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} \left[ e^{f(z)/(\lambda^*\epsilon)} f(z) \right]}{\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} \left[ e^{f(z)/(\lambda^*\epsilon)} \right]} d\widehat{\mathbb{P}}(x). \quad (5)$$

Now we are ready to prove Theorem 1.

*Proof of Theorem 1(III) under Condition 1 with  $\bar{\rho} > 0$ .* 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 the transport mapping  $\gamma_*$  such that

$$\frac{d\gamma_*(x, z)}{d\widehat{\mathbb{P}}(x) d\nu(z)} = \alpha_x \exp \left( \frac{1}{\lambda^*\epsilon} \phi(\lambda^*; x, z) \right), \quad \text{where } \phi(\lambda; x, z) = f(z) - \lambda c(x, z),$$

and  $\alpha_x := \left[ \int \exp \left( \frac{1}{\lambda^*\epsilon} \phi(\lambda^*; x, z) \right) d\nu(z) \right]^{-1}$  is a normalizing constant such that  $\operatorname{Proj}_{1\#} \gamma_* = \widehat{\mathbb{P}}$ . Also define the primal (approximate) optimal distribution  $\mathbb{P}_* := \operatorname{Proj}_{2\#} \gamma_*$ . Recall the expression of the Sinkhorn distance in Definition 1, one can verify that

$$\begin{aligned} & \mathcal{W}_{\epsilon}(\widehat{\mathbb{P}}, \mathbb{P}_*) \\ &= \inf_{\gamma \in \Gamma(\widehat{\mathbb{P}}, \mathbb{P}_*)} \left\{ \mathbb{E}_{\gamma} \left[ c(x, z) + \epsilon \log \left( \frac{d\gamma(x, z)}{d\widehat{\mathbb{P}}(x) d\nu(z)} \right) \right] \right\} \\ &\leq \mathbb{E}_{\gamma_*} \left[ c(x, z) + \epsilon \log \left( \frac{d\gamma_*(x, z)}{d\widehat{\mathbb{P}}(x) d\nu(z)} \right) \right] \\ &= \mathbb{E}_{\gamma_*} \left[ c(x, z) + \epsilon \log \left( \frac{\exp \left( \frac{\phi(\lambda^*; x, z)}{\lambda^*\epsilon} \right)}{\int \exp \left( \frac{\phi(\lambda^*; x, u)}{\lambda^*\epsilon} \right) d\nu(u)} \right) \right] \\ &= \frac{1}{\lambda^*} \left\{ \iint \frac{f(z) \exp \left( \frac{\phi(\lambda^*; x, z)}{\lambda^*\epsilon} \right)}{\int \exp \left( \frac{\phi(\lambda^*; x, z)}{\lambda^*\epsilon} \right) d\nu(z)} d\nu(z) d\widehat{\mathbb{P}}(x) - \lambda^*\epsilon \int \log \left( \int \exp \left( \frac{\phi(\lambda^*; x, u)}{\lambda^*\epsilon} \right) d\nu(u) \right) d\widehat{\mathbb{P}}(x) \right\}, \end{aligned}$$

where the second relation is because  $\gamma_*$  is a feasible solution in  $\Gamma(\widehat{\mathbb{P}}, \mathbb{P}_*)$ , the third and the fourth relation is by substituting the expression of  $\gamma_*$ . Since  $\bar{\rho} > 0$  and the dual minimizer  $\lambda^* > 0$ , the optimality condition in (5) holds, which implies that  $\mathcal{W}_\epsilon(\widehat{\mathbb{P}}, \mathbb{P}_*) \leq \rho$ , 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:

$$\begin{aligned} V &\geq \mathbb{E}_{\mathbb{P}_*}[f(z)] = \int f(z) d\gamma_*(x, z) \\ &= \iint f(z) \left( \frac{d\gamma_*(x, z)}{d\widehat{\mathbb{P}}(x) d\nu(z)} \right) d\nu(z) d\widehat{\mathbb{P}}(x) \\ &= \iint f(z) \frac{\exp\left(\frac{\phi(\lambda^*; x, z)}{\lambda^* \epsilon}\right)}{\int \exp\left(\frac{\phi(\lambda^*; x, u)}{\lambda^* \epsilon}\right) d\nu(u)} d\nu(z) d\widehat{\mathbb{P}}(x) \\ &= \lambda^* \left[ \rho + \epsilon \int \log \left( \int \exp \left[ \frac{\phi(\lambda^*; x, z)}{\lambda^* \epsilon} \right] d\nu(z) \right) d\widehat{\mathbb{P}}(x) \right] \\ &= V_D, \end{aligned}$$

where the third equality is based on the optimality condition in Lemma 5. This, together with the weak duality result, completes the proof for  $\lambda^* > 0$ .

When  $\lambda^* = 0$ , the optimality condition in Lemma 4 holds. We construct the primal (approximate) solution  $\mathbb{P}_* = \text{Proj}_{2\#} \gamma_*$ , where  $\gamma_*$  satisfies

$$d\gamma_*(x, z) = d\gamma_*^x(z) d\widehat{\mathbb{P}}(x), \quad \text{where } d\gamma_*^x(y) = \begin{cases} 0, & \text{if } z \notin A, \\ \frac{e^{-c(x, z)/\epsilon} d\nu(z)}{\int e^{-c(x, u)/\epsilon} 1_A d\nu(u)}, & \text{if } z \in A. \end{cases}$$

We can verify easily that the primal solution is feasible based on the optimality condition  $\bar{\rho}' \geq 0$  in Lemma 4. Moreover, we can check that the primal optimal value is lower bounded by the dual optimal value:

$$V \geq \int f(z) d\gamma_*(x, z) = \iint f(z) d\gamma_*^x(z) d\widehat{\mathbb{P}}(x) = \iint \text{ess sup}_\nu f d\gamma_*^x(z) d\widehat{\mathbb{P}}(x) = \text{ess sup}_\nu f = V_D,$$

where the second equality is because that  $z \in A$  so that  $f(z) = \text{ess sup}_\nu f$ . This, together with the weak duality result, completes the proof for  $\lambda^* = 0$ .  $\square$

#### 4. Efficient First-order Algorithm for Sinkhorn Robust Optimization

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

$$\inf_{\theta \in \Theta} \sup_{\mathbb{P} \in \mathbb{B}_{\rho, \epsilon}(\widehat{\mathbb{P}})} \mathbb{E}_{z \sim \mathbb{P}}[f_\theta(z)]. \quad (6)$$

Here the feasible set  $\Theta \subseteq \mathbb{R}^{d_\theta}$  is *closed and convex* containing all possible candidates of decision vector  $\theta$ , and the Sinkhorn uncertainty set is centered around a given nominal distribution  $\widehat{\mathbb{P}}$ , e.g., it can be an empirical distribution from samples. Based on our strong dual (Dual) expression, we reformulate (6) as

$$\inf_{\lambda \geq 0} \left\{ \lambda \bar{\rho} + \inf_{\theta \in \Theta} \mathbb{E}_{x \sim \widehat{\mathbb{P}}} \left[ \lambda \epsilon \log \left( \mathbb{E}_{\mathbb{Q}_{x, \epsilon}} \left[ e^{f_\theta(z)/(\lambda \epsilon)} \right] \right) \right] \right\}, \quad (7)$$

where the constant  $\bar{\rho}$  and the distribution  $\mathbb{Q}_{x, \epsilon}$  are defined in (1) and (2), respectively. In Example 1 and 2, we have seen instances of (7) where we can get closed-form expressions for the above integration. Generally, we present a stochastic mirror descent with bisection search algorithm to solve this problem when a closed-form expression is not available. Throughout this section, we assume the loss function  $f_\theta(z)$  is convex in  $\theta$ .

---

**Algorithm 1** Bisection search algorithm for finding optimal multiplier of (7)

---

**Require:** Interval  $[\lambda_\ell, \lambda_u]$ , maximum outer iterations  $T_{\text{out}}$ , inexact objective oracle of (7) (denoted as  $\widehat{F}^*(\cdot)$ , constructed from Algorithm 2).

```

1:  $\lambda^{(0)} \leftarrow \lambda_\ell, y_\ell^{(0)} \leftarrow \lambda_\ell, y_u^{(0)} \leftarrow \lambda_u.$ 
2: for  $t = 1, \dots, T_{\text{out}}$  do
3:   Update  $z_\ell^{(t)} \leftarrow \frac{1}{3}[2y_\ell^{(t-1)} + y_u^{(t-1)}]$  and  $z_u^{(t)} \leftarrow \frac{1}{3}[y_\ell^{(t-1)} + 2y_u^{(t-1)}].$ 
4:   if  $\widehat{F}(z_\ell^{(t)}) \leq \widehat{F}(z_u^{(t)})$  then
5:     Update  $(y_\ell^{(t)}, y_u^{(t)}) \leftarrow (y_\ell^{(t-1)}, z_u^{(t)}).$ 
6:     if  $\widehat{F}(z_\ell^{(t)}) \leq \widehat{F}(\lambda^{(t-1)})$ , update  $\lambda^{(t)} \leftarrow z_\ell^{(t)}.$ 
7:   else if  $\widehat{F}(z_\ell^{(t)}) > \widehat{F}(z_u^{(t)})$  then
8:     Update  $(y_\ell^{(t)}, y_u^{(t)}) \leftarrow (z_\ell^{(t)}, y_u^{(t-1)}).$ 
9:     if  $\widehat{F}(z_u^{(t)}) \leq \widehat{F}(\lambda^{(t-1)})$ , update  $\lambda^{(t)} \leftarrow z_u^{(t)}.$ 
10:  end if
11: end for
Output  $\lambda^{(\text{Last})}.$ 

```

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---

**Algorithm 2** BSMD with Sampling for finding the inexact objective oracle of (7)

---

**Require:** Batch size  $m$ , maximum inner iterations  $T_{\text{in}}$ , constant step size  $\gamma$ , initial guess  $\theta_1$ , fixed multiplier  $\lambda$ .

```

1: for  $i = 1, \dots, m$  do
2:   for  $t = 0, 1, \dots, T_{\text{in}} - 1$  do                                     # Step 2-6: BSMD Step
3:     Formulate (biased) gradient estimate of  $F(\theta_t; \lambda)$ , denoted as  $v(\theta_t; \lambda).$ 
4:     Update  $\theta_{t+1} = \text{Prox}_{\theta_t}(\gamma v(\theta_t; \lambda)).$ 
5:   end for
6:   Obtain estimate of optimal solution  $\widehat{\theta}_i = \frac{1}{T_{\text{in}}} \sum_{t=1}^{T_{\text{in}}} \theta_t.$ 
7:   Formulate objective estimate of  $F(\widehat{\theta}_i; \lambda)$ , denoted as  $V(\widehat{\theta}_i; \lambda).$                                      # Sampling Step
8: end for
Output the estimator  $\min_{i \in [m]} V(\widehat{\theta}_i; \lambda).$ 

```

---

#### 4.1. Algorithm Description

We present several notations before outlining the main algorithm. Define the objective value of (7) as

$$F^*(\lambda) := \lambda \bar{\rho} + \inf_{\theta \in \Theta} \left\{ F(\theta; \lambda) := \mathbb{E}_{x \sim \widehat{\mathbb{P}}} \left[ \lambda \epsilon \log \left( \mathbb{E}_{\mathbb{Q}_{x, \epsilon}} \left[ e^{f_{\theta}(z)/(\lambda \epsilon)} \right] \right) \right] \right\}. \quad (8)$$

Let  $\omega : \Theta \rightarrow \mathbb{R}$  be a distance generating function that is continuously differentiable and  $\kappa$ -strongly convex on  $\Theta$  with respect to norm  $\|\cdot\|$ , where the norm function  $\|\cdot\|$  satisfies that the dual norm  $\|\cdot\|_* \leq c \|\cdot\|_2$ . This induces the Bregman divergence  $D_\omega(\theta, \theta') : \Theta \times \Theta \rightarrow \mathbb{R}_+$ :

$$D_\omega(\theta, \theta') = \omega(\theta') - [\omega(\theta) + \langle \nabla \omega(\theta), \theta' - \theta \rangle].$$

Next, we define the *prox-mapping*  $\text{Prox} : \mathbb{R}^{d_\theta} \rightarrow \Theta$  as

$$\text{Prox}_\theta(y) = \arg \min_{\theta' \in \Theta} \{ \langle y, \theta' - \theta \rangle + D_\omega(\theta, \theta') \}.$$

With those notations in hand, we present our algorithm, which consists of outer and inner iterations. At the outer iterations, we apply the bisection search algorithm to seek a near-optimal multiplier in (7) provided that an inexact objective oracle of (7) is given. The inner iterations find such an oracle based on the following steps:



**BSMD Step:** First, we propose a **Stochastic Mirror Descent** algorithm with **Biased** gradient estimators (BSMD) to obtain a near-optimal decision of (8) for a given multiplier  $\lambda$ .

**Sampling Step:** Next, we present a sampling-based algorithm to estimate the objective value of (8) for a given decision  $\theta$  and multiplier  $\lambda$ .

Combining these two steps gives us an inexact objective oracle of (7). We summarize the algorithm at outer and inner iterations in Algorithm 1 and 2, respectively. In the following, we elaborate how to formulate gradient estimators in BSMD step and how to formulate objective estimators in sampling step.

**4.1.1. Configuration of Gradient Simulation in BSMD Step** Observe that the objective function of (8) involves a nonlinear transformation of the expectation, thus an unbiased gradient estimate could be challenging to obtain when  $\mathbb{Q}_{x,\epsilon}$  is a general probability distribution. Based on a batch of simulated samples from  $\mathbb{Q}_{x,\epsilon}$ , we provide stochastic gradient estimators that are possibly biased. As we will elaborate in Section 4.2.1, by properly tuning the hyper-parameters of these estimators to balance their bias and variance trade-off, the BSMD step can efficiently find a near-optimal decision of (8). Since the multiplier  $\lambda$  is fixed in (8), we omit the dependence of  $\lambda$  when defining objective or gradient terms in the remaining of this section.

**REMARK 7 (SAMPLING FROM  $\mathbb{Q}_{x,\epsilon}$ ).** In many cases, generating samples from  $\mathbb{Q}_{x,\epsilon}$  is easy. When the cost function  $c(\cdot, \cdot) = \frac{1}{2} \|\cdot - \cdot\|_2^2$  and  $\mathcal{Z} = \mathbb{R}^d$ , then the distribution  $\mathbb{Q}_{x,\epsilon}$  becomes a Gaussian distribution  $\mathcal{N}(x, \epsilon I_d)$ . When the cost function  $c(\cdot, \cdot)$  is decomposable in each coordinate, we can apply the acceptance-rejection method [5] to generate samples in each coordinate independently, the complexity of which only increases linearly in the data dimension. When the cost function  $c(x, y) = \frac{1}{q} \|x - y\|_p^q$ , the complexity of sampling based on Lagenvin Monte Carlo method for obtaining a  $\tau$ -close sample point is of  $O(d/\tau)$ . See the detailed algorithm of sampling in Appendix EC.6.3.

We follow the idea of multi-level Monte-Carlo (MLMC) simulation in [55] to tackle the difficulty of simulating gradient estimate. First, we construct a sequence of approximation functions  $\{F^\ell(\theta)\}_{\ell \geq 0}$  instead, where

$$F^\ell(\theta) = \mathbb{E}_{x^\ell} \mathbb{E}_{\{z_j^\ell\}_{j \in [2^\ell]} | x^\ell} \left[ \lambda \epsilon \log \left( \frac{1}{2^\ell} \sum_{j \in [2^\ell]} \exp \left( \frac{f_\theta(z_j^\ell)}{\lambda \epsilon} \right) \right) \right]. \quad (9)$$

Here the random variable  $x^\ell$  follows distribution  $\widehat{\mathbb{P}}$ , and for fixed value of  $x^\ell$ ,  $\{z_j^\ell\}_{j \in [2^\ell]}$  are independent and identically distributed samples from  $\mathbb{Q}_{x^\ell, \epsilon}$ . Unlike the original objective  $F(\theta)$ , unbiased gradient estimators of its approximation  $F^\ell(\theta)$  can be easily obtained. Denote by  $\zeta^\ell = (x^\ell, \{z_j^\ell\}_{j \in [2^\ell]})$  the collection of random sampling parameters, and

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

For fixed parameter  $\theta$ , we define

$$g^\ell(\theta, \zeta^\ell) = \nabla_\theta U_{1:2^\ell}(\theta, \zeta^\ell), \quad (10)$$

$$G^\ell(\theta, \zeta^\ell) = \nabla_\theta \left[ U_{1:2^\ell}(\theta, \zeta^\ell) - \frac{1}{2} U_{1:2^{\ell-1}}(\theta, \zeta^\ell) - \frac{1}{2} U_{2^{\ell-1}+1:2^\ell}(\theta, \zeta^\ell) \right]. \quad (11)$$

The random vector  $g^\ell(\theta, \zeta^\ell)$  is an unbiased estimator of  $\nabla F^\ell(\theta)$ , while the vector  $G^\ell(\theta, \zeta^\ell)$  is an unbiased estimator of  $\nabla F^\ell(\theta) - \nabla F^{\ell-1}(\theta)$ . Since  $\nabla F^\ell(\theta)$  and  $\nabla F^{\ell-1}(\theta)$  are close to each other for large  $\ell$ , stochastic estimators of them using the same random sampling parameters  $\zeta^\ell$  will be highly correlated. Consequently, the gradient estimator  $G^\ell(\theta, \zeta^\ell)$  will have small variance for large  $\ell$ , making it a suitable recipe for stochastic optimization. We list the following choices of MLMC-based gradient estimator in Step 3 of Algorithm 2 using  $g^\ell(\theta, \zeta^\ell)$  and  $G^\ell(\theta, \zeta^\ell)$ :

**Vanilla Stochastic Gradient Descent (V-SGD) Estimator:** at point  $\theta$ , query oracle for  $n_L^\circ$  times to obtain  $\{g^L(\theta, \zeta_i^L)\}_{i=1}^{n_L^\circ}$  and construct

$$v^{\text{V-SGD}}(\theta) = \frac{1}{n_L^\circ} \sum_{i=1}^{n_L^\circ} g^L(\theta, \zeta_i^L). \quad (12a)$$

**Vanilla MLMC Estimator (V-MLMC):** at point  $\theta$ , for each  $\ell$  we query oracle for  $n_\ell := \lceil 2^{-\ell} N \rceil$  times to obtain  $\{G^\ell(\theta, \zeta_i^\ell)\}_{i=1}^{n_\ell}$  and construct

$$v^{\text{V-MLMC}}(\theta) = \sum_{\ell=0}^L \frac{1}{n_\ell} \sum_{i=1}^{n_\ell} G^\ell(\theta, \zeta_i^\ell). \quad (12b)$$

**Randomized Truncation MLMC (RT-MLMC) Estimator:** at point  $\theta$ , we sample *random levels* for  $n_L^\circ$  times, denoted as  $\iota_1, \dots, \iota_{n_L^\circ}$ , following distribution  $Q_{\text{RT}} = \{q_\ell\}_{\ell=0}^L$  with  $\mathbb{P}(\iota = \ell) = q_\ell$ , where the probability mass value  $q_\ell \propto 2^{-\ell}$ . Then construct

$$v^{\text{RT-MLMC}}(\theta) = \frac{1}{n_L^\circ} \sum_{i=1}^{n_L^\circ} \frac{1}{q_{\iota_i}} G^{\iota_i}(\theta, \zeta^{\iota_i}). \quad (12c)$$

In the convergence analysis part in Section 4.2.1, we demonstrate V-MLMC and RT-MLMC estimators are more computationally efficient than V-SGD estimator provided that the loss function  $f_\theta(z)$  is smooth in  $\theta$ . Once gradient recipes  $G^{\iota_i}(\theta, \zeta^{\iota_i})$  are fixed, the V-MLMC estimator is a deterministic way for gradient simulation while the RT-MLMC estimator is a randomized approach.

