Modified Frank Wolfe in Probability Space

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Abstract

We propose a novel Frank-Wolfe (FW) procedure for the optimization of infinite-dimensional functionals of probability measures - a task which arises naturally in a wide range of areas including statistical learning (e.g. variational inference) and artificial intelligence (e.g. generative adversarial networks). Our FW procedure takes advantage of Wasserstein gradient flows and strong duality results recently developed in Distributionally Robust Optimization so that gradient steps (in the Wasserstein space) can be efficiently computed using finite-dimensional, convex optimization methods. We show how to choose the step sizes in order to guarantee exponentially fast iteration convergence, under mild assumptions on the functional to optimize. We apply our algorithm to a range of functionals arising from applications in nonparametric estimation.

1 Introduction

Problems in artificial intelligence, statistics, and optimization often find a common root as an infinite dimensional optimization problem in the form

$$\inf \left\{ J(\mu) : \mu \in \mathcal{P}\left(\mathbb{R}^d\right) \right\}, \tag{1}$$

for the space $\mathcal{P}\left(\mathbb{R}^d\right)$ of Borel probability measures over $\mathbb{R}^d$. In recent years, quantitative statistical and algorithmic treatments of these formulations have produced insights into modern computational methods– resulting in novel approaches to difficult, open problems. Recent works in robust optimization [6, 44, 54, 55], probabilistic fairness [57, 53], reinforcement learning [63, 64], and generative adversarial networks [42, 18, 19] highlight these gains and are linked by the following theme: problems in the form of (1) provide access to rich infinite dimensional structure that sidesteps brittle artifacts of finite dimensional formulations.

This paper provides the construction and analysis of a modified Frank-Wolfe algorithm for (1) that operates from this infinite dimensional perspective and yields concrete convergence and complexity guarantees for a sub-family of problems (1) which are well-behaved with respect to the Wasserstein distance of order 2 (see Algorithm 1 and Theorem 1). Under canonical conditions of smoothness and convexity we recover linear rates of convergence while, even for functionals which exhibit low degrees of smoothness and for conditions that go beyond convexity, we recover sublinear rates that are to be expected from finite dimensional analogues [36] (see Section 2.2).

The vanilla Frank-Wolfe method cannot work in probability space, in general, since the planar derivative (i.e. the first variation also known as the influence function) can be unbounded when distributions do not have compact support. To overcome this issue, we conduct a natural modification

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to introduce a tractable, local, linear constraint– inspired by efforts in DRO [44, 6, 25, 54]. Specifically, the modified Frank-Wolfe step admits the prototypical DRO formulation as below,

$$\sup \left\{ \int f \, d\mu : D_c(\mu, \mu_0) \leq \delta \right\}, \tag{2}$$

where $D_c(\mu, \mu_0)$ is the optimal transport cost between μ and μ_0 (a reference measure) under some cost function c. The form of (2), itself, immediately suggests the basis of an infinite dimensional Frank-Wolfe procedure since it provides a "linear" objective subject to a local, "trust-region" constraint– centered at μ_0. The relevance of (2) in distributionally robust optimization (DRO) and mathematical finance has resulted in a multitude of computational schemes [44, 34, 37, 54, 61] for solving (2). However, hitherto, such works have failed to consider (2) within the context of a general variational method for (1). What makes these efforts notable, within the scope of this work, is that they emphasize that the solution of (2) can be highly non-trivial. Indeed, without particular assumptions, (2) can disguise an computationally hard problem– despite being convex in a Banach sense on $\mathcal{P}(\mathbb{R}^d)$. Even in the case where the cost is the squared Euclidean norm $c(x, y) = \|x - y\|^2$ (the case of primary concern for this work), computational trouble can lie dormant– an artifact of inherently difficult problems in unconstrained optimization [14]. This should not be surprising, however, given specters of computational hardness dating back to early formulations of DRO [22]. To resolve these issues, we also provide a novel analysis of techniques from distributionally robust optimization (DRO) which illustrate how such formulations can be used, in a computationally tractable way, to construct first-order, variational methods. By localizing the problem to a Wasserstein ball, the new Local Linear Minimization Oracle (LLMO) that we make in this paper not only makes the vanilla Frank-Wolfe problem sensible, but it also renders the problem computationally tractable via finite dimensional convex optimization.

1.1 Previous work

Distributionally robust optimization To navigate such pitfalls, one can consider particular instances of (2) where the objective and constraints are sufficiently structured to preclude computational intractability and permit solution via methods adapted to the provided structure. Early work with this line [27, 22, 60], has recently been supplemented by approaches [13, 26, 7, 46, 37, 67, 35] which focus directly on DRO formulations from particular contexts in machine learning and operations research. Unfortunately, the techniques offered by these efforts require assumptions which are too restrictive for this work. These assumptions typically relate to a specific form for the objective function or constraints in (2) (e.g. linear/convex functions/piecewise-convex objectives or constraints with support or density requirements, see [31, 66, 44, 34, 65, 4, 58] for additional examples). In this instance, such limitations preclude their applicability since, in general, a "gradient object" for a functional J (see Section 2) need not satisfy these conditions.

A second, more relevant, approach to compute DRO problems (2) is to restrict the level of robustness δ for which the problem is solved. This technique has been used in works such as [6, 54] and we apply this principle in a similar spirit to [54]. In that work, smoothness of the objective in (2) is used to, qualitatively, argue that a sufficiently small δ provides a computationally-tractable optimization problem. In contrast, we provide quantification of the level of robustness required to achieve this tractability and we demonstrate that this level robustness is sufficiently large to achieve canonical convergence rates for an infinite-dimensional Frank-Wolfe algorithm.