**4.1.2. Configuration of Objective Simulation in Sampling Step** Similar to the gradient simulation part, we list MLMC-based sampling methods for estimating the objective value in (8) for fixed  $\theta$ . For notation simplicity, define

$$A^\ell(\theta, \zeta^\ell) = U_{1:2^\ell}(\theta, \zeta^\ell) - \frac{1}{2} U_{1:2^{\ell-1}}(\theta, \zeta^\ell) - \frac{1}{2} U_{2^{\ell-1}+1:2^\ell}(\theta, \zeta^\ell). \quad (13)$$

**V-MLMC Estimator:** at point  $\theta$ , for each  $\ell$  we query oracle for  $n_\ell := \lceil 2^{-\ell} N \rceil$  times to obtain  $\{A^\ell(\theta, \zeta_i^\ell)\}_{i=1}^{n_\ell}$  and construct

$$V^{\text{V-MLMC}}(\theta) = \sum_{\ell=0}^L \frac{1}{n_\ell} \sum_{i=1}^{n_\ell} A^\ell(\theta, \zeta_i^\ell). \quad (14a)$$

**RT-MLMC Estimator:** at point  $\theta$ , we sample *random levels* for  $n_L^\circ$  times, denoted as  $\iota_1, \dots, \iota_{n_L^\circ}$ , following distribution  $Q_{\text{RT}} = \{q_\ell\}_{\ell=0}^L$  with  $\mathbb{P}(\iota = \ell) = q_\ell$ , where the probability mass value  $q_\ell \propto 2^{-\ell}$ . Then construct

$$V^{\text{RT-MLMC}}(\theta) = \frac{1}{n_L^\circ} \sum_{i=1}^{n_L^\circ} \frac{1}{q_{\iota_i}} A^{\iota_i}(\theta, \zeta^{\iota_i}). \quad (14b)$$

## 4.2. Convergence Properties

With our algorithm described, we now describe its convergence properties. We begin with the following assumptions regarding the loss function  $f_\theta$ :

**ASSUMPTION 2.** (I) (*Convexity*): The loss function  $f_\theta(z)$  is convex in  $\theta$ .

(II) (*Boundedness*): The loss function  $f_\theta(z)$  satisfies  $0 \leq f_\theta(z) \leq B$  for any  $\theta \in \Theta$  and  $z \in \mathcal{Z}$ .

(III) (*Lipschitz Continuity*): For fixed  $z$  and  $\theta_1, \theta_2$ , it holds that  $|f_{\theta_1}(z) - f_{\theta_2}(z)| \leq L_f \|\theta_1 - \theta_2\|_2$ .

(IV) (*Lipschitz Smoothness*): The loss function  $f_\theta(z)$  is continuously differentiable and for fixed  $z$  and  $\theta_1, \theta_2$ , it holds that  $\|\nabla f_{\theta_1}(z) - \nabla f_{\theta_2}(z)\|_2 \leq S_f \|\theta_1 - \theta_2\|_2$ .

From Section 4.1.1 and 4.1.2, we can see the computational and storage bottleneck of our algorithm is on the random sampling parameter  $\zeta^\ell = (x^\ell, \{z_j^\ell\}_{j \in [2^\ell]})$ . To this end, we quantify the computation cost of our algorithm as *the (expected) number of queries for generating the random sampling parameter*, and the memory cost as *the stored (expected) number of random sampling parameter in data buffer*.

**Table 2** Configuration of optimization hyper-parameters together with the computational/memory cost for obtaining  $\delta$ -optimal solution of (8) in Theorem 2. Here "Comp." and "Memo." are the abbreviations of "Computation" and "Memory", respectively.

Smooth?	V-SGD		V-MLMC		RT-MLMC	
	Parameter	Comp./Memo.	Parameter	Comp./Memo.	Parameter	Comp./Memo.
No	$L = O(\log \frac{1}{\delta})$ $T_{\text{in}} = O(1/\delta^2)$ $n_L^o = O(1)$ $\gamma = O(\delta)$	Comp. = $O(Tn_L^o 2^L)$ = $O(1/\delta^3)$ Memo. = $O(n_L^o 2^L)$ = $O(1/\delta)$	N/A	N/A	N/A	N/A
Yes	$L = O(\log \frac{1}{\delta})$ $T_{\text{in}} = O(1/\delta^2)$ $n_L^o = O(1)$ $\gamma = O(\delta)$	Comp. = $O(Tn_L^o 2^L)$ = $O(1/\delta^3)$ Memo. = $O(n_L^o 2^L)$ = $O(1/\delta)$	$L = O(\log \frac{1}{\delta})$ $T_{\text{in}} = O(1/\delta)$ $N = O(1/\delta)$ $\gamma = O(1)$	Comp. = $O(T(NL + 2^L))$ = $\tilde{O}(1/\delta^2)$ Memo. = $O(NL + 2^L)$ = $\tilde{O}(1/\delta)$	$L = O(\log \frac{1}{\delta})$ $T_{\text{in}} = \tilde{O}(1/\delta^2)$ $n_L^o = O(1)$ $\gamma = O(\delta)$	Comp. = $O(T(n_L^o L))$ = $\tilde{O}(1/\delta^2)$ Memo. = $O(n_L^o L)$ = $\tilde{O}(1)$

**4.2.1. BSMD Step at Inner Iterations** In this part, we discuss the BSMD step (see Step 2-6 in Algorithm 2) for estimating an optimal solution of (8). By Corollary 1, the formulation (8) corresponds to the Sinkhorn robust learning problem with a softened Sinkhorn ball constraint. To quantify the quality of the obtained solution, we say a given random vector  $\theta$  is a  $\delta$ -optimal solution if  $\mathbb{E}[F(\theta)] - F(\theta^*) \leq \delta$ , where  $\theta^*$  is the optimal solution of (8).

The BSMD step iteratively obtains a stochastic gradient estimate (not necessarily unbiased) of the objective function and then performs a proximal gradient update. By properly tuning hyper-parameters to balance the trade-off between bias and variance of gradient estimate, we establish performance guarantees for our proposed BSMD step in Theorem 2. A detailed proof and formal statement can be found in Appendix EC.6.

**THEOREM 2 (Complexity Analysis of BSMD Step).** *Under Assumption 2(I), 2(II), and 2(III), with properly chosen hyper-parameters of gradient estimators in (12), the following results hold:*

- (I) *When the loss function  $f_\theta(z)$  is nonsmooth in  $\theta$ , the computation cost of V-SGD scheme for finding  $\delta$ -optimal solution is of  $O(\delta^{-3})$ , with memory cost  $O(1/\delta)$ .*
- (II) *Additionally assume Assumption 2(IV) holds, then the computation cost of V-SGD scheme for finding  $\delta$ -optimal solution is of  $O(\delta^{-3})$ , with memory cost  $O(1/\delta)$ ; the computation cost of V-MLMC scheme is of  $O(\delta^{-2})$ , with memory cost  $\tilde{O}(1/\delta)$ ; and the computation cost of RT-MLMC scheme is of  $O(\delta^{-2})$ , with memory cost  $\tilde{O}(1)$ .*

The configuration of optimization hyper-parameters is provided in Table 2.

Theorem 2 indicates that the computation cost of BSMD algorithm for solving (8) is of  $O(\delta^{-3})$ . When the additional smoothness assumption of loss function holds, the computation cost further reduces to  $\tilde{O}(\delta^{-2})$  using V-MLMC or RT-MLMC gradient estimators. This complexity is near-optimal for solving general convex and smooth optimization problems [14]. It is an open question whether the BSMD step with V-SGD gradient estimator is optimal for solving (8) with convex and nonsmooth loss functions. In comparison with V-MLMC scheme, the RT-MLMC scheme has the same order of computation cost but achieves cheaper memory cost  $\tilde{O}(1)$ , which is nearly error tolerance-independent.

Moreover, we note that the problem (8) can be viewed as a special case of the conditional stochastic optimization (CSO) studied in [54, 56, 55]. As far as we have known, the stochastic approximation-based idea proposed in [55] is the most efficient algorithm to solve the generic CSO problem. Although we follow the similar idea to design BSMD step, the difference is that we consider a more practical constrained optimization scenario, while Hu et al. [55] focused on unconstrained optimization only.

**REMARK 8 (COMPARISON WITH BIASED SAMPLE AVERAGE APPROXIMATION APPROACH).** Another way for solving the formulation (8) is to formulate sample estimates of the inner expectation and then optimize the biased sample estimate of the objective function instead, called the biased sample average approximation (BSAA) technique. Applying [54, Corollary 4.2], it can be shown that the total computation cost and memory cost for BSAA formulation of achieving  $\delta$ -optimal solution are both of  $\tilde{O}(\delta^{-3})$  for Lipschitz continuous loss functions (See formal statement in Appendix EC.6.4). The

**Table 3** Configuration of optimization hyper-parameters together with the computational/memory cost for estimating optimal value in (8) in Theorem 2. Here the "cost in Step 7" refers to both the computation and memory cost when implementing V-MLMC or RT-MLMC sampling method.

V-MLMC		RT-MLMC	
Parameter	Cost in Step 7	Parameter	Cost in Step 7
$L = O(\log \frac{1}{\delta})$	$O(NL + 2^L)$	$L = O(\log \frac{1}{\delta})$	$O(n_L^\circ L)$
$N = \tilde{O}(\frac{1}{\delta^2} \log \frac{1}{\alpha})$	$=\tilde{O}(\delta^{-2})$	$n_L^\circ = \tilde{O}(\frac{1}{\delta^2} \log \frac{1}{\alpha})$	$=\tilde{O}(\delta^{-2})$

storage complexity for BSAA is always worse compared with the proposed BSMD approach which is at most in the order of  $\delta^{-1}$ . The computation complexity for BSAA formulation is worse compared with the proposed BSMD approach when the loss functions are also Lipschitz smooth. Also, the BSAA method still requires a solution of the approximated optimization problem. Hence, it typically takes considerably less time and memory to run the BSMD step rather than solving for the BSAA formulation. ♣

**4.2.2. Sampling Step at Inner Iterations** After a near-optimal solution of (8) is obtained, we estimate its objective value in sampling step. With properly chosen hyper-parameters, the output of Algorithm 2 gives an estimation of the optimal value in (8) with negligible error with high probability. The complexity analysis of Algorithm 2 is provided in Theorem 3.

**THEOREM 3 (Complexity for Estimating Optimal Value in (8)).** Fix an error probability  $\eta \in (0, 1)$  and specify  $m = \lceil \log_2 \frac{2}{\eta} \rceil$ . Assume that Assumption 2(I), 2(II), and 2(III) hold, then with properly chosen hyper-parameters, the output in Algorithm 2 satisfies

$$\Pr \left\{ \left| \min_{i \in [m]} V(\hat{\theta}_i) - F(\theta^*) \right| \leq 3\delta \right\} \geq 1 - \eta.$$

In addition,

- (I) The computation cost of Algorithm 2 with V-SGD scheme for BSMD step and V-MLMC (or RT-MLMC) objective estimator is of  $O(\delta^{-3} \cdot \text{polylog} \frac{1}{\eta})$ , with memory cost  $\tilde{O}(\delta^{-2} \cdot \text{polylog} \frac{1}{\eta})$ .
- (II) Additionally assume Assumption 2(IV) holds, then the computation cost of Algorithm 2 with V-MLMC (or RT-MLMC) scheme for BSMD step and V-MLMC (or RT-MLMC) objective estimator is of  $\tilde{O}(\delta^{-2} \cdot \text{polylog} \frac{1}{\eta})$ , with memory cost  $\tilde{O}(\delta^{-2} \cdot \text{polylog} \frac{1}{\eta})$ .

Optimization hyper-parameters in BSMD step in Algorithm 2 follow the discussion in Section 4.2.1. The configuration of optimization hyper-parameters in sampling step is provided in Table 3.

Hu et al. [54, Theorem 4.1] proposed and analyzed the V-SGD estimator for estimating the objective value of generic CSO problem. Specially, the complexity of this estimator for estimating the optimal value in (8) with accuracy error  $\delta$  is of  $O(\delta^{-3})$ , while our proposed V-MLMC and RT-MLMC estimators have improved sample complexity  $\tilde{O}(\delta^{-2})$ .

**4.2.3. Bisection Search at Outer Iterations** In Algorithm 1, we propose a bisection search algorithm for solving (7) by iteratively querying the oracle for estimating the optimal value of (8). It can be shown that under mild assumptions, we can solve the constrained DRO formulation (7) to accuracy  $\delta$  by computing  $O(\delta)$ -accurate optimal values of (8) for  $O(\log \frac{1}{\delta})$  times.

**THEOREM 4 (Complexity of Bisection Search).** Fix an error probability  $\eta \in (0, 1)$ . Assume that Assumption 2(I) and 2(II) hold, and one can pick  $\lambda_\ell, \lambda_u$  such that the Lagrangian multiplier  $\lambda^*$  in (7) satisfies  $0 < \lambda_\ell \leq \lambda^* \leq \lambda_u < \infty$ . Specify hyper-parameters in Algorithm 1 as

$$T_{\text{out}} = \left\lceil \log_{3/2} \frac{4L_\lambda(\lambda_u - \lambda_\ell)}{\delta} \right\rceil, \quad \eta' = \frac{\eta}{1 + 2T_{\text{out}}}, \quad L_\lambda = \bar{\rho} + \frac{B}{\lambda_\ell} [1 + e^{B/(\lambda_\ell \epsilon)}].$$

Suppose there exists an oracle  $\widehat{F}$  such that for any  $\lambda > 0$ , it gives estimation of the optimal value in (8) up to accuracy  $\delta/4$  with probability at least  $1 - \eta'$ , then with probability at least  $1 - \eta$ , Algorithm 1 finds the optimal multiplier up to accuracy  $\delta$  by calling the inexact oracle  $\widehat{F}$  for  $O(\log \frac{1}{\delta})$  times.

In particular, Algorithm 2 presents a way for constructing the oracle required by Algorithm 1. Combining Theorem 3 and 4, the overall computation cost for obtaining a  $\delta$ -optimal solution of (7) with probability at least  $1 - \eta$  is of  $\tilde{O}\left(\delta^{-3} \cdot \text{polylog} \frac{1}{\eta}\right)$ , with memory cost  $\tilde{O}\left(\delta^{-2} \cdot \text{polylog} \frac{1}{\eta}\right)$ . Additionally, when the smoothness condition Assumption 2(IV) holds, the computation cost reduces to  $\tilde{O}\left(\delta^{-2} \cdot \text{polylog} \frac{1}{\eta}\right)$ .

REMARK 9 (COMPARISON WITH WASSERSTEIN DRO). In comparison with our proposed algorithm for Sinkhorn DRO, one should note that Wasserstein DRO is not always tractable. Especially, the Wasserstein robust optimization problem with nominal distribution  $\widehat{\mathbb{P}} = \frac{1}{n} \sum_{i=1}^n \delta_{\hat{x}_i}$  corresponding to (7) can be formulated as the minimax problem

$$\min_{\theta \in \Theta, \lambda \geq 0} \max_{z_i \in \mathbb{R}^d, i \in [n]} \lambda \rho + \frac{1}{n} \sum_{i=1}^n [f_{\theta}(z_i) - \lambda c(\hat{x}_i, z_i)].$$

However, when  $f_{\theta}(z)$  is not concave in  $z$ , the above problem generally reduces to the convex-non-concave minimax learning problem and it is difficult to obtain the global optimum. See Table 1a for detailed summary on the tractability of Wasserstein DRO formulation under some special cases. Even when the Wasserstein DRO formulation is tractable, its complexity usually has non-negligible dependence on the sample size  $n$  (see [46, Remark 9] and references therein for more discussions). In contrast, the complexity for solving the Sinkhorn DRO formulation is *sample size independent*. ♣

Also, in many scenarios one need to tune the Sinkhorn radius  $\bar{\rho}$  for problem (7) to achieve satisfactory out-of-sample performance. It will often make sense to directly tune the Lagrangian multiplier  $\lambda$  in (8) rather than a target radius  $\bar{\rho}$ . In other words, it is more computationally efficient to solve the subproblem (8) with a tuned Lagrangian multiplier  $\lambda$  directly instead of problem (7) with a tuned Sinkhorn radius  $\bar{\rho}$ .

## 5. Applications

In this section, we apply our methodology on three applications: the newsvendor model, mean-risk portfolio optimization, and multi-class classification. We examine the performance of the (Sinkhorn DRO) model by comparing it with four benchmarks: (i) the classical sample average approximation (SAA) model; (ii) the Wasserstein DRO model; and (iii) the KL-divergence DRO model. We choose the cost function  $c(\cdot, \cdot) = \|\cdot - \cdot\|_1^1$  for 1-Wasserstein or 1-Sinkhorn DRO model, and  $c(\cdot, \cdot) = \frac{1}{2} \|\cdot - \cdot\|^2$  for 2-Wasserstein or 2-Sinkhorn DRO model. Unless otherwise specified, we take 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 hyper-parameters of DRO models using the  $K$ -fold cross-validation method with  $K = 5$ . We run the repeated experiments for 200 independent trials.

In Section 5.1 and Section 5.2, we measure the out-of-sample performance of a solution  $\theta$  based on training dataset  $\mathcal{D}$  using the coefficient of prescriptiveness in [11]:

$$\text{Prescriptiveness}(\theta) = 1 - \frac{J(\theta) - J^*}{J(\theta_{\mathcal{D}}^{\text{SAA}}) - J^*},$$

where  $J^*$  denotes the true optimal value when the true distribution is known exactly,  $\theta_{\mathcal{D}}^{\text{SAA}}$  denotes the decision from SAA approach with dataset  $\mathcal{D}$ , and  $J(\theta)$  denotes the expected loss of the solution  $\theta$  under the true distribution, estimated through an SAA objective value with  $10^5$  testing samples. Thus, the higher this coefficient is, the better out-of-sample performance the solution has. Further details and additional experiments are included in Appendix EC.1 and EC.2, respectively.