Variational methods Although formulation of a Frank-Wolfe method for (1) (with quantitative bounds on complexity and convergence) has not appeared in previous literature, certain, tangentially-related variational methods offer conceptual similarity. The first of these methods is [41], which draws similar inspiration from finite-dimensional Frank-Wolfe procedures. However, the notion of first-order variation in [41] appears to be induced by the total variation distance– requiring compact support assumptions for the problem. Alternatively, we exploit Wasserstein geometry to provide a weaker notion of first-order variation, namely, Wasserstein differentiability– allowing us to eliminate restrictions to compact support. Hence, by balancing tractability of the analysis and fidelity of the procedure, the proposed algorithm scheme can be applied a broad class of computational examples. Indeed, [41] only discussed the Sinkhorn barycenter problem and it is still unclear how it can be applied to our setting. The second, more closely related effort, is [39] where similar, infinite-dimensional conditions (Section 2.2) are used to study particle-based methods for computing Nash equilibria of zero-sum games. While the setting and procedures developed in this work are completely

different, we note that, as a special case, our Frank-Wolfe method can also produce a particle-based optimization procedure. This hints at possible insightful connections with other particle methods [40, 24, 11, 10] which are left for future consideration.

2 Wasserstein geometry

This work considers the problem

$$\min_{\nu \in \mathcal{P}_2(\mathbb{R}^d)} J(\nu) \tag{3}$$

for functionals $J : \mathcal{P}_2(\mathbb{R}^d) \to \bar{\mathbb{R}}$ over the subset of Borel measures $\mathcal{P}(\mathbb{R}^d)$ defined by

$$\mathcal{P}_2(\mathbb{R}^d) := \left\{ \mu \in \mathcal{P}(\mathbb{R}^d) : \int_{\mathbb{R}^d} \|x\|^2 \, d\mu(x) < \infty \right\} \tag{4}$$

In particular, we consider functionals J that are differentiable (Definition 1) with respect to Wasserstein distance of order 2

$$\mathcal{W}^2(\mu, \nu) := \inf_{\gamma \in \Pi(\mu,\nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^2 \, d\gamma(x, y) \tag{5}$$

where $\Pi(\mu, \nu)$ is the set of all joint couplings with marginals $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$. Common examples of functionals that can be cast within this framework are as follows.

Example 1 (Divergences)**.** For any convex, lower-semicontinuous function $f : \mathbb{R}_+ \to \mathbb{R}$ such that $f(1) = 0$, one can consider a "f-divergence" of the form

$$J(\mu) := D_f(\mu||\nu) = \int_{\mathbb{R}^d} f\left(\frac{d\mu}{d\nu}\right) d\nu. \tag{6}$$

For instance, if $f(t) = t \log t$, (6) reduces to Kullback-Leibler divergence D_{KL}.

Example 2 (Integral Probability Metrics)**.** For a set of real valued functions F on $\mathbb{R}^d$ one can define the discrepancy

$$J(\mu) := \text{IPM}\,(\mu, \nu) = \sup_{f \in F} \int_{\mathbb{R}^d} f \, d\mu - \int_{\mathbb{R}^d} f \, d\nu \tag{7}$$

for $\mu, \nu \in \mathcal{P}\left(\mathbb{R}^d\right)$, where ν is a fixed, reference measure. Such discrepancies are termed Integral Probability Metrics (IPMs), although they may not strictly satisfy the requirements of a metric– say, by failing to distinguish all pairs of measures. Instead, for a pair of measures $\mu, \nu \in \mathcal{P}\left(\mathbb{R}^d\right)$, IPMs can be interpreted as measuring the extent to which μ and ν differ on functions in F– or, rather, measuring the extent to which μ and ν can be distinguished by F. Concretely, consider $F = \{f : \|f\|_H \leq 1\}$ where H is a reproducing kernel hilbert space (RKHS). In this case, one obtains the dual formulation of Maximum Mean Discrepancy (MMD).

2.1 Properties and differentiability for Wasserstein space

Under the Wasserstein distance, $\mathcal{P}_2(\mathbb{R}^d)$ is a Polish space [59] and, more importantly, it is a *geodesic* space. That is, for every $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$, there exists a constant-speed geodesic curve $\mu_t : [0, 1] \to \mathcal{P}_2(\mathbb{R}^d)$ where $\mu_0 = \mu$, $\mu_1 = \nu$ and

$$\mathcal{W}(\mu_t, \mu_s) = |t - s|\mathcal{W}(\mu_0, \mu_1) \tag{8}$$

Moreover, there is a bijection between constant-speed geodesics and optimal transport plans [1, Theorem 7.2.2]. Every geodesic corresponds to a unique, optimal transport plan $\gamma \in \Pi\,(\mu, \nu)$ such that

$$\mu_t = ((1 - t)x + ty)_{\#}\,\gamma \qquad \text{where} \quad \mathcal{W}^2(\mu, \nu) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^2 \, d\gamma(x, y), \tag{9}$$

and μ_t is the distribution of the random variable $(1 - t)X + tY$ with the pair (X, Y) following distribution γ. Conversely, every optimal transport plan gives rise to a unique geodesic via (9).

Since our Frank-Wolfe method minimizes a sequence of linear approximations, one must define the notion of a gradient (of a functional J) to be compatible with respect to the geometry of these geodesics. In particular, as $\mathcal{P}_2(\mathbb{R}^d)$ is curved under $\mathcal{W}$ (see Appendix A), gradients must be defined in terms of a selection in an appropriate cotangent bundle. For Wasserstein space, this cotangent bundle (denoted $\text{CoTan}_{\mathcal{P}_2(\mathbb{R}^d)}$) is essentially the set of vector fields on $\mathbb{R}^d$ that can be approximated by gradients of smooth functions (see Appendix A for details). This results in the following definition.