### 5.1. Newsvendor Model

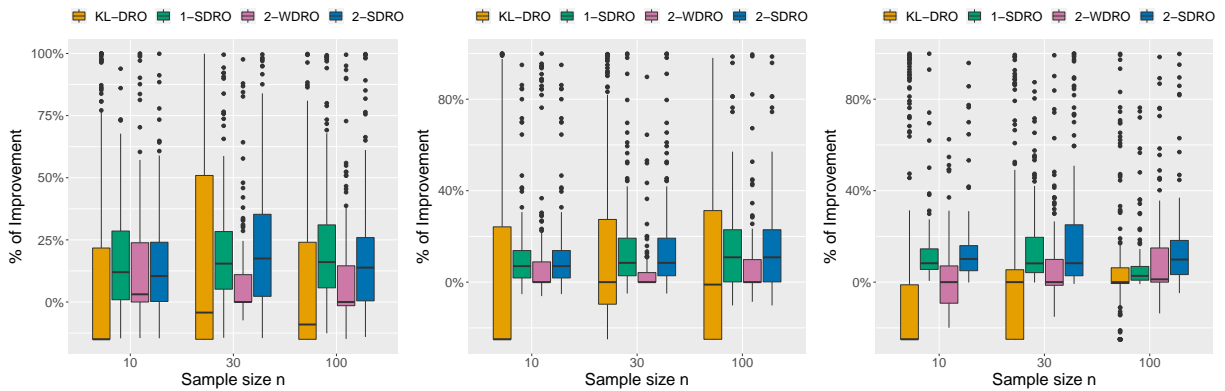
We consider the following distributionally robust newsvendor model:

$$\min_{\theta} \max_{\mathbb{P} \in \mathbb{B}_{\rho, \epsilon}(\hat{\mathbb{P}})} \mathbb{E}_{\mathbb{P}} [k\theta - u \min(\theta, z)],$$

where the random variable  $z$  stands for the random demand; its empirical distribution  $\hat{\mathbb{P}}$  consists of  $n$  independent samples from the data distribution  $\mathbb{P}_*$ ; the decision variable  $\theta$  represents the inventory level; and  $k = 5, u = 7$  are constants corresponding to overage and underage costs, respectively. In this experiment, we examine the performance of DRO models for various sample size  $n \in \{10, 30, 100\}$  and under three different types of data distribution: (i) the exponential distribution with rate parameter 1, (ii) the gamma distribution with shape parameter 2 and scale parameter 1.5, (iii) the equiprobable mixture of two truncated normal distributions  $\mathcal{N}(\mu = 1, \sigma = 1, a = 0, b = 10)$  and  $\mathcal{N}(\mu = 6, \sigma = 1, a = 0, b = 10)$ . In particular, we do not report the performance for 1-Wasserstein DRO model in this example, because this model shares the same formulation as the SAA approach [67, Remark 6.7]. Since 2-Wasserstein DRO is computationally intractable in this example, we solve the corresponding formulation by approximating the support of distribution using discrete grid points.

**Table 4** Average computational time (in seconds) per problem instance for the newsvendor problem.

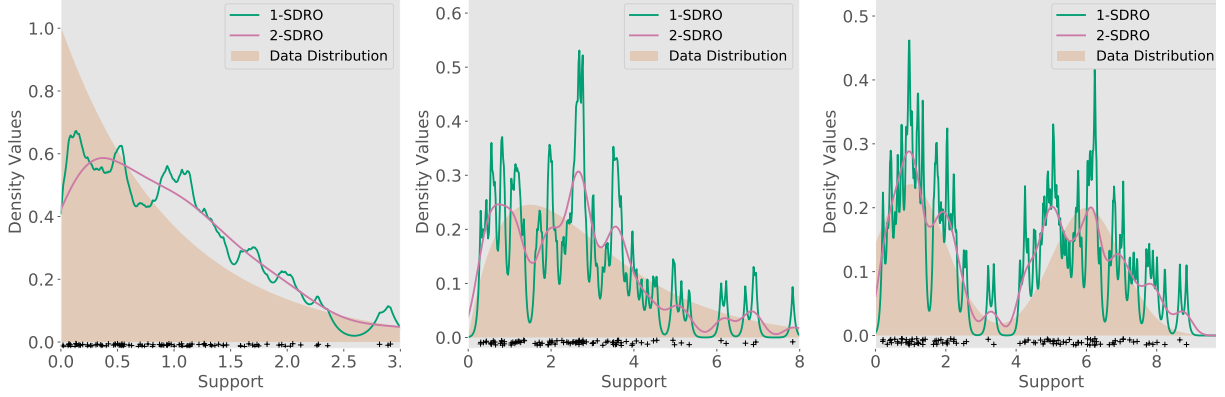
Model	Exponential			Gamma			Gaussian Mixture		
	$n = 10$	$n = 30$	$n = 100$	$n = 10$	$n = 30$	$n = 100$	$n = 10$	$n = 30$	$n = 100$
SAA	0.017	0.017	0.018	0.019	0.019	0.019	0.023	0.024	0.024
KL-DRO	0.027	0.029	0.040	0.027	0.028	0.039	0.027	0.028	0.038
1-SDRO	0.118	0.131	0.185	0.119	0.133	0.187	0.122	0.132	0.181
2-WDRO	0.123	0.358	1.307	0.128	0.354	1.337	0.134	0.402	1.428
2-SDRO	0.070	0.077	0.120	0.117	0.132	0.177	0.108	0.127	0.178



**Figure 1** Out-of-sample performances for the newsvendor model with parameters  $s \in \{0.25, 0.5, 0.75, 1, 2, 4\}$  and the fixed sample size  $n = 20$ . For figures from left to right, we specify the data distribution as exponential distribution, gamma distribution, and equiprobable mixture of two truncated normal distributions, respectively.

We report the box plots for the percentage of improvement across different DRO approaches in Fig. 1. We find that Sinkhorn DRO has the best out-of-sample performance in all figures. We report





**Figure 2** Plots for the density of worst-case distributions generated by the 1-SDRO or 2-SDRO model. In all figures we fix the sample size  $n = 100$ . For figures from left to right, we specify the data distribution as exponential distribution, gamma distribution, and equiprobable mixture of two truncated normal distributions, respectively.

the computational time for various approaches in Table 4. We observe that the training time of 2-Wasserstein DRO model increases quickly as the sample size increases, while the training time of other DRO models increases mildly in the training sample size. Finally, we plot the density of worst-case distributions for 1-SDRO or 2-SDRO model in Fig. 2. When specifying the data distribution as exponential, gamma, or Gaussian mixture, one can check the corresponding worst-case distributions capture the shape of the ground truth distribution reasonably well. Since the worst-case distributions from Sinkhorn DRO models are more reasonable, the corresponding decisions are less conservative compared to those from Wasserstein DRO models.

## 5.2. Mean-risk Portfolio Optimization

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

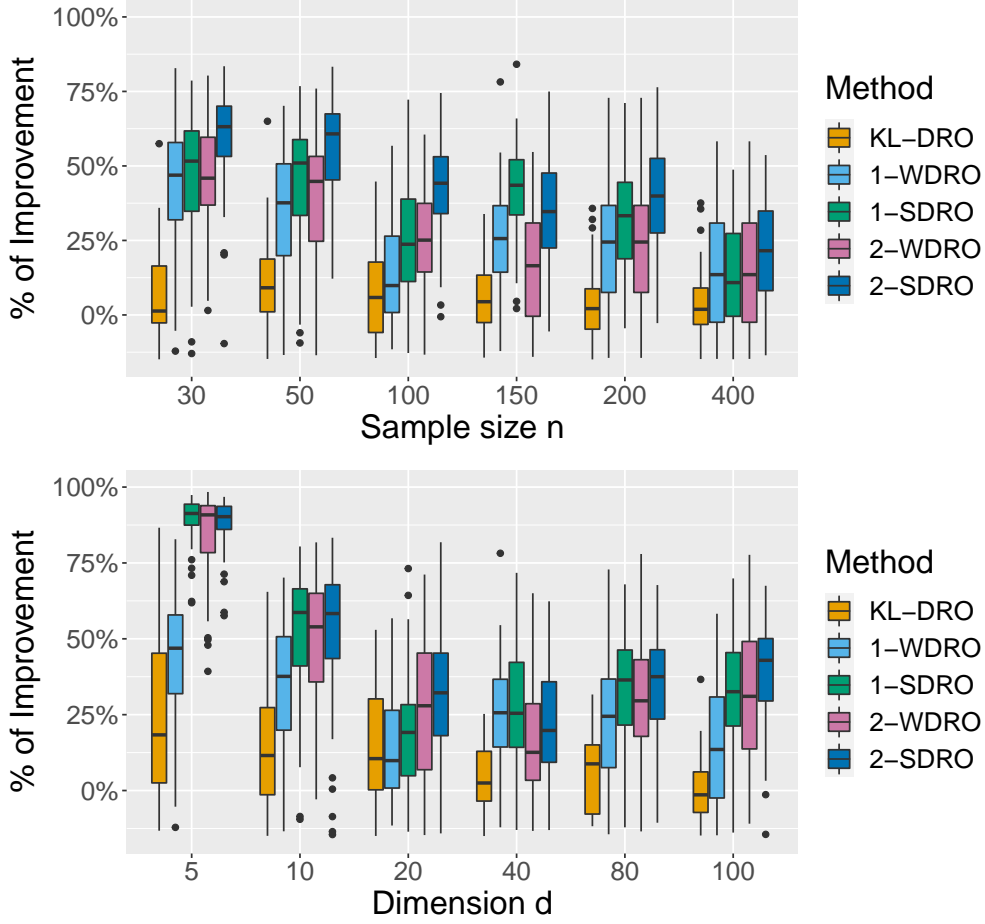
$$\begin{aligned} \min_{\theta} \max_{\mathbb{P} \in \mathbb{B}_{\rho, \epsilon}(\hat{\mathbb{P}})} \quad & \mathbb{E}_{\mathbb{P}_*}[-\theta^T z] + \varrho \cdot \mathbb{P}\text{-CVaR}_{\alpha}(-\theta^T z) \\ \text{s.t.} \quad & \theta \in \Theta = \{\theta \in \mathbb{R}_+^d : \theta^T \mathbf{1} = 1\}, \end{aligned}$$

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 [83], i.e., the average of the  $\alpha \times 100\%$  worst portfolio losses under the distribution  $\mathbb{P}$ . We follow a similar setup as in [67]. Specifically, we set  $\alpha = 0.2, \varrho = 10$ . The random asset  $z \sim \mathbb{P}_*$  can be decomposed into a systematic risk factor  $\psi \in \mathbb{R}$  and idiosyncratic risk factors  $\epsilon \in \mathbb{R}^d$ :

$$z_i = \psi + \epsilon_i, \quad i = 1, 2, \dots, d,$$

where  $\psi \sim \mathcal{N}(0, 0.02)$  and  $\epsilon_i \sim \mathcal{N}(i \times 0.03, i \times 0.025)$ . We solve this problem by taking the Bregman divergence  $D_{\omega}$  as the KL-divergence, so that the proximal gradient update can be implemented efficiently. Fig. 3a) reports the scenario where the data dimension  $d = 30$  is fixed and sample size  $n \in \{30, 50, 100, 150, 200, 400\}$ , and Fig. 3b) reports the scenario where the sample size  $n = 100$  is fixed and the number of assets  $d \in \{5, 10, 20, 40, 80, 100\}$ . Those box plots are generated from 200 independent trials, from which we can see that for all problem instances, the 1-SDRO or 2-SDRO model outperforms other DRO baselines.

Table 5 reports the average computational time for various DRO models. We observe that when data dimension is fixed and sample size varies from 30 to 400, the computational time for all approaches does not differ too much. When the data dimension increases and sample size is fixed, the computational time for 1-SDRO or 2-SDRO model increases linearly while other DRO models increases mildly.



**Figure 3** Box plot for the the portfolio optimization problem, where we try 200 independent trials for each problem instance. The  $x$ -axis indicates the number of observed samples  $n$  or the data dimension  $d$ , and the  $y$ -axis indicates the percentage of improvement in comparison with the SAA baseline. Upper:  $d = 30$  and  $n \in \{30, 50, 100, 150, 200, 400\}$ . Bottom:  $n = 100$  and  $d \in \{5, 10, 20, 40, 80, 100\}$ .

One possible explanation is that in this example, other DRO models have tractable finite-dimensional conic programming formulations so that off-the-shelf softwares can solve them efficiently. In contrast, Sinkhorn DRO models do not have special reformulation, but they can still be solved in reasonable amount of time.

### 5.3. Linear Classification Incorporating Structural Information

Finally, we investigate the multi-class logistic classification to illustrate the computational benefits of Sinkhorn DRO. Given a feature vector  $x \in \mathbb{R}^d$  and its label  $y \in [C]$ , we denote  $\vec{y} \in \{0, 1\}^C$  as the corresponding one-hot label vector, and define the following negative likelihood loss:

$$h_B(x, \vec{y}) = -\vec{y}^T B^T x + \log(1^T e^{B^T x}),$$

where  $B := [w_1, \dots, w_K]$  stands for the linear classifier. Then the DRO model aims to solve the following formulation:

$$\min_B \max_{\mathbb{P} \in \mathbb{B}_{\rho, \epsilon}(\hat{\mathbb{P}})} \mathbb{E}_{\mathbb{P}}[h_B(x, \vec{y})]$$

Assume only the feature vector  $x$  has uncertainty but not the label  $y$ . Also, assume the feature vector  $x$  lie in a subset of Euclidean space  $\Xi$  so that its infinity norm is bounded by 1. We specify the measure  $\nu$  as Lebesgue measure supported on  $\Xi$ .

**Table 5** Average computational time (in seconds) per problem instance for portfolio optimization problem.

$(n, d)$ Values	SAA	KL-DRO	1-WDRO	1-SDRO	2-WDRO	2-SDRO
(30, 30)	0.013	0.038	0.018	0.161	0.015	0.148
(50, 30)	0.014	0.042	0.020	0.209	0.016	0.175
(100, 30)	0.017	0.065	0.024	0.204	0.021	0.261
(150, 30)	0.019	0.084	0.029	0.203	0.027	0.258
(200, 30)	0.023	0.115	0.035	0.201	0.032	0.263
(400, 30)	0.045	0.136	0.061	0.205	0.056	0.257
(100, 5)	0.014	0.043	0.017	0.108	0.015	0.175
(100, 10)	0.014	0.045	0.018	0.133	0.015	0.229
(100, 20)	0.014	0.048	0.021	0.169	0.017	0.295
(100, 40)	0.017	0.068	0.027	0.233	0.022	0.432
(100, 80)	0.021	0.103	0.052	0.420	0.044	0.758
(100, 100)	0.023	0.116	0.070	0.500	0.059	0.836

This experiment is conducted using 6 real datasets from LIBSVM website. For the data preprocessing step, we learn the linear embedding of feature vectors using neural networks such that feature vectors have bounded infinity norm and the mis-classification risk for SAA approach is controlled within 50%. Detailed statistics on pre-processed datasets can be found in Table EC.1 in Appendix EC.1. We use the testing error for new observations to quantify the performance for the obtained classifiers.

Classification results for these different approaches are reported in Table 6, 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. We can see that in all problem instances SDRO models outperform the corresponding WDRO models, and either 1-SDRO or 2-SDRO model has the best classification performance. The average computational time for various approaches is reported in Table 7, from which we can see that Sinkhorn DRO models has shorter computational time than Wasserstein DRO models. In this example, Wasserstein DRO models can be reformulated as convex non-concave minimax problems. We try gradient descent ascent heuristics (see Algorithm 3 in Appendix EC.1) to approximately solve those formulations, but they are not computationally efficient to obtain satisfactory classifiers. For small boxes highlighted in Table 6, we find the Wasserstein DRO models in some cases even have worse performance than the traditional SAA model.

**Table 6** Classification results on real datasets. Each experiment is repeated for 200 independent trials, and 95% confidence intervals of classification errors for worse-case subgroup are reported for different approaches.

Dataset	SAA	KL-DRO	1-WDRO	1-SDRO	2-WDRO	2-SDRO
MNIST	.075 ± .002	.067 ± .002	.037 ± .003	<b>.035 ± .002</b>	.047 ± .003	<b>.041 ± .002</b>
IRIS	.396 ± .024	.351 ± .015	.321 ± .021	<b>.308 ± .021</b>	.378 ± .023	<b>.342 ± .022</b>
wine	.089 ± .010	.086 ± .010	.082 ± .005	<b>.077 ± .005</b>	.078 ± .005	<b>.076 ± .005</b>
vowel	.481 ± .012	.478 ± .011	.492 ± .012	<b>.456 ± .011</b>	.476 ± .012	<b>.443 ± .012</b>
vehicle	.379 ± .007	.368 ± .007	.481 ± .014	<b>.343 ± .006</b>	.434 ± .009	<b>.349 ± .007</b>
svmguide4	.427 ± .009	.418 ± .009	.430 ± .010	<b>.417 ± .009</b>	.425 ± .009	<b>.393 ± .011</b>

**Table 7** Average computational time (in seconds) per problem instance for multi-class classification problem

Dataset	SAA	KL-DRO	1-WDRO	1-SDRO	2-WDRO	2-SDRO
MNIST	2.423	5.245	5.826	4.810	4.920	2.606
IRIS	0.986	1.612	1.803	1.243	1.226	1.033
wine	1.669	2.331	2.104	1.813	1.905	1.826
vowel	19.507	23.438	26.826	25.343	29.447	26.123
vehicle	3.620	7.177	17.789	14.337	18.837	18.146
svmguide4	27.189	29.988	39.635	31.576	37.132	31.361

## 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. A meaningful research question is the choice of the optimal hyper-parameters in Sinkhorn DRO, such as the radius of the ambiguity set  $\bar{\rho}$ , the entropic regularization parameters  $\epsilon$ , and reference measures  $\nu$ . This paper focuses on regularizing Wasserstein distance with the entropic regularization – the Sinkhorn distance, but extensions to other types of regularization are possible. Exploring and discovering the benefits of Sinkhorn DRO in other types of applications may lead to future research directions.

### Appendix A: Sufficient condition for Condition 1

**PROPOSITION 1.** *Condition 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*

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

(III) *Assumption 1(III) holds, and there exists  $\lambda > 0$  such that*

$$\int e^{f(z)/(\lambda\epsilon)} e^{-2^{1-p}c(\bar{x}, z)/\epsilon} d\nu(z) < \infty.$$

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 1.

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## Supplementary for “Sinkhorn Distributionally Robust Optimization”

### Appendix EC.1: Detailed Experiment Setup

All the experiments are preformed on a MacBook Pro laptop with 32GB of memory running python 3.7. Unless otherwise specified, the SAA, Wasserstein DRO, and KL-divergence DRO baseline models are solved exactly based on the interior point method-based solver Mosek [4]. Optimization hyper-parameters (including step size, maximum iterations, number of levels, etc.) are tuned such that the training error after 100 iterations is decreased the fastest. To solve the Sinkhorn DRO model, we use V-SGD gradient estimator for newsvendor and portfolio optimization problems, and use V-MLMC estimator for multi-class classification problem. When solving the subproblem (8), the iteration is terminated when  $\frac{\|\text{obj}_{\ell+1} - \text{obj}_{\ell}\|}{1 + \|\text{obj}_{\ell}\|} \leq 1e-2$ , where  $\text{obj}_{\ell}$  denotes the objective function obtained at the  $\ell$ -th iteration. We also use the *warm starting* strategy during the iterative procedure: we set the initial guess of parameter  $\theta$  at the beginning of outer iteration as the one obtained from the SAA approach. At other outer iterations, the initial guess of parameter  $\theta$  is set to be the final obtained solution  $\theta$  at the last outer iteration. The following subsections outline some special reformulations or optimization algorithms for solving baseline models.