Definition 1 (Wasserstein differentiability)**.** Let S be a geodesically convex set; that is, $\mu_t \in S$ for any geodesic μ_t between $\mu, \nu \in S$. A functional $J : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ is Wasserstein differentiable on S if there is a map $F : \mathcal{P}_2(\mathbb{R}^d) \to \mathrm{CoTan}_{\mathcal{P}_2(\mathbb{R}^d)}$ such that for all $\mu, \nu \in S$ and a geodesic $\mu_t : [0,1] \to \mathcal{P}_2\left(\mathbb{R}^d\right)$ between μ and ν, one has

$$\lim_{\alpha \to 0^+} \frac{J\left(\mu_\alpha\right) - J(\mu)}{\alpha} = \int_{\mathbb{R}^d \times \mathbb{R}^d} F(\mu; x)^T (y - x)\, d\gamma(x, y), \tag{10}$$

where γ is the unique optimal transport plan (9) corresponding to μ_t. Note that $F(\mu; x) = \left(F(\mu)\right)(x)$ provides an aesthetic way of representing the evaluation at $x \in \mathbb{R}^d$ of the output of F at μ. The map F is called the Wasserstein derivative of J.

Remark 1. The description of differentiability provided by Definition 1 falls within the general framework of metric derivatives and Wasserstein gradient flows, largely codified in [1]. This framework is now a well-established component of the theory of Wasserstein spaces, while the relation (10), itself, presents only a narrow structuring of ideas from this framework. Definition 1, however, is often how works in statistical and algorithmic fields interact with this broader area [56, 16, 38, 39]. Moreover, this literature demonstrates the most motivating feature of (10): a large number of functionals of interest for machine learning and statistical inference exhibit Wasserstein gradients in the sense of (10). The curious reader is referred to [1, 52, 9] for precise statements of conditions under which (10) is guaranteed. However, F is intimately relative to the Gateaux differential for J [52, 56]. Recall, the Gateaux differential for a functional J exists when there is an appropriate, dual space D^* on a closed subspace $D \subseteq \mathcal{P}(\mathbb{R}^d)$ such that

$$\langle dJ(\mu), \nu - \mu \rangle = \lim_{\alpha \to 0^+} \frac{J\left(\mu + \alpha(\nu - \mu)\right) - J(\mu)}{\alpha} \tag{11}$$

for some $dJ(\mu) \in D^*$ and all μ in some set S such that $S - S \subseteq D$. In instances where the Gauteaux differential $dJ(\mu)$ exists, the Wasserstein derivative F will usually exist [39] and be given by $\nabla dJ(\mu)$. Here, we use the finite dimensional gradient operator $\nabla(\cdot)$ formally, and omit a rigorous exposition on this operation in the context of $\mathrm{CoTan}_{\mathcal{P}_2(\mathbb{R}^d)}$.

It should be noted that computation of the Wasserstein derivative might be difficult. Indeed, for a J in a variational form such as (7), computation of the Wasserstein derivative is equivalent to finding a *witness* function that achieves the supremum [52]. In the case of a pathological sets (in (7)), such a task might be intractable. To resolve this issue, and to simplify our treatment, this work utilizes the existence of an oracle for the computation of a Wasserstein gradient. This oracle permits a unified description of our Frank-Wolfe algorithm and abstracts away variation in functional-specific computational cost. Recall that a function in the Hölder space $C^1(\mathbb{R}^d)$ is called L-smooth if has L-Lipschitz gradients.

Definition 2 (Wasserstein Derivative Oracle)**.** Let $J : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ be a Wasserstein differentiable functional on a set S with Wasserstein derivative $F : \mathcal{P}_2(\mathbb{R}^d) \to \mathrm{CoTan}_{\mathcal{P}_2(\mathbb{R}^d)}$. A L-smooth Wasserstein derivative oracle over S is an oracle which, given sample access to a distribution $\mu \in S$ and an error parameter ϵ, returns an L-smooth function $\widehat{\phi}_\mu \in C^1(\mathbb{R}^d)$ satisfying

$$\left\| \nabla \widehat{\phi}_\mu - F(\mu) \right\|_{L^2(\mu)} \leq \epsilon \tag{12}$$

where $\|\cdot\|_{L^2(\mu)}$ is the canonical norm on the space $L^2(\mu)$ of square integrable functions with respect to $\mu \in \mathcal{P}(\mathbb{R}^d)$. In this work, the output of this oracle is represented as $\Theta(\mu, \epsilon)$.

Remark 2. The qualification that the Wasserstein derivative oracle return an L-smooth function is necessary to exclude the, aforementioned, possibility of a pathological Wasserstein derivative– that would be intractable for use in a computational procedure. In some ways, this is representative of the fact that the cotangent space $\mathrm{CoTan}(\mu)$ at a point μ is too large. Such a condition is common in other variational methods [3, 19, 64, 20] and is relatively superficial– when coupled with the degree of approximation afforded by ϵ. Via smoothing techniques [51, 11, 38], functionals can often be assumed to have Wasserstein derivatives which are $C^1(\mathbb{R}^d)$ or are well-approximable by $C^1(\mathbb{R}^d)$ functions.

2.2 Smoothness and Łojasiewicz inequalities

In finite dimensions, iterative, gradient-based methods typically require the specification of two conditions in order to achieve convergence.

- The accuracy of local, linear approximations that are provided by the gradient.
- The extent to which local descent makes global progress on the objective.

Here, we state these conditions in the context of functionals over Wasserstein space.