#### EC.1.1. Setup for Newsvendor Problem

To solve the 2-Wasserstein DRO model with radius  $\rho$ , we approximate the support of worst-case distribution using discrete grid points. Denote by  $\mathcal{D}_n = \{x_1, \dots, x_n\}$  the set of observed  $n$  samples and  $\mathcal{G}_{200-n}$  the set of  $200 - n$  points evenly supported on the interval  $[0, 10]$ . Then the support of worst-case distribution is restricted to  $\mathcal{D}_n \cup \mathcal{G}_{200-n} := \{\hat{z}_1, \dots, \hat{z}_{200}\}$ . The corresponding 2-Wasserstein DRO problem has the following linear programming reformulation:

$$\begin{aligned} \min_{\theta, \lambda, s} \quad & \lambda\rho + \frac{1}{n} \sum_{i=1}^n s_i \\ \text{s.t.} \quad & k\theta - u \min(\theta, \hat{z}_j) - \lambda(x_i - \hat{z}_j)^2 \leq s_i, \quad \forall i \in [n], \forall j \in [200]. \end{aligned}$$

#### EC.1.2. Setup for Mean-risk Portfolio Optimization

From [67, Eq. (27)] we can see that the 1-Wasserstein DRO formulation with radius  $\rho$  for the portfolio optimization problem becomes

$$\begin{aligned} \min_{\theta, \tau, \lambda, s} \quad & \lambda\rho + \frac{1}{n} \sum_{i=1}^n s_i \\ \text{s.t.} \quad & \theta \in \Theta, \\ & b_j\tau + a_j \langle \theta, \hat{z}_i \rangle \leq s_i, \quad i \in [n], j \in [H], \\ & \|a_j\theta\|_2 \leq \lambda, \quad j \in [H]. \end{aligned}$$

Also, we argue that the 2-Wasserstein DRO formulation with radius  $\rho$  for the portfolio optimization problem has a finite convex reformulation:

$$\begin{aligned} & \inf_{\theta \in \Theta, \tau} \sup_{\mathbb{P}: W_2(\mathbb{P}, \mathbb{P}_n) \leq \rho} \mathbb{E}_{\mathbb{P}} \left[ \max_{j \in [H]} a_j \langle \theta, z \rangle + b_j \tau \right] \\ = & \inf_{\theta \in \Theta, \tau, \lambda \geq 0} \left\{ \lambda\rho^2 + \frac{1}{n} \sum_{i=1}^n \sup_{s_i} \left\{ \max_{j \in [H]} a_j \langle \theta, s_i \rangle + b_j \tau - \lambda \|s_i - \hat{z}_i\|_2^2 \right\} \right\}. \end{aligned}$$

**Table EC.1** Basic statistics of classification datasets

Dataset	# of Features	# of Classes	Training Size	Testing Size
MNIST	50	10	345	69655
IRIS	10	3	37	133
wine	13	3	44	134
vowel	30	11	594	396
vehicle	20	4	507	339
svmguid4	50	6	367	245

In particular, the inner subproblem has the following reformulation:

$$\begin{aligned}
& \sup_{s_i} \left\{ \max_{j \in [H]} a_j \langle \theta, s_i \rangle + b_j \tau - \lambda \|s_i - \hat{z}_i\|_2^2 \right\} \\
&= \max_{j \in [H]} b_j \tau + \sup_{s_i} \left\{ a_j \langle \theta, s_i \rangle - \lambda \|s_i - \hat{z}_i\|_2^2 \right\} \\
&= \max_{j \in [H]} b_j \tau + \frac{a_j^2}{4\lambda} \|\theta\|_2^2 + a_j \langle \theta, \hat{z}_i \rangle.
\end{aligned}$$

Hence, the 2-Wasserstein DRO can be reformulated as

$$\begin{aligned}
& \min_{\theta, \tau, \lambda, s} \lambda \rho^2 + \frac{1}{n} \sum_{i=1}^n s_i \\
& \text{s.t. } \theta \in \Theta, \\
& b_j \tau + a_j \langle \theta, \hat{z}_i \rangle + \frac{a_j^2}{4\lambda} \|\theta\|_2^2 \leq s_i, \quad i \in [n], j \in [H].
\end{aligned}$$

### EC.1.3. Setup for Linear Classification Incorporating Structural Information

In this example, we solve the SAA, KL-divergence DRO problem using stochastic gradient descent. Also, Wasserstein DRO models can be reformulated as

$$\min_{B, \lambda \geq 0} \max_{\|z_i\|_\infty \leq 1, i \in [n]} \lambda \rho + \frac{1}{N} \sum_{i=1}^n [h_B(z_i) - \lambda c(\hat{x}_i, z_i)]. \quad (\text{EC.1})$$

To approximately solve such a convex-non-concave problem, we implement a gradient descent ascent heuristic outlined in Algorithm 3. Finally, we report basic statistics of classification datasets in this example in Table EC.1.



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**Algorithm 3** Heuristic Gradient Descent Ascent algorithm for solving (EC.1). We use default values

$\alpha = 5\text{e-}6, m = 64, n_{\text{critic}} = 5$ .

---

**Require:** Learning rate  $\alpha$ , batch size  $m$ , number of inner iterations  $n_{\text{critic}}$ , initial guess  $(\theta, \lambda)$ .

```

1: while  $(\theta, \lambda)$  not converged do
2:   for  $t = 0, 1, \dots, n_{\text{critic}}$  do
3:     Sample a subset of indices  $\{n_i\}_{i=1}^m$  from  $[n]$ .
4:     Compute  $g_{n_i} \leftarrow \frac{1}{N} \nabla_{z_{n_i}} [h_B(z_{n_i}) - \lambda c(\hat{z}_{n_i}, z_{n_i})]$  for  $i \in [m]$ .
5:     Update  $z_{n_i} \leftarrow \text{Proj}_{\mathcal{Z}} [z_{n_i} + \alpha \text{RMSProp}(z_{n_i}, g_{n_i})]$ .
6:   end for
7:   Sample a subset of indices  $\{n_i\}_{i=1}^m$  from  $[n]$ .
8:   Compute  $g_\lambda \leftarrow \nabla_\lambda \left\{ \lambda \rho + \frac{1}{m} \sum_{i=1}^m [h_B(z_{n_i}) - \lambda c(\hat{z}_{n_i}, z_{n_i})] \right\}$ .
9:   Compute  $g_B \leftarrow \nabla_B \left\{ \frac{1}{m} \sum_{i=1}^m h_B(z_{n_i}) \right\}$ .
10:  Update  $\lambda \leftarrow (\lambda - \alpha \text{RMSProp}(\lambda, g_\lambda))_+$ .
11:  Update  $B \leftarrow B - \alpha \text{RMSProp}(B, g_B)$ .
12: end while
Output  $(\lambda, B)$ .
```

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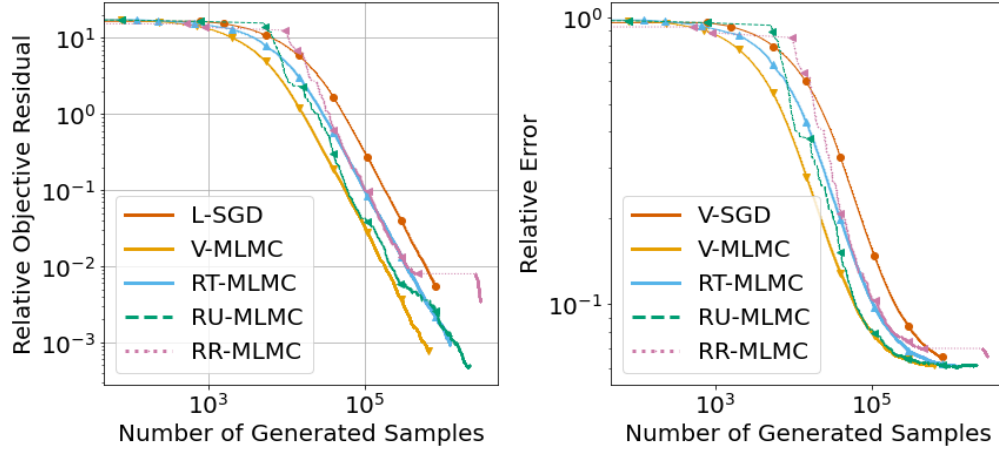
## Appendix EC.2: Additional Validation Experiments

### EC.2.1. Comparison of Optimization Algorithms

To examine the performance of different gradient estimators, we study the problem of distributionally robust linear regression (see the setup in Example 2). We take the nominal distribution  $\hat{\mathbb{P}}$  as the empirical one based on samples  $\{(a_i, b_i)\}_{i=1}^n$ . As a consequence, the inner objective function in (8) has the closed form expression:

$$F(\theta) = \frac{1}{n} \sum_{i=1}^n (a_i^T \theta - b_i)^2 + \frac{\frac{1}{n} \sum_{i=1}^n (a_i^T \theta - b_i)^2}{\frac{1}{2} \lambda \|\theta\|_2^{-2} - 1} - \frac{\lambda \epsilon}{2} \log \det \left( I - \frac{\theta \theta^T}{\frac{1}{2} \lambda} \right), \quad \text{if } \|\theta\|_2^2 < \frac{\lambda}{2},$$

and otherwise  $F(\theta) = \infty$ . We take the constraint set  $\Theta = \{\theta : \|\theta\|_2^2 \leq 0.999 \cdot \frac{\lambda}{2}\}$ . For the data generation procedure, we first generate a ground truth predictor  $\theta^* \sim \mathcal{N}(0, 100 \cdot I_d)$ . We then generate inputs  $a_i \sim \mathcal{N}(0, I_d)$  and  $b_i = \langle a_i, \theta^* \rangle + \zeta_i$ , where the noise  $\zeta_i$  follows the Gaussian distribution such that the response  $b_i$  has the signal-to-noise ratio 0.2. In this experiment, we take the training sample size  $n = 500$  and data dimension  $d = 50$ .



**Figure EC.1** Comparison results of V-SGD, V-MLMC, RT-MLMC, RU-MLMC, and RR-MLMC on robust linear regression in terms of relative objective residual (left plot) and relative prediction error (right plot).

The quality of proposed gradient estimators is examined in a single BSMD step with specified hyper-parameters  $(\lambda, \epsilon) = (5 \cdot 10^3, 10^{-2})$ . For baseline comparison, we also study the performance of two unbiased gradient estimators in literature [55]. However, the variance of them are unbounded, so that there is no convergence analysis for those two methods.

**RU-MLMC Estimator:** at point  $\theta$ , first sample a *random level*  $\iota$  following distribution  $Q_{\text{RU}} = \{q_\ell\}_{\ell=0}^\infty$  with  $\mathbb{P}(\iota = \ell) = q_\ell$ , then construct

$$v^{\text{RU-MLMC}}(\theta) := \frac{1}{q_\iota} G^\iota(\theta, \zeta^\iota). \quad (\text{EC.2})$$

**RR-MLMC Estimator:** at point  $\theta$ , first sample a *random level*  $L$  following distribution  $Q_{\text{RR}} = \{q_\ell\}_{\ell=0}^\infty$  with  $\mathbb{P}(L = \ell) = q_\ell$ , then construct

$$v^{\text{RR-MLMC}}(\theta) := \sum_{\ell=0}^L p_\ell G^\ell(x, \zeta^\ell), \quad (\text{EC.3})$$

where  $p_\ell := \frac{1}{1 - \sum_{\ell'=0:\ell-1} q_{\ell'}}$  and  $\sum_{\ell'=0}^{-1} q_{\ell'} = 0$ .

---

To quantify the performance of a given solution  $\theta$ , we denote the relative objective residual as  $\frac{F(\theta) - F(\theta^*)}{1 + |F(\theta^*)|}$ , where  $\theta^*$  is the optimal solution of  $F$ . We compute this optimal solution by optimizing the closed-form expression of  $F$  directly via OSMM software [91]. We also denote the relative error of  $\theta$  as  $\frac{\|\theta - \theta^*\|}{1 + \|\theta^*\|}$ , where  $\theta^*$  is the ground truth optimal solution when the data distribution is known. Fig. EC.1 reports the relative objective residual and relative error in terms of the number of generated samples. From the plot, we can see the V-SGD scheme does not have competitive performance, which is consistent with our theoretical analysis that V-SGD has the worst complexity order. In contrast, using other MLMC methods, we can obtain optimal solutions with small sample complexity. Although the RU-MLMC and RR-MLMC schemes have competitive performance, we can see there exist some oscillations during the optimization procedure. One possible explanation is that the variance values of those gradient estimators are unbounded, making those two approaches unstable.

### EC.2.2. Sensitivity of Regularization Parameters

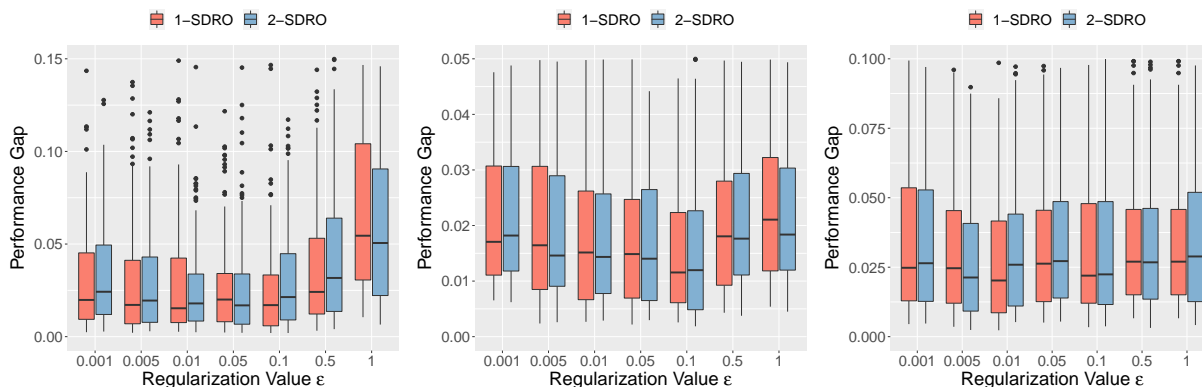
In this subsection, we validate the impact of regularization parameter  $\epsilon$  on the performance of the Sinkhorn DRO model in two numerical examples: newsvendor and portfolio optimization problem. We examine the performance of 1-SDRO or 2-SDRO models for different regularization parameters chosen from the candidate set  $\mathcal{A}$ :

$$\mathcal{A} = \begin{cases} \{10^{-3}, 5 \cdot 10^{-3}, 10^{-2}, 5 \cdot 10^{-2}, 10^{-1}, 5 \cdot 10^{-1}, 10^0\}, & \text{for newsvendor problem,} \\ \{5 \cdot 10^{-2}, 10^{-1}, 5 \cdot 10^{-1}, 10^0, 3 \cdot 10^0, 5 \cdot 10^0, 10^1\}, & \text{for portfolio optimization.} \end{cases}$$

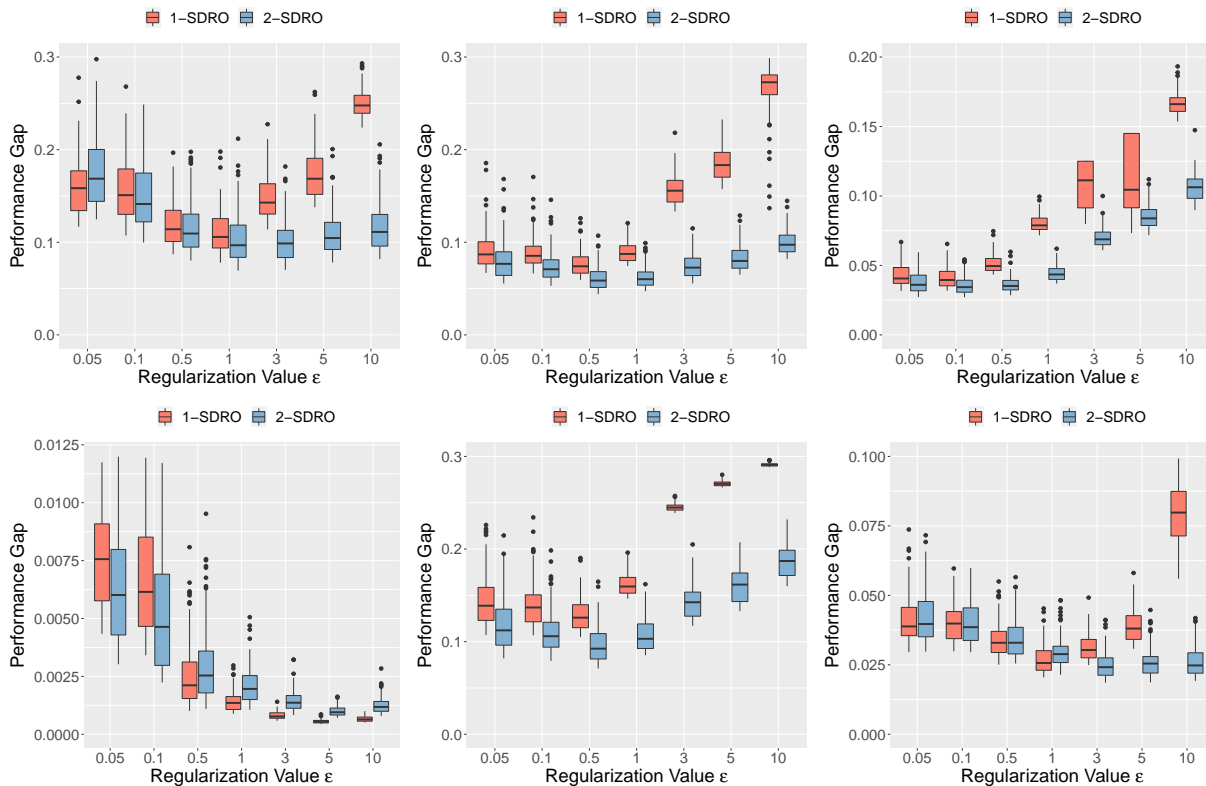
For each fixed regularization parameter  $\epsilon$ , we tune the corresponding Sinkhorn DRO radius  $\bar{\rho}$  by cross validation. We quantify the performance of a given solution  $\theta$  obtained from DRO models using the *performance gap* metric  $\frac{J(\theta) - J^*}{1 + |J^*|}$ , where notations  $J^*$  and  $J(\theta)$  are defined at the beginning of Section 5. Hence, the smaller the metric is, the better the given decision has.

Fig. EC.2 shows box plots on the performance of Sinkhorn DRO models across different choices of regularization values with different data distributions on the newsvendor problem. We can see as the regularization value increases, the performance of Sinkhorn DRO models generally improves first and then degrades.

Fig. EC.3 shows performance on the portfolio optimization problem with different choices of problem parameters  $(n, d)$ , where  $n$  denotes the sample size and  $d$  denotes the data dimension. Compared with the newsvendor problem, we find a more clear trend that the model performance improves and then degrades as the regularization value increases. In this special example, we also find 2-SDRO model has more stable and satisfactory performance compared with 1-SDRO model.



**Figure EC.2** Performance of Sinkhorn DRO models for newsvendor problem versus different choices of regularization values  $\epsilon$ . For figures from left to right, we specify the data distribution as exponential distribution, gamma distribution, and equiprobable mixture of two truncated normal distributions, respectively.



**Figure EC.3** Performance of Sinkhorn DRO models for portfolio problem versus different choices of regularization values  $\epsilon$ . For those fix figures from left to right, from top to bottom, we specify the problem parameters (sample size  $n$  and data dimension  $d$ ) as  $(30, 30)$ ,  $(100, 30)$ ,  $(400, 30)$ ,  $(100, 5)$ ,  $(100, 20)$ ,  $(100, 100)$ , respectively.

### Appendix EC.3: Proofs of Technical Results in Section 3.2

*Proof of Remark 4* 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 limit for the second term in  $v(\lambda; \epsilon)$  to obtain:

$$\begin{aligned} & \lim_{\epsilon \rightarrow 0} \lambda\epsilon \int \log \left( \int \exp \left( \frac{f(z) - \lambda c(x, z)}{\lambda\epsilon} \right) d\nu(z) \right) d\widehat{\mathbb{P}}(x) \\ &= \int \lim_{\beta \rightarrow \infty} \frac{\lambda}{\beta} \log \left( \int \exp \left( \frac{[f(z) - \lambda c(x, z)]\beta}{\lambda} \right) d\nu(z) \right) d\widehat{\mathbb{P}}(x) \\ &= \int \lim_{\beta \rightarrow \infty} \lambda \nabla \log \left( \int \exp \left( \frac{[f(z) - \lambda c(x, z)]\beta}{\lambda} \right) d\nu(z) \right) d\widehat{\mathbb{P}}(x) \\ &= \int \left[ \lim_{\beta \rightarrow \infty} \frac{\int \exp \left( \frac{[f(z) - \lambda c(x, z)]\beta}{\lambda} \right) [f(z) - \lambda c(x, z)] d\nu(y)}{\int \exp \left( \frac{[f(z) - \lambda c(x, z)]\beta}{\lambda} \right) d\nu(y)} \right] d\widehat{\mathbb{P}}(x) \\ &= \int \operatorname{ess\,sup}_{\nu} [f(\cdot) - \lambda c(x, \cdot)] d\widehat{\mathbb{P}}(x). \end{aligned}$$

Particularly, when  $\operatorname{supp}(\nu) = \mathcal{Z}$ , it holds that

$$\operatorname{ess\,sup}_{\nu} [f(\cdot) - \lambda c(x, \cdot)] = \sup_z [f(z) - \lambda c(x, z)],$$

and in this case the dual objective function of the Sinkhorn DRO problem converges into that of the Wasserstein DRO problem.  $\square$

*Proof of Example 2* In this example, the dual objective becomes

$$V_D = \inf_{\lambda \geq 0} \left\{ \lambda \bar{\rho} + \mathbb{E}_{(a,b) \sim \widehat{\mathbb{P}}} \left[ \lambda \epsilon \log \left( \mathbb{E}_{a' \sim \mathcal{N}(a, \eta I_d)} \exp \left( \frac{(\theta^T a' - b)^2}{\lambda \epsilon} \right) \right) \right] \right\}. \quad (\text{EC.4})$$

Specially, for any  $a \in \mathbb{R}^d, b \in \mathbb{R}, \theta \in \mathbb{R}^d$ , it holds that

$$\begin{aligned} & \lambda \epsilon \log \left( \mathbb{E}_{a' \sim \mathcal{N}(a, \eta I_d)} \exp \left( \frac{(\theta^T a' - b)^2}{\lambda \epsilon} \right) \right) \\ &= \lambda \epsilon \log \left( \mathbb{E}_{\Delta_a \sim \mathcal{N}(0, I_d)} \exp \left( \frac{[(\theta^T a - b) + (\sqrt{\eta} \theta)^T \Delta_a]^2}{\lambda \epsilon} \right) \right) \\ &= (\theta^T a - b)^2 + \lambda \epsilon \log \left( \underbrace{\mathbb{E}_{\Delta_a \sim \mathcal{N}(0, I_d)} \exp \left( \frac{\eta(\theta^T \Delta_a)^2 - 2(b - \theta^T a)\sqrt{\eta} \theta^T \Delta_a}{\lambda \epsilon} \right)}_{\text{(I)}} \right). \end{aligned}$$

Note that the term (I) can be simplified using integral of exponential functions:

$$\begin{aligned} \text{(I)} &= (2\pi)^{-d/2} \int_{\mathbb{R}^d} \exp \left( -\frac{1}{2} \Delta_a^T \Delta_a + \frac{(\theta^T \Delta_a)^2}{\lambda} - 2 \frac{(b - \theta^T a)\theta^T}{\lambda \sqrt{\epsilon}} \Delta_a \right) d\Delta_a \\ &= (2\pi)^{-d/2} \int_{\mathbb{R}^d} \exp \left( -\frac{1}{2} \Delta_a^T A \Delta_a + J^T \Delta_a \right) d\Delta_a, \end{aligned}$$

where the matrix  $A = I - \frac{2\theta\theta^T}{\lambda}$  and vector  $J = 2\frac{(\theta^T a - b)\theta}{\lambda\sqrt{\epsilon}}$ . As a consequence, when  $\|\theta\|_2^2 < \frac{\lambda}{2}$ , it holds that

$$\begin{aligned} (\mathbf{I}) &= \det(A)^{-1/2} \exp\left(\frac{1}{2}J^T A^{-1}J\right) \\ &= \det\left(I - \frac{2\theta\theta^T}{\lambda}\right)^{-1/2} \exp\left(2\frac{(\theta^T a - b)^2}{\lambda^2\epsilon}\theta^T A^{-1}\theta\right). \end{aligned}$$

Finally, we arrive at

$$\begin{aligned} &\lambda\epsilon \log\left(\mathbb{E}_{a' \sim \mathcal{N}(a, \eta I_d)} \exp\left(\frac{(\theta^T a' - b)^2}{\lambda\epsilon}\right)\right) \\ &= (\theta^T a - b)^2 + \frac{(\theta^T a - b)^2}{\frac{1}{2}\lambda\|\theta\|_2^2 - 1} - \frac{\lambda\epsilon}{2} \log \det\left(I - \frac{2\theta\theta^T}{\lambda}\right), \quad \text{if } \|\theta\|_2^2 < \frac{\lambda}{2}. \end{aligned}$$

Substituting this expression into (EC.4) gives the desired result.  $\square$

*Proof of Corollary 2* We now introduce the epi-graphical variables  $s_i, i = 1, \dots, n$  to reformulate  $V_D$  as

$$V_D = \begin{cases} \inf_{\lambda \geq 0, s_i} & \lambda\bar{\rho} + \frac{1}{n} \sum_{i=1}^n s_i \\ \text{s.t.} & \lambda\epsilon \log(\mathbb{E}_{\mathbb{Q}_{i,\epsilon}} [e^{f(z)/(\lambda\epsilon)}]) \leq s_i, \forall i \end{cases}$$

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

$$\begin{aligned} &\left\{ \exp\left(\frac{s_i}{\lambda\epsilon}\right) \geq \mathbb{E}_{\mathbb{Q}_{i,\epsilon}} [e^{f(z)/(\lambda\epsilon)}] \right\} \\ &= \left\{ 1 \geq \mathbb{E}_{\mathbb{Q}_{i,\epsilon}} \left[ e^{[f(z) - s_i]/(\lambda\epsilon)} \right] \right\} \\ &= \left\{ \lambda\epsilon \geq \mathbb{E}_{\mathbb{Q}_{i,\epsilon}} \left[ \lambda\epsilon e^{[f(z) - s_i]/(\lambda\epsilon)} \right] \right\} \\ &= \left\{ \lambda\epsilon \geq \sum_{\ell=1}^L \mathbb{Q}_{i,\epsilon}(z_\ell) a_{i,\ell} \right\} \cap \left\{ a_{i,\ell} \geq \lambda\epsilon \exp\left(\frac{f(z_\ell) - s_i}{\lambda\epsilon}\right), \forall \ell \right\}, \end{aligned}$$

where the second constraint set can be formulated as

$$(\lambda\epsilon, a_{i,\ell}, f(z_\ell) - s_i) \in \mathcal{K}_{\text{exp}}.$$

Substituting this expression into  $V_D$  completes the proof.  $\square$



## Appendix EC.4: Proofs of Technical Results in Section 3.3

We rely on the following technical lemma to derive our strong duality result.

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

$$v(\tau) = \sup_{\mathbb{P} \in \mathcal{P}(\mathcal{Z})} \left\{ \mathbb{E}_{\mathbb{P}} \left[ f(z) - \tau \log \left( \frac{d\mathbb{P}}{d\mathbb{Q}}(z) \right) \right] \right\}. \quad (\text{EC.5})$$

(I) When  $\tau = 0$ ,

$$v(0) = \operatorname{ess\,sup}_{\mathbb{Q}}(f) \triangleq \inf \{ t \in \mathbb{R} : \Pr_{z \sim \mathbb{Q}} \{ f(z) > t \} = 0 \}.$$

(II) When  $\tau > 0$  and

$$\mathbb{E}_{\mathbb{Q}} [e^{f(z)/\tau}] < \infty,$$

it holds that

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

and  $\lim_{\tau \downarrow 0} v(\tau) = v(0)$ . The optimal solution in (EC.5) has the expression

$$d\mathbb{P}(z) = \frac{e^{f(z)/\tau}}{\int e^{f(u)/\tau} d\mathbb{Q}(u)} d\mathbb{Q}(z).$$

(III) When  $\tau > 0$  and

$$\mathbb{E}_{\mathbb{Q}} [e^{f(z)/\tau}] = \infty,$$

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

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

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

Then the remaining part follows the discussion in [57, Section 2.1].  $\square$

*Proof of Lemma 1* Based on Definition 1 of Sinkhorn distance, we reformulate  $V$  as

$$V = \sup_{\gamma \in \mathcal{P}(\mathcal{Z} \times \mathcal{Z}) : \operatorname{Proj}_1 \# \gamma = \widehat{\mathbb{P}}} \left\{ \mathbb{E}_{\gamma} [f(z)] : \mathbb{E}_{\gamma} \left[ c(x, z) + \epsilon \log \left( \frac{d\gamma(x, z)}{d\widehat{\mathbb{P}}(x) d\nu(z)} \right) \right] \leq \rho \right\}.$$

By the disintegration theorem [23] we represent the joint distribution  $\gamma$  such that  $d\gamma(x, z) = d\widehat{\mathbb{P}}(x) d\gamma_x(z)$  holds for any  $(x, z)$ , where  $\gamma_x$  is the conditional distribution of  $\gamma$  given the first marginal of  $\gamma$  equals  $x$ . Thereby the constraint is equivalent to

$$\int \mathbb{E}_{\gamma_x} \left[ c(x, z) + \epsilon \log \left( \frac{d\gamma_x(z)}{d\nu(z)} \right) \right] d\widehat{\mathbb{P}}(x) \leq \rho, \quad \gamma_x \in \mathcal{P}(\mathcal{Z}), x \in \operatorname{supp}(\widehat{\mathbb{P}}).$$

We remark that any feasible solution  $\gamma$  satisfies that  $\gamma \ll \widehat{\mathbb{P}} \otimes \nu$  and hence  $\gamma_x \ll \nu$ . Consequently the term  $\log \left( \frac{d\gamma_x(z)}{d\nu(z)} \right)$  is well-defined. Based on the change-of-measure identity  $\log \left( \frac{d\gamma_x(z)}{d\nu(z)} \right) = \log \left( \frac{d\mathbb{Q}_{x, \epsilon}(z)}{d\nu(z)} \right) + \log \left( \frac{d\gamma_x(z)}{d\mathbb{Q}_{x, \epsilon}(z)} \right)$  and the expression of  $\mathbb{Q}_{x, \epsilon}$ , the constraint can be reformulated as

$$\int \mathbb{E}_{\gamma_x} \left[ c(x, z) + \epsilon \log \left( \frac{e^{-c(x, z)/\epsilon}}{\int e^{-c(x, u)/\epsilon} d\nu(u)} \right) + \epsilon \log \left( \frac{d\gamma_x(z)}{d\mathbb{Q}_{x, \epsilon}(z)} \right) \right] d\widehat{\mathbb{P}}(x) \leq \rho,$$

$$\gamma_x \in \mathcal{P}(\mathcal{Z}), x \in \operatorname{supp}(\widehat{\mathbb{P}}).$$

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

$$\epsilon \int \mathbb{E}_{\gamma_x} \left[ \log \left( \frac{d\gamma_x(z)}{d\mathbb{Q}_{x,\epsilon}(z)} \right) \right] d\hat{\mathbb{P}}(x) \leq \bar{\rho}, \quad \gamma_x \in \mathcal{P}(\mathcal{Z}), x \in \text{supp}(\hat{\mathbb{P}}).$$

Similarly, the objective function of ([Sinkhorn DRO](#)) can be written as  $\int \mathbb{E}_{\gamma_x} [f(z)] d\hat{\mathbb{P}}(x)$ . Consequently, the primal problem ([Sinkhorn DRO](#)) can be reformulated as a generalized KL-divergence DRO problem

$$V = \sup_{\gamma_x \in \mathcal{P}(\mathcal{Z}), x \in \text{supp}(\hat{\mathbb{P}})} \left\{ \int \mathbb{E}_{\gamma_x} [f(z)] d\hat{\mathbb{P}}(x) : \epsilon \int \mathbb{E}_{\gamma_x} \left[ \log \left( \frac{d\gamma_x(z)}{d\mathbb{Q}_{x,\epsilon}(z)} \right) \right] d\hat{\mathbb{P}}(x) \leq \bar{\rho} \right\}.$$

□

*Proof of Lemma 2* Recall from [Remark 5](#) that the primal problem  $V$  can be reformulated as

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

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

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

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

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

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

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

and swap the supremum and the integration, we obtain

$$V \leq \inf_{\lambda \geq 0} \left\{ \lambda \bar{\rho} + \int v_x(\lambda) d\hat{\mathbb{P}}(x) \right\}. \quad (\text{EC.6})$$

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,

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

Substituting this expression into [\(EC.6\)](#) implies that  $V \leq V_D < \infty$ . Suppose on the contrary that for any  $\lambda > 0$ ,

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

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

□

*Proof of Lemma 3* We first show that  $\lambda^* < \infty$ . Denote by  $v(\lambda)$  the objective function for the dual problem, then

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

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

$$\begin{aligned}
& \lim_{\lambda \rightarrow \infty} \lambda \epsilon \int \log \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} \left[ e^{f(z)/(\lambda\epsilon)} \right] \right) d\widehat{\mathbb{P}}(x) \\
&= \int \lim_{\beta \rightarrow 0} \frac{\epsilon}{\beta} \log \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} \left[ e^{\beta f(z)/\epsilon} \right] \right) d\widehat{\mathbb{P}}(x) \\
&= \int \lim_{\beta \rightarrow 0} \epsilon \nabla_{\beta} \log \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} \left[ e^{\beta f(z)/\epsilon} \right] \right) d\widehat{\mathbb{P}}(x) \\
&= \int \lim_{\beta \rightarrow 0} \epsilon \frac{1}{\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} \left[ e^{\beta f(z)/\epsilon} \right]} \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} \left[ \frac{f(z)}{\epsilon} e^{(\beta f(z))/\epsilon} \right] \right) d\widehat{\mathbb{P}}(x) \\
&= \int \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [f(z)] d\widehat{\mathbb{P}}(x),
\end{aligned}$$

where the first equality follows from the change-of-variable technique with  $\beta = 1/\lambda$ , the second equality follows from the definition of derivative, the third and the last equality follows from the dominated convergence theorem. As a consequence, as long as  $\bar{\rho} > 0$ , we have

$$\lim_{\lambda \rightarrow \infty} v(\lambda) = \infty.$$

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.  $\square$

*Proof of Lemma 4* Suppose the dual minimizer  $\lambda^* = 0$ , then taking the limit of the dual objective function gives

$$\lim_{\lambda \rightarrow 0} v(\lambda) = \int H^u(x) d\widehat{\mathbb{P}}(x) < \infty,$$

where

$$H^u(x) := \inf \{ t : \mathbb{Q}_{x,\epsilon} \{ f(z) > t \} = 0 \} \triangleq \operatorname{ess\,sup}_{\mathbb{Q}_{x,\epsilon}} f.$$

For notational simplicity we take  $H^u = \operatorname{ess\,sup} f$ . One can check that  $H^u(x) \equiv H^u$  for any  $x \in \operatorname{supp}(\widehat{\mathbb{P}})$ : for any  $t$  so that  $\mathbb{Q}_{x,\epsilon} \{ f(z) > t \} = 0$ , we have that

$$\int 1\{f(z) > t\} e^{-c(x,z)/\epsilon} d\nu(z) = 0,$$

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

$$\int 1\{f(z) > t\} d\nu(z) = 0.$$

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

$$0 \leq \int 1\{f(z) > t\} e^{-c(x,z)/\epsilon} d\nu(z) \leq \int 1\{f(z) > t\} d\nu(z) = 0,$$

where the second inequality is because that  $\nu\{c(x,z) \geq 0\} = 1$ . As a consequence,  $\mathbb{Q}_{x,\epsilon} \{ f(z) > t \} = 0$ . Hence we can assert that  $H^u(x) = H^u$  for all  $x \in \operatorname{supp}(\widehat{\mathbb{P}})$ , which implies

$$\lim_{\lambda \rightarrow 0} v(\lambda) = H^u < \infty.$$

Then we show that almost surely for all  $x$ ,

$$\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [1_A] > 0, \quad \text{where } A = \{z : f(z) = H^u\}.$$

Denote by  $D$  the collection of samples  $x$  so that  $\mathbb{E}_{\mathbb{Q}_{x,\epsilon}}[1_A] = 0$ . Assume the condition above does not hold, which means that  $\widehat{\mathbb{P}}\{D\} > 0$ . For any  $\tau > 0$  and  $x \in D$ , there exists  $H^l(x) < H^u$  such that

$$0 < \mathfrak{h}_x := \mathbb{E}_{\mathbb{Q}_{x,\epsilon}}[1_{B(x)}] \leq \tau, \quad \text{where } B(x) = \{z : H^l(x) \leq f(z) \leq H^u\}.$$

Define  $H^{\text{gap}}(x) = H^u - H^l(x)$ ,  $\mathfrak{h}_x^c = 1 - \mathfrak{h}_x$ . Then we find that for  $x \in D$ ,

$$\begin{aligned} v_x(\lambda) &= \lambda\epsilon \log \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} \left[ e^{f(z)/(\lambda\epsilon)} 1_{B(x)} \right] + \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} \left[ e^{f(z)/(\lambda\epsilon)} 1_{B(x)^c} \right] \right) \\ &\leq H^u + \lambda\epsilon \log \left( \mathfrak{h}_x + e^{-H^{\text{gap}}(x)/(\lambda\epsilon)} \mathfrak{h}_x^c \right). \end{aligned}$$

Since  $\widehat{\mathbb{P}}\{D\} > 0$ , the dual objective function for  $\lambda > 0$  is upper bounded as

$$\begin{aligned} v(\lambda) &= \lambda\bar{\rho} + \int v_x(\lambda) d\widehat{\mathbb{P}}(x) \\ &\leq H^u + \lambda\bar{\rho} + \lambda\epsilon \int_D \log \left( \mathfrak{h}_x + e^{-H^{\text{gap}}(x)/(\lambda\epsilon)} \mathfrak{h}_x^c \right) d\widehat{\mathbb{P}}(x). \end{aligned}$$

We can see that

$$\lim_{\lambda \rightarrow 0} \lambda\bar{\rho} + \lambda\epsilon \int_D \log \left( \mathfrak{h}_x + e^{-H^{\text{gap}}(x)/(\lambda\epsilon)} \mathfrak{h}_x^c \right) d\widehat{\mathbb{P}}(x) = 0,$$

and

$$\begin{aligned} &\lim_{\lambda \rightarrow 0} \nabla \left[ \lambda\bar{\rho} + \lambda\epsilon \int_D \log \left( \mathfrak{h}_x + e^{-H^{\text{gap}}(x)/(\lambda\epsilon)} \mathfrak{h}_x^c \right) d\widehat{\mathbb{P}}(x) \right] \\ &= \bar{\rho} + \epsilon \int_D \log(\mathfrak{h}_x) d\widehat{\mathbb{P}}(x) \\ &\leq \bar{\rho} + \epsilon \log(\tau) \widehat{\mathbb{P}}\{D\} \leq -\bar{\rho} < 0, \end{aligned}$$

where the second inequality is by taking the constant  $\tau = \exp\left(-\frac{2\bar{\rho}}{\epsilon\widehat{\mathbb{P}}\{D\}}\right)$ . Hence, there exists  $\bar{\lambda} > 0$  such that

$$v(\bar{\lambda}) \leq H^u + \bar{\lambda}\bar{\rho} + \bar{\lambda}\epsilon \int_D \log \left( \mathfrak{h}_x + e^{-H^{\text{gap}}(x)/(\bar{\lambda}\epsilon)} \mathfrak{h}_x^c \right) d\widehat{\mathbb{P}}(x) < v(0),$$

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

$$\mathbb{E}_{\mathbb{Q}_{x,\epsilon}}[1_A] > 0.$$

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

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

The gradient of  $v(\lambda)$  becomes

$$\begin{aligned} \nabla v(\lambda) &= \bar{\rho} + \epsilon \int \left[ \log \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}}[1_A] + \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} \left[ e^{[f(z)-H^u]/(\lambda\epsilon)} 1_{A^c} \right] \right) \right] d\widehat{\mathbb{P}}(x) \\ &\quad + \int \frac{\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} \left[ e^{[f(z)-H^u]/(\lambda\epsilon)} 1_{A^c} (H^u - f(z)) / (\lambda) \right]}{\mathbb{E}_{\mathbb{Q}_{x,\epsilon}}[1_A] + \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} \left[ e^{[f(z)-H^u]/(\lambda\epsilon)} 1_{A^c} \right]} d\widehat{\mathbb{P}}(x). \end{aligned}$$

We can see that  $\lim_{\lambda \rightarrow \infty} \nabla v(\lambda) = \bar{\rho}$ . Take

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

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

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

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

$$\lim_{\lambda \rightarrow 0} \nabla v(\lambda) = \bar{\rho} + \epsilon \int \log(\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [\mathbf{1}_A]) d\widehat{\mathbb{P}}(x) = \bar{\rho}'.$$

Hence, if the last condition is violated, based on the mean value theorem, we can find  $\bar{\lambda} > 0$  so that  $\nabla v(\bar{\lambda}) = 0$ , which contradicts to the optimality of  $\lambda^* = 0$ .