Definition 3 (α-Hölder smoothness)**.** Let S be a geodesically convex set and let $J : \mathcal{P}_2\left(\mathbb{R}^d\right) \to \mathbb{R}$ be a functional which is continuously Wasserstein differentiable on the set S. J is said to be locally α-Holder smooth on S with parameters T and Δ if for all $\mu \in S$ and all $\nu \in S$ such that $\mathcal{W}(\mu, \nu) \leq \Delta$, there exists an optimal transport plan $\gamma \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d)$ such that

$$J(\nu) \leq J(\mu) + \int_{\mathbb{R}^d \times \mathbb{R}^d} F(\mu; x)^T (y - x) \, d\gamma(x, y) + \frac{T}{1+\alpha} \mathcal{W}^{1+\alpha}(\nu, \mu) \tag{13}$$

Definition 4 (Łojasiewicz inequality)**.** A Wasserstein differentiable functional J on a set $S \subseteq \mathcal{P}_2(\mathbb{R}^d)$ is said to satisfy a *Łojasiewicz inequality* with parameter τ and exponent θ if for all $\mu \in S$ and $J_* := \inf_{\mu \in S} J(\mu)$

$$\tau \left(J(\mu) - J_*\right)^\theta \leq \|F(\mu)\|_{L^2(\mu)} \tag{14}$$

where F is the Wasserstein derivative (10) of J.

Remark 3. More restrictive versions of both (13) and (14) commonly appear in previous literature to establish the explicit converence rate [3, 32, 39, 19, 15]. In most cases, the α-Hölder smoothness condition (13) is stated for $\alpha = 1$ and required to hold globally ($\Delta = \infty$). This smoothness criterion is considerably weaker since it requires that the Wasserstein gradient only provide a local approximation that is slightly more than first-order accurate. Moreover, such a condition can be necessary when the Wasserstein derivative (10) is not Lipschitz with respect to $\mathcal{W}$ in the cotangent space norm on $\mathrm{CoTan}_{\mathcal{P}_2(\mathbb{R}^d)}$– see [43] for such an example. Additionally, statement of the Łojasiewicz inequality (14) is broader than canonical treatments due to the presence of the auxiliary power θ. Most often, the specific instances of either $\theta = 1/2$ or $\theta = 1$ are considered. The case $\theta = 1$ is implied for (geodesically) convex functionals J with a $\mathcal{W}$-bounded level set, while $\theta = 1/2$ is implied for strongly convex J [1, 32]. Although the notions of Holder smoothness condition (14) and Łojasiewicz inequalities (13) have been well-studied in the literature [33, 5], the use of both of these conditions with explicitly determined exponents α and θ to provide concrete convergence rates for a computationally-implemented, infinite-dimensional descent method does not appear in related literature as far as the authors are aware.

3 Modified Frank-Wolfe algorithm

Algorithm 1 provides our modified Frank-Wolfe procedure along with its associated convergence guarantees and sample complexities in Theorem 1 and Proposition 1. It is worth mentioning that the algorithm itself only requires a much weaker notion of differentiability to be applicable, namely, Gateaux differentiability (i.e., $dJ(\mu)$ in (11) exists). In Section 4, we will provide several computational examples which may not satisfy the following assumptions but work well in practice. We have to admit there is a theoretical and computational gap. We will leave it as an open question for our future work. However, to conduct the convergence analysis, we require the following assumptions–phrased in the language from Section 2.

Assumption 1 (Smoothness assumption)**.** The functional $J : \mathcal{P}_2(\mathbb{R}^d) \to \bar{\mathbb{R}}$ is Wasserstein differentiable (Definition 1) and locally α-*Holder smooth* (Definition 3) on a set $S \subseteq \mathcal{P}_2(\mathbb{R}^d)$ with parameters T and $\Delta_1 > 0$ (Definition 3). Further, an L-smooth Wasserstein derivative oracle (Definition 2) for J exists.

Assumption 2 (Local richness)**.** The set S is rich enough to contain the solution to (2) for $\mu \in S$, L-smooth $-f$, and $\delta \leq \Delta_2$.

Remark 4. When S is not the whole set, it is necessary to invoke Assumption 2 to guarantee that the iterates produced by our algorithm remain in S. This is a result of the fact that the solution of (15) is optimal for some Wasserstein ball of size $\tilde{\delta} \leq \delta$. Hence, each of these iterates is guaranteed to lie in S so long as $\delta \leq \Delta_2$.

Assumption 3 (Łojasiewicz assumption)**.** The functional J satisfies a *Łojasiewicz inequality* (14) on $S \subseteq \mathcal{P}_2(\mathbb{R}^d)$ with parameters $\tau > 0$ and θ.

Algorithm 1 Modified Frank Wolfe for (3)

Input: Wasserstein derivative oracle Θ, initial distribution μ_0, smoothness parameter α, gradient error $\hat{\epsilon}$, estimation error $\bar{\epsilon}$, iterate error $\widetilde{\epsilon}$, stopping threshold r, step sizes $(\beta_1, \beta_2, \beta_3)$, number of iterations k

for $1 \leq i \leq k$ **do**

Let $\widehat{\phi}_{\mu_{i-1}} \leftarrow \Theta(\mu_{i-1}, \hat{\epsilon})$ (▷) Definition 2

Compute $\left\|\nabla\widehat{\phi}_{\mu_{i-1}}\right\|_{L^2(\mu_{i-1})} - \bar{\epsilon} \leq s \leq \left\|\nabla\widehat{\phi}_{\mu_{i-1}}\right\|_{L^2(\mu_{i-1})}$

if $s \leq r$, **then break**

else $\delta \leftarrow \min\left(\beta_1, \beta_2 s, \beta_3 s^{1/\alpha}\right)$, $\zeta \leftarrow \delta\widetilde{\epsilon}$

Compute μ_i satisfying $W(\mu_i, \mu_{i-1}) \leq \delta$ and (▷) Proposition 1

$$\int \widehat{\phi}_{\mu_{i-1}}\, d\mu_i - \inf_{\mathcal{W}(\nu,\mu_{i-1})\leq\delta} \int \widehat{\phi}_{\mu_{i-1}}\, d\nu \leq \zeta \tag{15}$$

return μ_i

Theorem 1. *Under Assumptions 1, 2, 3, and an appropriate choice of input parameters, Algorithm 1 computes a distribution μ^* satisfying*

$$r(\mu^*) := J(\mu^*) - \inf_{\mu\in S} J(\mu) \leq \epsilon \tag{16}$$

in at most

$$k = \widetilde{O}\left(\epsilon^{-p_-}\right) \tag{17}$$

iterations, where p_- denotes the negative part of $p = 1 - \alpha^*\theta$ for the dual exponent $\alpha^* = (1+\alpha)/\alpha$. The notation $\widetilde{O}(\cdot)$ omits logarithmic factors in it's arguments.