Now we show the converse direction. For any  $\lambda > 0$ , we find that

$$\nabla v(\lambda) = \bar{\rho} + \epsilon \int [\log(\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [\mathbf{1}_A] + v_{1,x}(\lambda))] d\widehat{\mathbb{P}}(x) + \int v_{2,x}(\lambda) d\widehat{\mathbb{P}}(x).$$

For fixed  $x$ , when  $\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [\mathbf{1}_A] = 1$ , we can see that  $v_{1,x}(\lambda) = v_{2,x}(\lambda) = 0$ , then

$$\bar{\rho} + \epsilon [\log(\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [\mathbf{1}_A] + v_{1,x}(\lambda))] + v_{2,x}(\lambda) = \bar{\rho} > 0.$$

When  $\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [\mathbf{1}_A] \in (0, 1)$ , we can see that  $v_{1,x}(\lambda) > 0$ ,  $v_{2,x}(\lambda) > 0$ . Then

$$\bar{\rho} + \epsilon [\log(\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [\mathbf{1}_A] + v_{1,x}(\lambda))] + v_{2,x}(\lambda) > \bar{\rho} + \epsilon \log(\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [\mathbf{1}_A]) = \bar{\rho}' \geq 0.$$

Therefore,  $\nabla v(\lambda) > 0$  for any  $\lambda > 0$ . By the convexity of  $v(\lambda)$ , we conclude that the dual minimizer  $\lambda^* = 0$ . □

*Proof of Lemma 5.* Since  $\lambda^* > 0$ , based on the optimality condition of the dual problem, we have that

$$0 = \nabla_{\lambda} \left[ \lambda \bar{\rho} + \lambda \epsilon \int \log(\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [e^{f(z)/(\lambda\epsilon)}]) d\widehat{\mathbb{P}}(x) \right] \Big|_{\lambda=\lambda^*}.$$

Or equivalently, we have that

$$\bar{\rho} + \epsilon \int \log(\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [e^{f(z)/(\lambda^*\epsilon)}]) d\widehat{\mathbb{P}}(x) - \int \frac{\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [e^{f(z)/(\lambda^*\epsilon)} f(z)]}{\lambda^* \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [e^{f(z)/(\lambda^*\epsilon)}]} d\widehat{\mathbb{P}}(x) = 0.$$

Re-arranging the term completes the proof. □

*Proof of Theorem 1.* The feasibility result in Theorem 1(I) can be easily shown by considering the reformulation of  $V$  in Lemma 1 and the non-negativity of KL-divergence. When  $\bar{\rho} = 0$ , one can see that

$$V_D \leq \lim_{\lambda \rightarrow \infty} \lambda \epsilon \int \log(\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [e^{f(z)/(\lambda\epsilon)}]) d\widehat{\mathbb{P}}(x) = \mathbb{E}_{z \sim \mathbb{P}^0} [f(z)] = V.$$

Therefore, the strong duality result holds in this case. The proof for  $\bar{\rho} > 0$  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  $\{R_j\}_j$  such that  $R_j \rightarrow \infty$  and take the objective function  $f_j(z) = f(z) \mathbf{1}\{z \leq R_j\}$ . Hence, there exists  $\lambda > 0$  satisfying  $\Pr_{x \sim \widehat{\mathbb{P}}} \{x : \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [e^{f_j(z)/(\lambda\epsilon)}] = \infty\} = 0$ . According to the necessary condition in Lemma 4, 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

$$\sup_{\mathbb{P} \in \mathbb{B}_{\bar{\rho}, \epsilon}(\widehat{\mathbb{P}})} \{\mathbb{E}_{z \sim \mathbb{P}} [f_j(z)]\} \geq \lambda_j^* \bar{\rho} + \lambda_j^* \epsilon \int \log(\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [e^{f_j(z)/(\lambda\epsilon)}]) d\widehat{\mathbb{P}}(x).$$

Taking  $j \rightarrow \infty$  both sides implies that  $V = \infty$ , which completes the proof. □

*Proof of Corollary 1* According to the definition of Sinkhorn distance, we first reformulate  $V_\lambda$  as

$$\begin{aligned} V_\lambda &= \sup_{\mathbb{P}, \gamma \in \Gamma(\widehat{\mathbb{P}}, \mathbb{P})} \left\{ \mathbb{E}_{z \sim \mathbb{P}}[f(z)] - \lambda \mathbb{E}_\gamma \left[ c(x, z) + \epsilon \log \left( \frac{d\gamma(x, z)}{d\widehat{\mathbb{P}}(x) d\nu(z)} \right) \right] \right\} \\ &= \sup_{\gamma_x \in \mathcal{P}(\Omega), x \in \mathcal{Z}} \left\{ \int \mathbb{E}_{\gamma_x} \left[ f(z) - \lambda \epsilon \log \left( \frac{d\gamma_x(z)}{d\mathbb{Q}_{x, \epsilon}(z)} \right) \right] d\widehat{\mathbb{P}}(x) \right\} \\ &\quad + \lambda \epsilon \int \log \left( \int e^{-c(x, u)/\epsilon} d\nu(u) \right) d\widehat{\mathbb{P}}(x), \end{aligned}$$

where the second relation is by decomposing  $\gamma$  with  $\gamma(x, z) = \widehat{\mathbb{P}}(x) \otimes \gamma_x(z)$ . By the principal of interchangability [89], it holds that

$$\begin{aligned} V_\lambda &= \int \sup_{\gamma_x \in \mathcal{P}(\Omega)} \mathbb{E}_{\gamma_x} \left[ f(z) - \lambda \epsilon \log \left( \frac{d\gamma_x(z)}{d\mathbb{Q}_{x, \epsilon}(z)} \right) \right] d\widehat{\mathbb{P}}(x) + C \\ &= \lambda \epsilon \int \log \left( \mathbb{E}_{\mathbb{Q}_{x, \epsilon}}[e^{f(z)/(\lambda \epsilon)}] \right) d\widehat{\mathbb{P}}(x) + C, \end{aligned}$$

where the last relation holds by applying Lemma EC.1. □

## Appendix EC.5: Preliminaries on Stochastic Mirror Descent (SMD)

In this section, we provide some preliminaries on SMD that can be useful for proving Theorem 2. Consider the minimization of the objective function  $F(\theta) = \mathbb{E}[f_\theta(z)]$  with  $\theta \in \Theta \subseteq \mathbb{R}^{d_\theta}$ . In particular, we assume the constraint set  $\Theta$  is non-empty, closed and convex. We also impose the following assumption regarding the (sub-)gradient oracles when using the SMD algorithm:

**ASSUMPTION EC.1 (Stochastic Oracles of Gradient Estimate).** (I) *The objective function  $F(\theta)$  is convex in  $\theta$ , and we have the stochastic oracle such that for given  $\theta$  we can generate a stochastic vector  $G(\theta, \xi)$  such that  $\mathbb{E}[G(\theta, \xi)] \in \partial F(\theta)$ , where  $\partial F(\theta)$  is the subdifferential set of  $F(\cdot)$  at  $\theta$ . Also, suppose there exists a constant  $M_* > 0$  so that*

$$\mathbb{E}[\|G(\theta, \xi)\|_*^2] \leq M_*^2, \quad \forall \theta \in \Theta.$$

(II) *Assume the objective function  $F(\theta)$  is  $S$ -smooth, and we have the stochastic oracle such that for given  $\theta$  we can generate a stochastic vector  $G(\theta, \xi)$  such that  $\mathbb{E}[G(\theta, \xi)] = \nabla F(\theta)$ . Also, suppose there exists  $\sigma > 0$  so that*

$$\text{Var}[G(\theta, \xi)] \leq \sigma^2, \quad \forall \theta \in \Theta.$$

Under the above assumption, the SMD algorithm generates the following iteration:

$$\theta_{t+1} = \text{Prox}_{\theta_t}(\gamma_t G(\theta_t, \xi^t)), \quad \theta_1 \in \Theta, \quad t = 1, \dots, T-1.$$

For simplicity of discussion, we employ constant step size policy  $\gamma_t := \gamma$  for  $t = 1, \dots, T-1$ . The following presents convergence results of the SMD algorithm. Similar results can be found in [89, 51, 70, 82]. For the sake of completeness, we provide the proof for the case where the loss function  $F(\theta)$  is smooth in  $\theta$ .

**LEMMA EC.2 (SMD for Nonsmooth Convex Optimization).** *Under Assumption EC.1(I), let the estimation of optimal solution at the iteration  $j$  be*

$$\tilde{\theta}_{1:j} = \frac{1}{j} \sum_{t=1}^j \theta_t.$$

When taking constant step size

$$\gamma = \sqrt{\frac{2\kappa V(\theta_1, \theta^*)}{TM_*^2}},$$

it holds that

$$\mathbb{E}[F(\tilde{\theta}_{1:T}) - F(\theta^*)] \leq M_* \sqrt{\frac{2V(\theta_1, \theta^*)}{\kappa T}}.$$

*Proof of Lemma EC.2* The proof follows from [89, Section 8.2.3]. □

**LEMMA EC.3 (SMD for Smooth Convex Optimization).** *Assume the loss function  $F(\theta)$  is convex in  $\theta$  and Assumption EC.1(II) holds. Let the estimation of optimal solution at the iteration  $j$  be  $\tilde{\theta}_{1:j} = \frac{1}{j} \sum_{t=1}^j \theta_t$ . Also, suppose the norm function  $\|\cdot\|$  satisfies that the dual norm  $\|\cdot\|_* \leq c\|\cdot\|_2$ . When taking constant step size  $\gamma \in (0, \kappa/(2Sc^2))$ , it holds that*

$$\mathbb{E}[F(\tilde{\theta}_{1:T}) - F(\theta^*)] \leq \frac{\gamma Sc^2 \sigma^2}{\kappa} + \frac{2V(\theta_1, \theta^*)}{\gamma T}.$$

*Proof of Lemma EC.3* For each  $u \in \Theta$  and  $\theta \in \Theta^*$ , and  $y \in \mathbb{R}^d$ , based on [89, Lemma 8.3], one has that

$$V(P_\theta(y), u) \leq V(\theta, u) + \langle y, u - \theta \rangle + \frac{1}{2\kappa} \|y\|_*^2. \quad (\text{EC.7})$$



Based on this identity with  $\theta := \theta_t$ ,  $y := \gamma G(\theta_t, \xi^t)$ , and  $u := \theta^*$ , we obtain

$$V(\theta_{t+1}, \theta^*) \leq V(\theta_t, \theta^*) + \gamma \langle G(\theta_t, \xi^t), \theta^* - \theta_t \rangle + \frac{\gamma^2}{2\kappa} \|G(\theta_t, \xi^t)\|_*^2. \quad (\text{EC.8})$$

As a consequence, we have the relation

$$\mathbb{E} \langle G(\theta_t, \xi^t), \theta_t - \theta^* \rangle \leq \frac{\mathbb{E}V(\theta_t, \theta^*) - \mathbb{E}V(\theta_{t+1}, \theta^*)}{\gamma} + \frac{\gamma}{2\kappa} \mathbb{E} \|G(\theta_t, \xi^t)\|_*^2.$$

On the other hand, conditioned on  $x_t$ , we have that

$$-\mathbb{E} \langle G(\theta_t, \xi^t), \theta_t - \theta^* \rangle = -\langle \nabla F(\theta_t), \theta_t - \theta^* \rangle \leq F(\theta^*) - F(\theta_t).$$

Based on those two relations above, we obtain that conditioned on  $x_t$ ,

$$\begin{aligned} F(\theta_t) - F(\theta^*) &\leq \frac{\mathbb{E}V(\theta_t, \theta^*) - \mathbb{E}V(\theta_{t+1}, \theta^*)}{\gamma} + \frac{\gamma}{2\kappa} \mathbb{E} \|G(\theta_t, \xi^t)\|_*^2 \\ &\leq \frac{\mathbb{E}V(\theta_t, \theta^*) - \mathbb{E}V(\theta_{t+1}, \theta^*)}{\gamma} + \frac{\gamma c^2}{2\kappa} \text{Var}(G(\theta_t, \xi^t)) + \frac{\gamma c^2}{2\kappa} \|\nabla F(\theta_t) - \nabla F(\theta^*)\|_2^2 \\ &\leq \frac{\mathbb{E}V(\theta_t, \theta^*) - \mathbb{E}V(\theta_{t+1}, \theta^*)}{\gamma} + \frac{\gamma c^2}{2\kappa} \text{Var}(G(\theta_t, \xi^t)) + \frac{\gamma S c^2}{\kappa} [F(\theta_t) - F(\theta^*)]. \end{aligned}$$

This implies that

$$\mathbb{E}[F(\theta_t) - F(\theta^*)] \leq \frac{1}{1 - \gamma S c^2 / \kappa} \left[ \frac{\mathbb{E}V(\theta_t, \theta^*) - \mathbb{E}V(\theta_{t+1}, \theta^*)}{\gamma} + \frac{\gamma S c^2}{2\kappa} \text{Var}(G(\theta_t, \xi^t)) \right].$$

When taking the step size  $\gamma \in (0, \kappa / (2S c^2)]$ , it holds that for any  $t$ ,

$$\mathbb{E}[F(\theta_t) - F(\theta^*)] \leq \frac{2 \{ \mathbb{E}V(\theta_t, \theta^*) - \mathbb{E}V(\theta_{t+1}, \theta^*) \}}{\gamma} + \frac{\gamma S c^2 \sigma^2}{\kappa}. \quad (\text{EC.9})$$

Finally, the estimate of optimal solution  $\tilde{\theta}_{1:T}$  satisfies that

$$\begin{aligned} \mathbb{E}[F(\tilde{\theta}_{1:T}) - F(\theta^*)] &= \mathbb{E} \left[ F \left( \frac{1}{T} \sum_{t=1}^T \theta_t \right) - F(\theta^*) \right] \\ &\leq \mathbb{E} \left[ \frac{1}{T} \sum_{t=1}^T F(\theta_t) - F(\theta^*) \right] = \frac{1}{T} \sum_{t=1}^T \mathbb{E}[F(\theta_t) - F(\theta^*)] \\ &\leq \frac{\gamma S c^2 \sigma^2}{\kappa} + \frac{2V(\theta_1, \theta^*)}{\gamma T}, \end{aligned}$$

where the first inequality is based on the Jensen's inequality and the convexity of  $F(\theta)$ , and the second inequality is by the relation (EC.9).  $\square$

## Appendix EC.6: Proofs of Technical Results in Section 4.2.1

**REMARK EC.1 (COMPUTATION COSTS OF GRADIENT ESTIMATORS).** The cost for generating V-SGD gradient estimator  $v^{\text{V-SGD}}(\theta)$  is of  $O(n_L^\circ 2^L)$ . For V-MLMC scheme, we set the number of inner approximation level  $n_\ell = \lceil 2^{-\ell} N \rceil$ . The cost for generating V-MLMC gradient estimator  $v^{\text{V-MLMC}}(\theta)$  is of  $O(NL + 2^L)$ . For RT-MLMC scheme, we take the probability  $q_\ell \propto 2^{-\ell}$ . The cost for generating RT-MLMC gradient estimator  $v^{\text{RT-MLMC}}(\theta)$  is of  $O(n_L^\circ L)$ .

*Proof of Remark EC.1* Since V-SGD estimator requires generating  $g^L(\theta, \zeta_i^L)$  for  $n_L^\circ$  times, and generating a single  $g^L(\theta, \zeta_i^L)$  requires generating the random sampling parameters  $\{z_j^\ell\}_{j \in [2^L]}$  of size  $2^\ell$ , we imply the cost of V-SGD estimator is of  $O(n_L^\circ 2^L)$ .

Since for fixed  $\ell$ , the cost of generating a single  $G^\ell(\theta, \zeta_i^\ell)$  requires generating the random sampling parameters  $\{z_j^\ell\}_{j \in [2^L]}$  of size  $2^\ell$ , the cost of V-MLMC estimator can be bounded as

$$O\left(\sum_{\ell=0}^L n_\ell^\circ 2^\ell\right) = O\left(\sum_{\ell=0}^L \lceil 2^{-\ell} N \rceil 2^\ell\right) = O\left(\sum_{\ell=0}^L (2^{-\ell} N + 1) 2^\ell\right) = O(NL + 2^L).$$

The cost of RT-MLMC estimator can be bounded as

$$O\left(n_L^\circ \sum_{\ell=0}^L q_\ell 2^\ell\right) = O\left(n_L^\circ \sum_{\ell=0}^L \frac{2^{-\ell}}{C} 2^\ell\right) = O(n_L^\circ L/C) = O(n_L^\circ L),$$

where the constant  $C = \sum_{\ell=0}^L 2^{-\ell} = O(1)$ . □

### EC.6.1. Proof of Theorem 2(I)

We first discuss sample complexity for nonsmooth convex optimization. Suppose for a given  $\theta$ , the gradient estimate of  $F(\theta)$ , denoted as  $v(\theta)$ , satisfies

$$\mathbb{E}[v(\theta)] = \nabla \bar{F}(\theta), \quad \mathbb{E}[\|v(\theta)\|_*^2] \leq M_*^2.$$

Assume the bias of objective satisfies

$$\Delta_F := \sup_{\theta \in \Theta} |\bar{F}(\theta) - F(\theta)|.$$

Denote by  $\bar{\theta}^*$  an global optimum of  $\bar{F}$ . Then we have the following result.

**PROPOSITION EC.1 (BSMD for Nonsmooth Convex Optimization).** *When taking the step size  $\gamma = \sqrt{\frac{2\kappa V(\theta_1, \bar{\theta}^*)}{TM_*^2}}$ , it holds that*

$$\mathbb{E}[F(\tilde{\theta}_{1:T}) - F(\theta^*)] \leq 2\Delta_F + M_* \sqrt{\frac{2V(\theta_1, \bar{\theta}^*)}{\kappa T}}.$$

*Proof of Proposition EC.1* Note that we can establish the following error bound:

$$\begin{aligned} \mathbb{E}[F(\tilde{\theta}_{1:T}) - F(\theta^*)] &= \mathbb{E}[F(\tilde{\theta}_{1:T}) - \bar{F}(\tilde{\theta}_{1:T})] + \mathbb{E}[\bar{F}(\tilde{\theta}_{1:T}) - \bar{F}(\theta^*)] + \mathbb{E}[\bar{F}(\theta^*) - F(\theta^*)] \\ &\leq 2\Delta_F + \mathbb{E}[\bar{F}(\tilde{\theta}_{1:T}) - \bar{F}(\theta^*)] \\ &\leq 2\Delta_F + \mathbb{E}[\bar{F}(\tilde{\theta}_{1:T}) - \bar{F}(\bar{\theta}^*)], \end{aligned}$$

where the first inequality is due to the bias approximation error bound, and the second inequality is due to the sub-optimality of  $\theta^*$  for the objective  $\bar{F}$ . According to Lemma EC.2, if we take the step size  $\gamma = \sqrt{\frac{2\kappa V(\theta_1, \bar{\theta}^*)}{TM_*^2}}$ , then it holds that

$$\mathbb{E}[\bar{F}(\tilde{\theta}_{1:T}) - \bar{F}(\bar{\theta}^*)] \leq M_* \sqrt{\frac{2V(\theta_1, \bar{\theta}^*)}{\kappa T}}.$$

□

Now we show complexity result for the V-SGD scheme. Without loss of generality, we take the batch size  $n_L^o = 1$ . According to Proposition EC.1, parameters for V-SGD scheme satisfy

$$\Delta_F := \lambda\epsilon \exp(2B/(\lambda\epsilon)) \cdot 2^{-(L+1)}, \quad M_*^2 := c^2 L_f^2.$$

To obtain  $\delta$ -optimal solution, we set

$$2\Delta_F \leq \frac{\delta}{2}, \quad M_* \sqrt{\frac{2V(\theta_1, \bar{\theta}^*)}{\kappa T_{\text{in}}}} \leq \frac{\delta}{2}.$$

As a consequence, we specify the following hyper-parameters to meet the above requirements:

$$L = \left\lceil \frac{1}{\log 2} \left[ \log \frac{2\lambda\epsilon \exp(2B/(\lambda\epsilon))}{\delta} \right] \right\rceil, \quad T_{\text{in}} = \left\lceil \frac{8c^2 L_f^2 V(\theta_1, \bar{\theta}^*)}{\kappa \delta^2} \right\rceil, \quad \gamma = \sqrt{\frac{2\kappa V(\theta_1, \bar{\theta}^*)}{c^2 T_{\text{in}} L_f^2}}.$$

### EC.6.2. Proof of Theorem 2(II)

Next, we discuss sample complexity for smooth convex optimization. Suppose for a given  $\theta$ , the gradient estimate of  $F(\theta)$ , denoted as  $v(\theta)$ , satisfies

$$\mathbb{E}[v(\theta)] = \nabla \bar{F}(\theta), \quad \text{Var}[v(\theta)] \leq \sigma^2.$$

Assume the bias of objective satisfies

$$\Delta_F := \sup_{\theta \in \Theta} |\bar{F}(\theta) - F(\theta)|.$$

Denote by  $\bar{\theta}^*$  an global optimum of  $\bar{F}$ . Then we have the following result.

**PROPOSITION EC.2 (BSMD for Smooth Convex Optimization).** *Assume that the approximation function  $\bar{F}$  is  $S$ -smooth. When taking constant step size  $\gamma = \sqrt{\frac{2\kappa V(\theta_1, \bar{\theta}^*)}{Sc^2\sigma^2T}}$ , it holds that*

$$\mathbb{E}[F(\tilde{\theta}_{1:T}) - F(\theta^*)] \leq 2\Delta_F + \sqrt{\frac{2Sc^2\sigma^2 V(\theta_1, \bar{\theta}^*)}{\kappa T}}.$$

Specially, we can show the approximation function  $F^\ell(\theta)$  defined in (9) is indeed smooth, and therefore Proposition EC.2 can be used to prove Theorem 2(II).

**LEMMA EC.4.** *Under Assumption 2(II), 2(III), and 2(IV), the functions  $F$  and  $F^\ell$  are  $S_F$ -smooth with*

$$S_F := (S_f + L_f^2/(\lambda\epsilon)) \exp(B/(\lambda\epsilon)) + L_f^2/(\lambda\epsilon) \exp(2B/(\lambda\epsilon)).$$

The proof of Lemma EC.4 follows the similar argument as in [55, Proposition 4.1]. We provide a full proof here for the sake of completeness.

*Proof of Lemma EC.4* Observe that

$$\begin{aligned}
& \|\nabla F(\theta_1) - \nabla F(\theta_2)\|_2 \\
& \leq (\lambda\epsilon)^{-1} \mathbb{E}_{\hat{\mathbb{P}}} \left\| \phi' \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_1}(z)/(\lambda\epsilon)} \right) \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_1}(z)/(\lambda\epsilon)} \nabla f_{\theta_1}(z) \right. \\
& \quad \left. - \phi' \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_2}(z)/(\lambda\epsilon)} \right) \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_2}(z)/(\lambda\epsilon)} \nabla f_{\theta_2}(z) \right\|_2 \\
& \leq (\lambda\epsilon)^{-1} \mathbb{E}_{\hat{\mathbb{P}}} \left\| \phi' \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_1}(z)/(\lambda\epsilon)} \right) \left[ \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_1}(z)/(\lambda\epsilon)} \nabla f_{\theta_1}(z) - \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_2}(z)/(\lambda\epsilon)} \nabla f_{\theta_2}(z) \right] \right\|_2 \\
& \quad + (\lambda\epsilon)^{-1} \mathbb{E}_{\hat{\mathbb{P}}} \left\| \left[ \phi' \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_1}(z)/(\lambda\epsilon)} \right) - \phi' \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_2}(z)/(\lambda\epsilon)} \right) \right] \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_2}(z)/(\lambda\epsilon)} \nabla f_{\theta_2}(z) \right\|_2
\end{aligned}$$

The first term on the RHS can be bounded as

$$\begin{aligned}
& \mathbb{E}_{\hat{\mathbb{P}}} \left\| \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_1}(z)/(\lambda\epsilon)} \nabla f_{\theta_1}(z) - \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_2}(z)/(\lambda\epsilon)} \nabla f_{\theta_2}(z) \right\|_2 \\
& \leq \mathbb{E}_{\hat{\mathbb{P}}} \left\| \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_1}(z)/(\lambda\epsilon)} \left[ \nabla f_{\theta_1}(z) - \nabla f_{\theta_2}(z) \right] \right\|_2 \\
& \quad + \mathbb{E}_{\hat{\mathbb{P}}} \left\| \left[ \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_1}(z)/(\lambda\epsilon)} - \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_2}(z)/(\lambda\epsilon)} \right] \nabla f_{\theta_2}(z) \right\|_2 \\
& \leq e^{B/(\lambda\epsilon)} S_f \|\theta_1 - \theta_2\| + L_f^2/(\lambda\epsilon) e^{B/(\lambda\epsilon)} \|\theta_1 - \theta_2\|_2,
\end{aligned}$$

where the last inequality is because  $f_\theta(z)$  is bounded by  $B$ ,  $L_f$ -Lipschitz, and  $S_f$ -smooth. The second term on the RHS can be bounded as

$$\begin{aligned}
& L_f/(\lambda\epsilon) e^{B/(\lambda\epsilon)} \mathbb{E}_{\hat{\mathbb{P}}} \left\| \phi' \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_1}(z)/(\lambda\epsilon)} \right) - \phi' \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_2}(z)/(\lambda\epsilon)} \right) \right\|_2 \\
& \leq L_f e^{B/(\lambda\epsilon)} \mathbb{E}_{\hat{\mathbb{P}}} \left\| \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_1}(z)/(\lambda\epsilon)} - \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta_2}(z)/(\lambda\epsilon)} \right\|_2 \\
& \leq L_f^2/(\lambda\epsilon) e^{2B/(\lambda\epsilon)} \|\theta_1 - \theta_2\|_2.
\end{aligned}$$

Hence, we conclude that the function  $F$  is  $S_F$ -smooth, where

$$S_F = L_f^2/(\lambda\epsilon) e^{2B/(\lambda\epsilon)} + e^{B/(\lambda\epsilon)} S_f + L_f^2/(\lambda\epsilon) e^{B/(\lambda\epsilon)}.$$

The smoothness of the function  $F^\ell$  can be finished in a similar manner.  $\square$

Now we are ready to show complexity results for V-SGD, V-MLMC, and RT-MLMC schemes. **V-SGD** Without loss of generality, we take the batch size  $n_L^\circ = 1$ . According to Proposition EC.2, parameters for V-SGD scheme satisfy

$$\Delta_F := \lambda\epsilon \exp(2B/(\lambda\epsilon)) \cdot 2^{-(L+1)}, \quad \sigma^2 := L_f^2.$$

To obtain  $\delta$ -optimal solution, we set

$$2\Delta_F \leq \frac{\delta}{2}, \quad \sqrt{\frac{2S_F c^2 \sigma^2 V(\theta_1, \bar{\theta}^*)}{\kappa T}} \leq \frac{\delta}{2}.$$

As a consequence, we specify the following hyper-parameters to meet the above requirements:

$$L = \left\lceil \frac{1}{\log 2} \left[ \log \frac{2\lambda\epsilon \exp(2B/(\lambda\epsilon))}{\delta} \right] \right\rceil, \quad T_{\text{in}} = \left\lceil \frac{8S_F c^2 L_f^2 V(\theta_1, \bar{\theta}^*)}{\kappa \delta^2} \right\rceil, \quad \gamma = \sqrt{\frac{2\kappa V(\theta_1, \bar{\theta}^*)}{S_F c^2 L_f^2 T_{\text{in}}}}.$$

**V-MLMC** When taking the inner approximation sample size  $n_\ell = \lceil 2^{-\ell} N \rceil$  for some  $N > 0$ , it holds that

$$\Delta_F := \lambda\epsilon \exp(2B/(\lambda\epsilon)) \cdot 2^{-(L+1)}, \quad \sigma^2 := L_f^2 \exp(4B/(\lambda\epsilon)) (L+1)N^{-1}.$$

To obtain  $\delta$ -optimal solution, we set

$$2\Delta_F \leq \frac{\delta}{2}, \quad \frac{2S_F c^2 V(\theta_1, \bar{\theta}^*)}{\kappa T_{\text{in}}} \leq \frac{\delta}{2}, \quad \sigma^2 \leq \frac{\delta}{2}.$$

As a consequence, we specify the following hyper-parameters to meet the above requirements:

$$L = \left\lceil \frac{1}{\log 2} \left[ \log \frac{2\lambda\epsilon \exp(2B/(\lambda\epsilon))}{\delta} \right] \right\rceil, \quad T_{\text{in}} = \left\lceil \frac{4S_F c^2 V(\theta_1, \bar{\theta}^*)}{\kappa \delta} \right\rceil, \quad N = \frac{2L_f^2 (L+1) e^{4B/(\lambda\epsilon)}}{\delta}.$$

**RT-MLMC** Without loss of generality, we take the batch size  $n_L^\circ = 1$ . When taking the probability  $q_\ell \propto 2^{-\ell}$ , it holds that

$$\Delta_F := \lambda\epsilon \exp(2B/(\lambda\epsilon)) \cdot 2^{-(L+1)}, \quad \sigma^2 := 2L_f^2 \exp(4B/(\lambda\epsilon)) (L+1),$$

To obtain  $\delta$ -optimal solution, we set

$$2\Delta_F \leq \frac{\delta}{2}, \quad \frac{2S_F c^2 \sigma^2 V(\theta_1, \bar{\theta}^*)}{\kappa T_{\text{in}}} \leq \frac{\delta^2}{4}.$$

As a consequence, we specify the following hyper-parameters to meet the above requirements:

$$L = \left\lceil \frac{1}{\log 2} \left[ \log \frac{2\lambda\epsilon \exp(2B/(\lambda\epsilon))}{\delta} \right] \right\rceil, \quad T_{\text{in}} = \left\lceil \frac{16S_F c^2 V(\theta_1, \bar{\theta}^*) L_f^2 \exp(4B/(\lambda\epsilon))}{\kappa \delta^2} \cdot (L+1) \right\rceil.$$

### EC.6.3. Sampling Algorithm in Remark 7

In this subsection, we present an algorithm that generates samples from  $\mathbb{Q}_\epsilon$ , where the density function

$$\frac{d\mathbb{Q}_\epsilon(z)}{dz} \propto \exp(-V_\epsilon(z)), \quad V_\epsilon(z) := \|z\|_p^2$$

One can use the unadjusted Langevin algorithm for sampling:

$$dX_t = -\nabla V_\epsilon(X_t) dt + \sqrt{2} dB_t,$$

where  $\{B_t\}$  is a multi-dimensional Brownian motion. As the time index  $t \rightarrow \infty$ , the distribution  $X_t$  will converges to a stationary distribution  $\mathbb{Q}_\epsilon$  exponentially fast. Also, for practical implementation we use the discretized version of SDE for sampling:

$$X_{k+1} = X_k - \gamma \nabla V_\epsilon(X_k) + \sqrt{2\gamma} Z_{k+1}, \quad \text{where } Z_{k+1} \sim \mathcal{N}(0, I_d). \quad (\text{EC.10})$$

In particular, the function  $V_\epsilon(z)$  is continuously differentiable with

$$\nabla V_\epsilon(z) = 2\|v\|_p^{2-p} \text{sign}(v)|v|^{p-1}.$$

Hence, the iteration (EC.10) returns a distribution that is  $\tau$ -close to  $\mathbb{Q}_\epsilon$  in terms of KL-divergence distance within  $O(1/\tau)$  iterations.

#### EC.6.4. Proof of Remark 8

If employing the BSAA technique, the estimation of optimal solution of (8) is given by the optimal value of the following problem, where the objective function is a biased estimate of the objective in (8):

$$\min_{\theta \in \Theta} \left\{ \hat{F}_{n,m}(\theta) := \frac{\lambda\epsilon}{n} \sum_{i=1}^n \log \left( \frac{1}{m} \sum_{j=1}^m e^{f_{\theta}(z_{i,j})/(\lambda\epsilon)} \right) \right\}. \quad (\text{EC.11})$$

Here  $\{x_i\}_{i=1}^n$  are samples i.i.d. generated from  $\hat{\mathbb{P}}$ , and for fixed  $x_i$ , samples  $\{z_{i,j}\}_{j=1}^m$  are i.i.d. generated from  $\mathbb{Q}_{x_i,\epsilon}$ . Leveraging existing results in [54, Corollary 4.2], we present the following sample complexity analysis of BSAA problem.

**PROPOSITION EC.3 (Sample Complexity for BSAA Problem).** *Assume the following conditions hold:*

- (I) *The constraint set  $\Theta$  is bounded with diameter  $D_{\Theta} < \infty$*
- (II) *For fixed  $z$  and  $\theta_1, \theta_2$ , it holds that  $|f_{\theta_1}(z) - f_{\theta_2}(z)| \leq L_f \|\theta_1 - \theta_2\|_2$ .*
- (III) *The loss function  $f$  satisfies  $0 \leq f_{\theta}(z) \leq B$  for any  $\theta \in \Theta$  and  $z \in \mathcal{Z}$ .*

Suppose we specify parameters for (EC.11) as

$$m = \left\lceil \frac{2\lambda\epsilon e^{2B/(\lambda\epsilon)}}{\delta} \right\rceil, n = O(1) \frac{B^2 + 4B\lambda\epsilon e^{2B/(\lambda\epsilon)}}{\delta^2} \left[ d \log \left( \frac{8e^{B/(\lambda\epsilon)} L_f D_{\Theta}}{\epsilon} \right) + \log \left( \frac{1}{\alpha} \right) \right],$$

then with probability at least  $1 - \alpha$ , the solution to the SAA problem (EC.11) is an  $\delta$ -optimal solution of (8).

The sample complexity of BSAA problem is of  $\tilde{O}(\delta^{-3})$ , which is much worse than  $\tilde{O}(\delta^{-2})$ , i.e., the complexity of first-order method used in our paper. Hence, we conclude that it takes considerably less time to implement the BSMD step directly rather than solving the SAA problem.

*Proof of Proposition EC.3* We first verify the technical assumption imposed in [54, Corollary 4.2]. Specifically, one can show that

- (a) The mapping  $\phi : [1, e^{B/(\lambda\epsilon)}] \rightarrow \mathbb{R}$  such that  $\phi(x) = \lambda\epsilon \log(x)$  is  $\lambda\epsilon$ -Lipschitz continuous and  $\lambda\epsilon$ -smooth, and the mapping  $g_z(\cdot, x) : \Theta \rightarrow \mathbb{R}$  such that  $g_z(\theta, x) = e^{f_{\theta}(z)/(\lambda\epsilon)}$  is  $e^{B/(\lambda\epsilon)} L_f / (\lambda\epsilon)$ -Lipschitz continuous.
- (b) The variance

$$\begin{aligned} & \max_{\theta \in \Theta} \text{Var}_{x \sim \hat{\mathbb{P}}} \left( \lambda\epsilon \log \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} \left[ e^{f_{\theta}(z)/(\lambda\epsilon)} \right] \right) \right) \\ & \leq \max_{\theta \in \Theta} \mathbb{E}_{x \sim \hat{\mathbb{P}}} \left( \lambda\epsilon \log \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} \left[ e^{f_{\theta}(z)/(\lambda\epsilon)} \right] \right) \right)^2 \\ & \leq B^2. \end{aligned}$$

- (c) The variance

$$\begin{aligned} & \max_{\theta \in \Theta, x \in \text{supp}(\hat{\mathbb{P}})} \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} \left( e^{f_{\theta}(z)/(\lambda\epsilon)} - \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta}(z)/(\lambda\epsilon)} \right)^2 \\ & \leq \max_{\theta \in \Theta, x \in \text{supp}(\hat{\mathbb{P}})} \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{2f_{\theta}(z)/(\lambda\epsilon)} \\ & \leq e^{2B/(\lambda\epsilon)}. \end{aligned}$$