Remark 5. In the case of a (geodescially) strongly-convex and 1-Hölder smooth functional J, the Łojasiewicz inequality (14) holds with $\theta = 1/2$ and one obtains standard $\widetilde{O}(1)$ complexity (in terms of ϵ). This is to be expected from finite dimensional analogues [36]. Similarly, for J which is only convex (with a $\mathcal{W}$-bounded level set), (14) holds with $\theta = 1$ and (17) yields a $\widetilde{O}(\epsilon^{-1})$ complexity that mimics canonical results. The step size required to achieve these complexities is illustrated by the choice of δ in Algorithm 1.

For functionals which are α-Hölder smooth for $\alpha < 1$, the dependence on the dual exponent α^* in (17) can be rather punishing for small α. It is natural to ask if this exponent could be improved within the scope of Assumptions 1, 2, and 3. Moreover, in finite dimensions, it is well known that first-order methods for convex and α-Hölder smooth functions (also known as weakly smooth functions) can obtain ϵ-optimal solutions in $O(\epsilon^{-2/(1+3\alpha)})$ iterations [47]. Hence, it could even be considered whether, given geodesic-convexity assumptions on J, a better iteration complexity for Algorithm 1 would be obtainable.

We conjecture that such improvements are unlikely - particularly those that would draw on analogy from finite dimensional techniques. The motivation for this is as follows. A common approach to establishing improved iteration complexities for convex, α-Hölder smooth functions, in finite dimensions is to consider their gradient oracles as inexact oracles for convex, 1-Hölder smooth functions [23]. Using either averaging arguments or accelerated methods, more rapid progress on an underlying objective can then be made with these inexact oracles. Our Frank-Wolfe method already utilizes an inexact step (15) so, conceptually, such an approach could be applied to Algorithm 1. Unfortunately, however, such finite dimensional analogies fail due to the difficulty of averaging distributions in Wasserstein space. Indeed, in finite dimensions, averaging is crucial to prevent error accumulation from outpacing objective progress. Since Wasserstein space is positively curved (Appendix A) computing analogous convex combinations of the μ_i in Algorithm 1 is, itself, a variational problem that might be as expensive to compute as the original problem (3).

3.1 Computation of the Frank-Wolfe step

An algorithm for computation of the Frank Wolfe step (15) is given in Appendix C and the net result of this procedure is as follows.

Proposition 1. *Under the assumptions of Theorem 1, there exists a stochastic algorithm which (with high probability) provides sample access to a distribution satisfying* (15)*. Moreover, in the setting of* (17)*, this algorithm requires* $\widetilde{O}\left(\epsilon^{-2\alpha^*\theta}\right)$ *samples and gradient evaluations.*

Crucially, the property enabling Proposition 1 is *duality*. The Frank-Wolfe problem (15) exhibits a dual of the form

$$\sup_{\lambda \geq 0} \quad \left[\int_{\mathbb{R}^d} \left(\inf_{y \in \mathbb{R}^d} f(y) + \frac{\lambda}{2} \left\| x - y \right\|^2 \right) d\mu(x) - \frac{\delta^2 \lambda}{2} \right] \tag{18}$$

and (18) is amenable to computation using techniques from finite dimensional optimization. This approach derives from distributionally robust optimization [6, 54, 25, 34] where such techniques have been used to produce methods in optimization and machine learning that are robust to adversarial perturbations.

In general, solution of (15) for any level of δ could be computationally hard [6, 54]. However, since a Frank-Wolfe procedure need only solve *local* problems, not *global* ones, we show: there is a δ which is, simultaneously, small enough to enable the efficient computation of (18)), yet large enough to produce (17). The techniques used to achieve these results most closely resemble ideas from [54]. However, we provide a precise quantification of the δ in (15) that is required to achieve computation tractability and develop a procedure which yields guarantees on the primal-dual gap of (15) and (18). In turn, the theoretical insights that we obtain suggest an empirical procedure in which λ in (18) can be updated relatively infrequently within our Frank-Wolfe algorithm, provided that it is chosen on a proper scale. Such an implementation is investigated in Section 4 and yields significant computational savings.

It is also worth noting that the implementation in Appendix C requires only sample access to μ_0 in order to provide sample access to a distribution satisfying (16). Thus, all operations in Algorithm 1 can be implemented using only sample access to μ_0. Practically, however, it is often more efficient to maintain approximations to the iterates μ_i via a non-parametric estimator. When this is done, it results in an additional, additive error in the residual (16) at each step of Algorithm 1. If this error is on the order of the error produced by the Wasserstein derivative oracle Θ, the iteration complexity (17) remains unaffected. Moreover, analysis of the error induced by a particular non-parametric approximation of the μ_i is highly problem dependent– so we do not consider it in the context of Theorem 1.

4 Computational examples

In this section, we demonstrate the application our Frank-Wolfe algorithm to several non-parametric estimation problems in statistics and machine learning. All simulations are implemented using Python 3.8 on a high performance computing server running Ubuntu 18.04 with a Gen10 Quad Intel(R) Xeon(R) Platinum 8268 CPU @ 2.90GHz processor. As we mentioned in Section 3, the proposed algorithm just needs a very weak of differentiability to be applied (i.e., Gateaux differentiability). The computational examples we conduct in this section aim to show attractive performance in applications where the assumptions required for theoretical convergence are unknown, instead of corroborating our theoretical results.

4.1 Gaussian deconvolution

A classical task in nonparametric statistics [12, 8] is to infer a latent, data-generating distribution $\mu \in \mathcal{P}_2\left(\mathbb{R}^d\right)$ from a set of observations that are corrupted by independent, additive Gaussian noise. For observations $Y_1, \ldots, Y_n$ such that $Y_i = X_i + Z_i$ where $X_i \sim \mu, Z_i \sim N\left(0, \sigma^2\right)$. One seeks to compute a non-parametric estimate of μ — the variance of the noise σ^2 is considered known. Since Z_i is independent of X_i, this task amounts to "deconvolving" μ from the distribution of Z_i. A natural candidate for μ is the maximum-likelihood estimator (MLE),

$$\widehat{\mu} := \underset{\mu \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\max} \sum_{i=1}^{n} \log \int_{\mathbb{R}^d} g_\sigma \left(Y_i - x\right) \, d\mu(x) \tag{19}$$

where g_σ is the density of Z_i. We refer the reader to [50, Section 3] for further details but note that it was shown in [50] that $\widehat{\mu}$ has an equivalent characterization

$$\hat{\mu} = \underset{\mu \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\min} \quad D_{\sigma^2}(\mu, \hat{P}_Y) \tag{20}$$

where

$$D_{\sigma^2}(\mu_1, \mu_2) := \inf_{\pi \in \Pi(\mu_1, \mu_2)} \frac{1}{2} \int \|x - y\|^2 \, d\pi(x, y) + \sigma^2 D_{KL}(\pi \,||\, \mu_1 \otimes \mu_2) \tag{21}$$

is the entropic optimal transportation distance [21] and $\hat{P}_Y$ is the empirical distribution of the Y_i. The problem (20) readily lies within the framework of (3) for $J(\mu) := D_{\sigma^2}(\mu, \hat{P}_Y)$. Moreover, it is known [41] that the Wasserstein derivative (10) of $D_{\sigma^2}(\mu, \hat{P}_Y)$ with respect μ is given by

$$\nabla \hat{\phi}_\mu(x) = \sigma^2 \log \left(\frac{1}{n} \sum_{i=1}^{n} \exp\left(\left(v_i^* - \|x - y_i\|^2 / 2 \right) / \sigma^2 \right) \right) \tag{22}$$

where $v^* \in \mathbb{R}^n$ is dual variable (corresponding to $\hat{P}_Y$) which is optimal for $D_{\sigma^2}(\mu, \hat{P}_Y)$. This provides a Wasserstein derivative oracle for (20) as the vector v^* can be readily approximated using sinkhorn or stochastic gradient algorithms [49].

Toy example On 2D Gaussian mixture A simple, two dimensional instance of (19) is shown in Figure 1 on a dataset Y_i of 50 samples with mixture of 4 Gaussians — illustrated by the kernel density estimator of the Y_i, shown in red. The behavior of our Frank-Wolfe Algorithm is depicted over the course of several iterations, where the foreground contours provide the density of the iterate, μ_i, that is maintained by the algorithm. It can be easily observed that despite the small overlap between our initial distribution and target one, our method reaches the global optima very quickly.

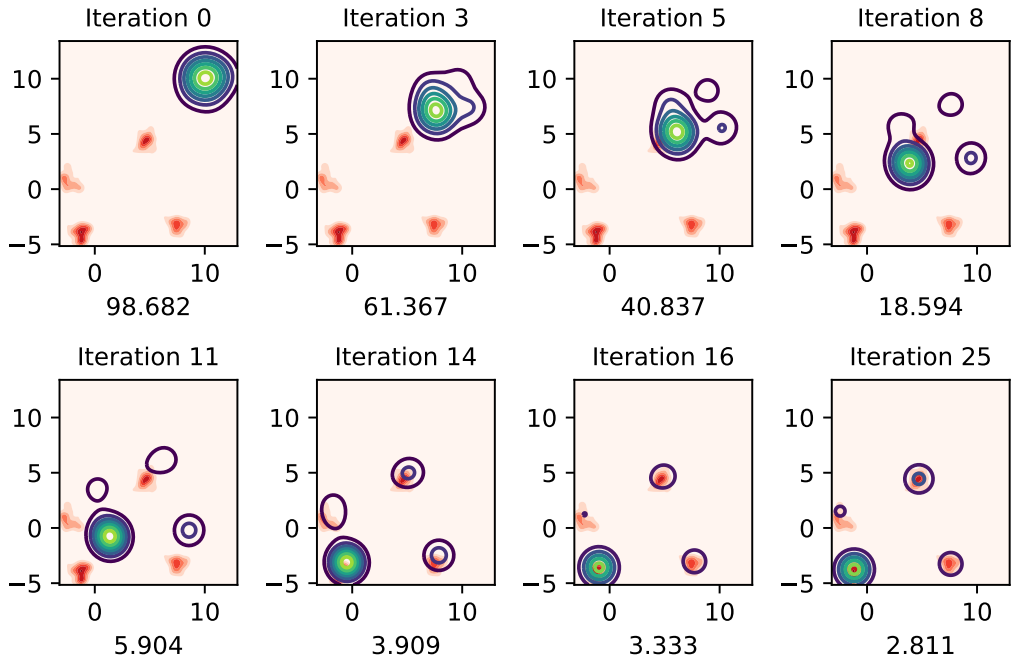
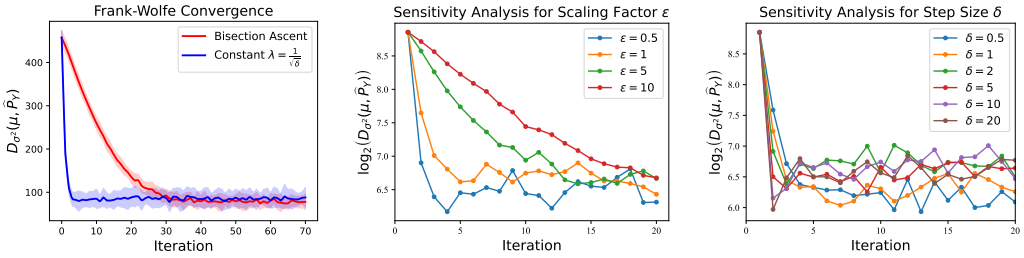