(d) The mapping  $\phi$  satisfies  $|\phi(\cdot)| \leq B$ , and the mapping  $g_z(\cdot, x)$  satisfies  $|g_z(\cdot, x)| \leq e^{B/(\lambda\epsilon)}$ . Therefore, from [54, Corollary 4.2], we know that to obtain  $\delta$ -optimal solution with probability at least  $1 - \alpha$ , sample sizes  $m, n$  need to satisfy

$$n \geq O(1) \frac{B^2 + 4B\lambda\epsilon e^{2B/(\lambda\epsilon)}}{\delta^2} \left[ d \log \left( \frac{8e^{B/(\lambda\epsilon)} L_f D_{\Theta}}{\epsilon} \right) + \log \left( \frac{1}{\alpha} \right) \right]$$

and

$$m \geq \frac{2\lambda\epsilon e^{2B/(\lambda\epsilon)}}{\delta}.$$

□



## Appendix EC.7: Proofs of Technical Results in Section 4.2.2

Here we provide bounds for two basic statistics:  $\text{Var}(a^\ell(\theta, \zeta^\ell))$  and  $\text{Var}(A^\ell(\theta, \zeta^\ell))$ . First,

$$\begin{aligned} \text{Var}(a^\ell(\theta, \zeta^\ell)) &\leq \mathbb{E}[a^\ell(\theta, \zeta^\ell)]^2 \\ &= \mathbb{E}\left[\lambda\epsilon \log\left(\frac{1}{2^\ell} \sum_{j \in [2^\ell]} \exp\left(\frac{f_\theta(z_j^\ell)}{\lambda\epsilon}\right)\right)\right]^2 \\ &\leq B^2, \end{aligned}$$

where the last inequality is because  $0 \leq f_\theta(z_j^\ell) \leq B$ . Next, we find

$$\begin{aligned} \text{Var}(A^\ell(\theta, \zeta^\ell)) &\leq \mathbb{E}[A^\ell(\theta, \zeta^\ell)]^2 \\ &= \mathbb{E}\left|\frac{1}{2}\left(U_{1:2^\ell}(\theta, \zeta^\ell) - U_{1:2^{\ell-1}}(\theta, \zeta^\ell)\right) + \frac{1}{2}\left(U_{1:2^\ell}(\theta, \zeta^\ell) - U_{2^{\ell-1}+1:2^\ell}(\theta, \zeta^\ell)\right)\right|^2 \\ &\leq \frac{1}{2}\mathbb{E}\left|U_{1:2^\ell}(\theta, \zeta^\ell) - U_{1:2^{\ell-1}}(\theta, \zeta^\ell)\right|^2 + \frac{1}{2}\mathbb{E}\left|U_{1:2^\ell}(\theta, \zeta^\ell) - U_{2^{\ell-1}+1:2^\ell}(\theta, \zeta^\ell)\right|^2 \\ &\leq \frac{\lambda^2\epsilon^2}{2}\mathbb{E}\left|\frac{1}{2^\ell} \sum_{j \in [2^\ell]} \exp\left(\frac{f_\theta(z_j^\ell)}{\lambda\epsilon}\right) - \frac{1}{2^{\ell-1}} \sum_{j \in [2^{\ell-1}]} \exp\left(\frac{f_\theta(z_j^\ell)}{\lambda\epsilon}\right)\right|^2 \\ &\quad + \frac{\lambda^2\epsilon^2}{2}\mathbb{E}\left|\frac{1}{2^\ell} \sum_{j \in [2^\ell]} \exp\left(\frac{f_\theta(z_j^\ell)}{\lambda\epsilon}\right) - \frac{1}{2^{\ell-1}} \sum_{j \in [2^{\ell-1}+1:2^\ell]} \exp\left(\frac{f_\theta(z_j^\ell)}{\lambda\epsilon}\right)\right|^2 \\ &= \frac{\lambda^2\epsilon^2}{4}\mathbb{E}\left|\frac{1}{2^{\ell-1}} \sum_{j \in [2^{\ell-1}]} \exp\left(\frac{f_\theta(z_j^\ell)}{\lambda\epsilon}\right) - \frac{1}{2^{\ell-1}} \sum_{j \in [2^{\ell-1}+1:2^\ell]} \exp\left(\frac{f_\theta(z_j^\ell)}{\lambda\epsilon}\right)\right|^2 \\ &\leq \frac{\lambda^2\epsilon^2}{4} \cdot \frac{2 \exp(2B/(\lambda\epsilon))}{2^{\ell-1}} \\ &= \lambda^2\epsilon^2 e^{2B/(\lambda\epsilon)} \cdot 2^{-\ell}. \end{aligned}$$

**LEMMA EC.5 (Cramer's Large Deviation Theorem).** *Let  $X_1, \dots, X_n$  be i.i.d. samples of zero-mean random variable  $X$  with finite variance  $\sigma^2$ . For any  $\delta > 0$ , there exists  $\epsilon_1 > 0$  such that for any  $\epsilon \in (0, \epsilon_1)$ , it holds that*

$$\Pr\left(\left|\frac{1}{n} \sum_{i=1}^n X_i\right| \geq \epsilon\right) \leq 2 \exp\left(-\frac{n\epsilon^2}{(2+\delta)\sigma^2}\right).$$

We first present the complexity of estimating objective value of a feasible solution  $\theta$  based on MLMC estimators.

**PROPOSITION EC.4 (Complexity of MLMC Objective Estimators).** *Assume that Assumption 2(II) holds, then with properly chosen hyper-parameters of objective estimators in (14), the following results hold:*

- (I) *The total cost of V-SGD scheme for estimating objective value for fixed  $\theta$  up to accuracy error  $\delta$ , with probability at least  $1 - \alpha$ , is of  $O\left(\log \frac{1}{\alpha} \cdot \delta^{-3}\right)$ ;*
- (II) *The total cost of V-MLMC or RT-MLMC scheme for estimating objective value for fixed  $\theta$  up to accuracy error  $\delta$ , with probability at least  $1 - \alpha$ , is of  $\tilde{O}\left(\log \frac{1}{\alpha} \cdot \delta^{-2}\right)$ .*

*The configuration of optimization hyper-parameters is provided in the following:*

$$\text{V-SGD: } L = O\left(\log \frac{1}{\delta}\right), n_L^o = O\left(\frac{1}{\delta^2} \cdot \log \frac{1}{\alpha}\right);$$

$$\begin{aligned} \text{V-MLMC: } L &= O\left(\log \frac{1}{\delta}\right), N = \tilde{O}\left(\frac{1}{\delta^2} \cdot \log \frac{1}{\alpha}\right); \\ \text{RT-MLMC: } L &= O\left(\log \frac{1}{\delta}\right), n_L^\circ = \tilde{O}\left(\frac{1}{\delta^2} \cdot \log \frac{1}{\alpha}\right). \end{aligned}$$

*Proof of Proposition EC.4* First, we pick  $L$  such that  $|F^L(\theta) - F(\theta)| \leq \frac{\delta}{4}$ , i.e.,

$$L = \left\lceil \frac{1}{\log 2} \left\lceil \log \frac{2\lambda\epsilon \exp(2B/(\lambda\epsilon))}{\delta} \right\rceil \right\rceil.$$

Assume we have the estimator  $V(\theta)$  such that  $\mathbb{E}[V(\theta)] = F^L(\theta)$  and  $\mathbb{V}\text{ar}(V(\theta)) < \infty$ .

$$\left\{ |F(\theta) - V(\theta)| > \frac{\delta}{2} \right\} \subseteq \left\{ |F^L(\theta) - V(\theta)| > \frac{\delta}{4} \right\}. \quad (\text{EC.12})$$

Then by the relation (EC.12) and Lemma EC.5, it holds that

$$\Pr \left\{ |F(\theta) - V(\theta)| > \frac{\delta}{2} \right\} \leq \Pr \left\{ |F^L(\theta) - V(\theta)| > \frac{\delta}{4} \right\} \leq 2 \exp \left( -\frac{\delta^2}{16(\delta' + 2)\mathbb{V}\text{ar}(V(\theta))} \right). \quad (\text{EC.13})$$

Specially, we find  $V^{\text{V-SGD}}(\theta)$ ,  $V^{\text{V-MLMC}}(\theta)$ ,  $V^{\text{RT-MLMC}}(\theta)$  are all unbiased estimators of  $F^L(\theta)$  with

$$\begin{aligned} \mathbb{V}\text{ar}(V^{\text{V-SGD}}(\theta)) &\leq \frac{1}{n_L^\circ} \mathbb{V}\text{ar}(a^L(\theta, \zeta_i^L)) \leq \frac{B^2}{n_L^\circ}, \\ \mathbb{V}\text{ar}(V^{\text{V-MLMC}}(\theta)) &\leq \sum_{\ell=0}^L \frac{1}{n_\ell} \mathbb{V}\text{ar}(A^\ell(\theta, \zeta_i^L)) \leq \lambda^2 \epsilon^2 e^{2B/(\lambda\epsilon)} \cdot (L+1)N^{-1}, \\ \mathbb{V}\text{ar}(V^{\text{RT-MLMC}}(\theta)) &\leq \frac{1}{n_L^\circ} \sum_{\ell=0}^L \frac{1}{q_\ell} \mathbb{V}\text{ar}(A^\ell(\theta, \zeta_i^L)) \leq \lambda^2 \epsilon^2 e^{2B/(\lambda\epsilon)} \cdot (L+1) \cdot (n_L^\circ)^{-1}. \end{aligned}$$

The concentration for V-SGD scheme becomes

$$\Pr \left\{ |F(\theta) - V^{\text{V-SGD}}(\theta)| > \frac{\delta}{2} \right\} \leq 2 \exp \left( -\frac{\delta^2 n_L^\circ}{16(\delta' + 2)B^2} \right).$$

To make the desired coverage probability, we take

$$n_L^\circ = \frac{16(\delta' + 2)B^2}{\delta^2} \cdot \log \frac{2}{\alpha}.$$

The concentration for V-MLMC scheme becomes

$$\Pr \left\{ |F(\theta) - V^{\text{V-MLMC}}(\theta)| > \frac{\delta}{2} \right\} \leq \exp \left( -\frac{N\delta^2}{16(\delta' + 2)\lambda^2 \epsilon^2 e^{2B/(\lambda\epsilon)}(L+1)} \right).$$

To make the desired coverage probability, we take

$$N = \frac{16(\delta' + 2)\lambda^2 \epsilon^2 e^{2B/(\lambda\epsilon)}(L+1)}{\delta^2} \cdot \log \frac{2}{\alpha}.$$

Similar to the analysis of V-MLMC scheme, we specify the following parameter to make RT-MLMC scheme satisfies the desired coverage probability:

$$n_L^\circ = \frac{16(\delta' + 2)\lambda^2 \epsilon^2 e^{2B/(\lambda\epsilon)}(L+1)}{\delta^2} \cdot \log \frac{2}{\alpha}.$$

Finally, we provide the proof for Theorem 3.

*Proof of Theorem 3* When running the BSMD step, we obtain  $\hat{\theta}$  such that

$$\mathbb{E}[F(\hat{\theta}) - F(\theta^*)] \leq \delta.$$

Based on Markov's inequality, it holds that

$$\Pr\left\{F(\hat{\theta}) - F(\theta^*) \leq 2\delta\right\} \geq \frac{1}{2}.$$

When running the BSMD step for  $m := \lceil \log_2 \frac{2}{\eta} \rceil$  times, it holds that

$$\Pr\left\{\min_{i \in [m]} F(\hat{\theta}_i) - F(\theta^*) \leq 2\delta\right\} \geq 1 - \frac{1}{2^m} \geq 1 - \frac{\eta}{2}.$$

We specify the error probability  $\alpha = \frac{\eta}{2^m}$  in Proposition EC.4 when running the sampling step. Then with probability at least  $1 - m\alpha = 1 - \frac{\eta}{2}$ , it holds that

$$\max_{i \in [m]} \left| F(\hat{\theta}_i) - V(\hat{\theta}_i) \right| \leq \delta.$$

Combining those two relations, it holds that

$$\Pr\left\{\left|\min_{i \in [m]} V(\hat{\theta}_i) - F(\theta^*)\right| \leq 3\delta\right\} \geq 1 - \frac{\eta}{2} - m\alpha = 1 - \eta.$$

The overall computation cost in Algorithm 2 is

$$m * \left\{ \text{Cost}(\text{estimating optimal solution of (8) once}) + \text{Cost}(\text{estimating objective value of (8) once}) \right\}.$$

The memory cost is

$$\max \left\{ \text{Cost}(\text{estimating optimal solution of (8) once}), \text{Cost}(\text{estimating objective value of (8) once}) \right\}.$$

- (I) When running the BSMD step with V-SGD scheme and estimating the objective values using V-MLMC or RT-MLMC scheme, the computation cost becomes

$$m * O(\delta^{-3}) + m * \tilde{O}\left(\delta^{-2} \cdot \log \frac{m}{\eta}\right) = O\left(\delta^{-3} \cdot \text{polylog} \frac{1}{\eta}\right).$$

The memory cost becomes

$$\max \left\{ O(\delta^{-1}), \tilde{O}\left(\delta^{-2} \cdot \log \frac{m}{\eta}\right) \right\} = \tilde{O}\left(\delta^{-2} \cdot \text{polylog} \frac{1}{\eta}\right).$$

- (II) When additionally the smoothness assumption holds, if running the BSMD step and estimating the objective values using V-MLMC or RT-MLMC scheme, the complexity becomes

$$m * \tilde{O}(\delta^{-2}) + m * \tilde{O}\left(\delta^{-2} \cdot \log \frac{m}{\eta}\right) = \tilde{O}\left(\delta^{-2} \cdot \text{polylog} \frac{1}{\eta}\right).$$

The memory cost becomes

$$\max \left\{ \tilde{O}(\delta^{-1}), \tilde{O}\left(\delta^{-2} \cdot \log \frac{m}{\eta}\right) \right\} = \tilde{O}\left(\delta^{-2} \cdot \text{polylog} \frac{1}{\eta}\right).$$

## Appendix EC.8: Proofs of Technical Results in Section 4.2.3

A key technique to show Theorem 4 is the following complexity result on bisection search with inexact oracles.

**LEMMA EC.6 (Complexity for Noisy Bisection [30, Lemma 33]).** *Let  $f : \mathbb{R} \rightarrow \mathbb{R}$  be a  $B$ -Lipschitz and convex function defined on the interval  $[\ell, u]$ , and  $\mathcal{G} : \mathbb{R} \rightarrow \mathbb{R}$  be an oracle so that  $|\mathcal{G}(y) - f(y)| \leq \tilde{\delta}$  for all  $y$ . With at most*

$$1 + 2 \left\lceil \log_{3/2} \frac{B(u - \ell)}{\tilde{\delta}} \right\rceil$$

*calls to  $\mathcal{G}$ , the algorithm `OneDimMinimier` [30, Algorithm 8] outputs  $y'$  so that*

$$f(y') - \min_y f(y) \leq 4\tilde{\delta}.$$

*Proof of Theorem 4* Since  $f_\theta(z)$  is convex in  $\theta$ , one can check that the objective  $F(\theta; \lambda)$  is jointly convex in  $(\theta, \lambda)$ , and therefore the objective  $F^*(\lambda)$  is convex in  $\lambda$ . Also, by danskin's theorem, we find

$$\frac{\partial}{\partial \lambda} F^*(\lambda) = \bar{\rho} + \mathbb{E}_{\hat{\mathbb{P}}} \left[ \epsilon \log \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta^*}(z)/(\lambda\epsilon)} \right) \right] - \mathbb{E}_{\hat{\mathbb{P}}} \left[ \frac{\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta^*}(z)/(\lambda\epsilon)} f_{\theta^*}(z)}{\lambda \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta^*}(z)/(\lambda\epsilon)}} \right].$$

Since  $0 \leq f_\theta(z) \leq B$ , we find

$$0 \leq \mathbb{E}_{\hat{\mathbb{P}}} \left[ \epsilon \log \left( \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta^*}(z)/(\lambda\epsilon)} \right) \right] \leq \frac{B}{\lambda} \leq \frac{B}{\lambda_\ell}$$

and

$$0 \leq \mathbb{E}_{\hat{\mathbb{P}}} \left[ \frac{\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta^*}(z)/(\lambda\epsilon)} f_{\theta^*}(z)}{\lambda \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} e^{f_{\theta^*}(z)/(\lambda\epsilon)}} \right] \leq \frac{e^{B/(\lambda_\ell\epsilon)} B}{\lambda} \leq \frac{e^{B/(\lambda_\ell\epsilon)} B}{\lambda_\ell}$$

Therefore, the subgradient of  $F^*(\lambda)$  is bounded:

$$\left| \frac{\partial}{\partial \lambda} F^*(\lambda) \right| \leq L_\lambda \triangleq \bar{\rho} + \frac{B}{\lambda_\ell} [1 + e^{B/(\lambda_\ell\epsilon)}].$$

In summary,  $F^*(\lambda)$  is a  $L_\lambda$ -Lipschitz and convex function defined on  $[\lambda_\ell, \lambda_u]$ . Applying Lemma EC.6 with  $\tilde{\delta} := \delta/4$  together with the union bound, we are able to find the optimal multiplier up to accuracy  $\delta$  with probability at least  $1 - \eta$  by calling the oracle  $\hat{F}$  for

$$1 + 2 \left\lceil \log_{3/2} \frac{4L_\lambda(\lambda_u - \lambda_\ell)}{\delta} \right\rceil$$

times.

## Appendix EC.9: Proof of the Technical Result in Appendix A

We first present an useful technical lemma before showing Proposition 1.

LEMMA EC.7. *Under the first condition of Proposition 1, for any  $x \in \mathcal{Z}$ , it holds that*

$$\int e^{-c(x,z)/\epsilon} d\nu(z) \geq e^{-2^{p-1}c(x,\bar{x})/\epsilon} \int e^{-2^{p-1}c(\bar{x},z)/\epsilon} d\nu(z).$$

*Proof of Lemma EC.7* 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  $c(x,z) \leq 2^{p-1}(c(\bar{x},z) + c(x,\bar{x}))$ , we can see that

$$\int e^{-c(x,z)/\epsilon} d\nu(z) \geq \exp(-2^{p-1}c(x,\bar{x})/\epsilon) \int e^{-2^{p-1}c(\bar{x},z)/\epsilon} d\nu(z).$$

The proof is completed. □

*Proof of Proposition 1* One can see that for any  $x \in \text{supp}(\widehat{\mathbb{P}})$ , it holds that

$$\begin{aligned} & \mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [e^{f(z)/(\lambda\epsilon)}] \\ &= \int e^{f(z)/(\lambda\epsilon)} \frac{e^{-c(x,z)/\epsilon}}{\int e^{-c(x,u)/\epsilon} d\nu(u)} d\nu(z) \\ &\leq \int e^{f(z)/(\lambda\epsilon)} \frac{e^{-c(x,z)/\epsilon}}{\int e^{-2^{p-1}c(\bar{x},z)/\epsilon} d\nu(z)} d\nu(z) \\ &\leq \int e^{f(z)/(\lambda\epsilon)} \frac{e^{-2^{1-p}c(\bar{x},z)/\epsilon} e^{c(x,\bar{x})/\epsilon}}{\int e^{-2^{p-1}c(\bar{x},z)/\epsilon} d\nu(z)} d\nu(z) \\ &= \frac{e^{c(x,\bar{x})(1+2^{p-1})/\epsilon}}{\int e^{-2^{p-1}c(\bar{x},z)/\epsilon} d\nu(z)} \int e^{f(z)/(\lambda\epsilon)} e^{-2^{1-p}c(\bar{x},z)/\epsilon} d\nu(z), \end{aligned}$$

where the first inequality is based on the lower bound in Lemma EC.7, the second inequality is based on the triangular inequality  $c(x,z) \geq 2^{1-p}c(\bar{x},z) - c(x,\bar{x})$ . Note that almost surely for all  $x \in \text{supp}(\widehat{\mathbb{P}})$ ,  $c(x,\bar{x}) < \infty$ . Moreover,

$$0 < \int e^{-2^{p-1}c(\bar{x},z)/\epsilon} d\nu(z) \leq \int e^{-c(\bar{x},z)/\epsilon} d\nu(z) < \infty,$$

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

$$\mathbb{E}_{\mathbb{Q}_{x,\epsilon}} [e^{f(z)/(\lambda\epsilon)}] \leq \frac{e^{c(x,\bar{x})(1+2^{p-1})/\epsilon}}{\int e^{-2^{p-1}c(\bar{x},z)/\epsilon} d\nu(z)} \int e^{f(z)/(\lambda\epsilon)} e^{-2^{1-p}c(\bar{x},z)/\epsilon} d\nu(z) < \infty$$

almost surely for all  $x \sim \widehat{\mathbb{P}}$ . □