Figure 1: Toy Example on a 2D Gaussian Mixture. Note that the initial distribution is set as $N([10, 10], \sigma^2 \mathbf{I})$ for $\sigma^2 = 0.4$ and the number of particles is 200. The bisection method of Appendix C is used with tolerance set to $1e^{-3}$. The objective value $D_{\sigma^2}(\mu_i, \hat{P}_y)$ is below to each sub-figure.

Uniform strategy for λ and sensitivity analysis on high-dimensional examples Since the number of bisection ascent step for λ in (18) that arises during the search can be large, the original algorithm may be computationally rather demanding for high-dimensional cases. Thus, we are



(a) Objective Value (b) Scaling Factor ε (c) Step size δ

Figure 2: High-dimensional Gaussian deconvolution for $d = 64$. For 50 data points, Y_i, sampled from a mixture of 7-Gaussians, 200 particles are used in a non-parametric estimate the μ_i. In Figure 2(a), the tolerance for the ascent method is $1e^{-3}$ and the shaded bands show the standard derivation over 10 independent runs with random initializations. In Figure 2(b), the step size δ is 0.5.

motivated to develop an approach that makes λ as a constant which only depends on the step size $\lambda = \varepsilon/\delta^{1/2}$ without other one-dimensional optimization methods as an inner solver, where ε is the scaling factor. Figure 2(a) provides a convergence behavior comparison between the vanilla Algorithm 1 and the modification leveraging this new uniform strategy. Not surprisingly, the modified Frank-Wolfe algorithm can get to the local region around the global optima faster but with a larger variance, as the uniform strategy is indeed a more aggressive strategy at the early stage. To further support the uniform strategy and our Frank-Wolfe framework, we conduct extensive sensitivity experiments on the hyperparameter (e.g., step size δ and scaling factor ε). Both Figure 2(b) and 2(c) demonstrate that our algorithm is robust to these crucial hyperparamter. We can also observe that it is better not to choose a relatively large step size although we can converge faster at the beginning but suffer from the risk of divergence, as the maximum step size is controlled by the smooth parameter in theory. Hence, our experiment results here also corroborate the theoretical findings.

It is worth mentioning that this new uniform strategy can make our Frank-Wolfe framework be extended to an asynchronous decentralized parallel setting easily and thus can further meet the requirements of large-scale applications. Based on the superior performance, we left its rigorous convergence analysis as an open question.

4.2 Nonparametric learning with student-teacher networks

The rise of generative adversarial networks (GANs) [28] and efforts connecting neural networks and kernel regression [17], have generated interest in maximum mean discrepancy (MMD), particularly with respect to it's role in constructing high-dimensional, distributional embeddings [20, 45]. This development is predicated on the observation that any neural network $(x, \theta) \to \psi(x, \theta)$, which produces an output $\psi(x, \theta) \in \mathbb{R}^d$ from input data $x \in X \subseteq \mathbb{R}^d$ and parameters $\theta \in \Theta \subseteq \mathbb{R}^m$, yields a kernel on the parameter set Θ:

$$k(\theta_1, \theta_2) := \mathbb{E}_x \left[\psi(x, \theta_1)^T \psi(x, \theta_2)\right] \tag{23}$$

where the expectation over x is taken with respect to a data generating distribution. Via MMD, $k(\cdot, \cdot)$ induces a natural discrepancy measure between distributions over network parameters θ. Thus, learning of a generative image model can be expressed as minimizing MMD with respect to latent, generative distribution for ν. We refer to [45, 3] for further descriptions of these applications.

Being an integral probability metric (7), squared MMD lies well within the framework of this paper

$$J(\mu) := \mathrm{MMD}^2(\mu, \nu). \tag{24}$$

and the Gateaux derivative (i.e., influence function) of J admits a natural expression [3] as the difference between the mean embeddings of μ and ν

$$f^*_\mu(x) = \mathbb{E}_{z\sim\mu}\left[k(z, x)\right] - \mathbb{E}_{z\sim\nu}\left[k(z, x)\right] \tag{25}$$

Indeed, f^*_μ can be readily computed via sampling methods– even when μ or ν are continuous or are large, discrete distributions [29]. Note that, as discussed in Remark 1, the Wasserstein

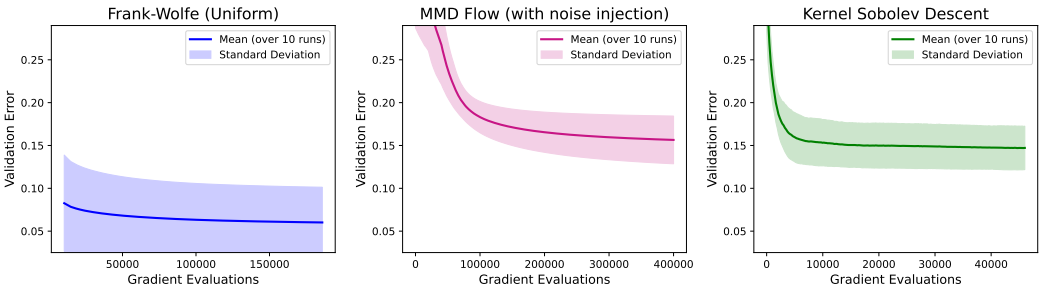


Figure 3: Student-Teacher Network; The detailed implementation set up is same as [3, Appendix G]. The left one is the result for our Frank-Wolfe method with the uniform strategy $\lambda = \frac{0.05}{\delta}$ and the step size δ is 0.5. The number of particle is 200.

derivative is, under sufficient regularity, the gradient of the Gateaux differential $\nabla f_\mu^*(\cdot)$. Perhaps the most advantageous consequence of (25), however, is that the Wasserstein gradient directly inherits regularity present in k. Indeed, should $\nabla_x k(x, y)$ be L-Lipschitz in x (uniformly for all y), J (24) is naturally L-smooth [3]. This has led to the development of several variational or particle-based methods for minimizing (24) [3, 45, 20].

Remark 6. For general MMD functionals, the smoothness and Łojasiewicz inequalities (i.e., Assumptions 1 and 3) are shown in [3]. Nevertheless, the MMD experiments in our paper, following the setup in [3], fail to satisfy the differentiability assumptions in [3] due to the ReLU terms present in the network defining the kernel.

However, despite a possible violation of the assumptions, Figure 3 demonstrates the competitive performance of our method with two of baselines showcased in [3] on Student-Teacher network problem. Our method is shown on the left, the center plot shows the "MMD gradient flow" algorithm from [3], and the right plot provides the "Sobolev Descent" algorithm of [45]. Performance is evaluated in terms of MMD error on a validation dataset and is shown as a function of the total gradient evaluations performed by each method. This provides a better proxy for relative performance and convergence since an iteration of Algorithm 1 performs multiple solves that are, each, similar in terms of gradient complexity to a single iteration of MMD gradient flow or Sobolev descent. Further, the total number of gradient evaluations should not be viewed as a proxy for wall-time as, for each gradient evaluation, the number of operations performed by each method can vary widely. Indeed, for each gradient evaluation in Sobolev descent an entire linear system solve is performed, which is computational demanding in practice. Also, note that, as both MMD gradient flow and Sobolev descent are particle-based, Algorithm 1 was, for the purposes of comparison, instantiated with a particle distribution of equal size.

5 Conclusion

This paper introduces and studies a Frank-Wolfe procedure for the minimization of functionals of probability measures. While these methods have been widely studied in the finite-dimensional setting; our current environment presents both significant benefits and opportunities. First, many problems of interest can be posed in terms of the types of formulations that we study [18, 19, 6, 54, 20, 39, 64, 55, 57, 11]. Second, our algorithm can naturally be asynchronously parallelized. This is a research avenue of significant promise that we plan to explore in future work, especially in connection with the wide range of applications mentioned earlier.

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes]
   (c) Did you discuss any potential negative societal impacts of your work? [No] The contributions of this work are mainly theoretical. We do not foresee any negative societal impact as a consequence.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes]
   (b) Did you include complete proofs of all theoretical results? [Yes] See the supplemental material
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results? [Yes] See the supplemental material
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes]
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes]
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes]
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [N/A]
   (b) Did you mention the license of the assets? [N/A]
   (c) Did you include any new assets either in the supplemental material or as a URL? [N/A]
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [N/A]
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5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]

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A Properties of Wasserstein space

The following properties of Wasserstein space make Definition 1 precise and are using in the convergence proofs in Appendix B.

Proposition 2 (Properties of Wasserstein space)**.**

- *For a constant-speed geodesic $\mu_t : [0,1] \to \mathcal{P}_2(\mathbb{R}^d)$ with respect to $\mathcal{W}$, there exists a (μ_t-almost surely) unique Borel vector field $v_t : [0,1] \times \mathbb{R}^d \to \mathbb{R}^d$ which satisfies*

$$\mathcal{W}^2(\mu_0, \mu_1) = \int_0^1 \int_{\mathbb{R}^d} \|v_t(x)\|^2 \, d\mu_t(x)\, dt = \min_{v_t \in V_\mu} \int_0^1 \int_{\mathbb{R}^d} \|v_t(x)\|^2 \, d\mu_t(x) \tag{26}$$

for

$$V_\mu := \left\{ v_t : \frac{d\mu_t}{dt} + \nabla \cdot (v_t \mu_t) = 0 \right\} \tag{27}$$

defined as the set of all Borel vector fields which solve the continuity equation for μ_t. The continuity equation is understood in duality with $C_c^\infty(\mathbb{R}^d)$.

- *For any constant-speed geodesic μ_t, the corresponding optimal transport plan $\gamma \in \Pi(\mu_0, \mu_1)$ and the corresponding vector field v_t (given by* (26)*) satisfy the relation*

$$v_t((1-t)x + ty) = y - x, \qquad \gamma\text{-almost surely} \tag{28}$$

for Lebesgue-almost every t.

- *The space $\mathcal{P}_2(\mathbb{R}^d)$ is positively curved under $\mathcal{W}$ and at each point $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, the tangent space*

$$\mathrm{Tan}(\mu) := \overline{\{\nabla\psi \ : \ \psi \in C_c^\infty(\mathbb{R}^d)\}}^{L^2(\mu)} \tag{29}$$

is the closure in $L^2(\mu)$ of the gradients of smooth functions with compact support. Via the Riesz isomorphism, $\mathrm{CoTan}(\mu) = \mathrm{Tan}(\mu)$ where $\mathrm{CoTan}(\mu)$ denotes the cotangent space. The tangent and cotangent bundles will be denoted $\mathrm{Tan}_{\mathcal{P}_2(\mathbb{R}^d)}$ and $\mathrm{CoTan}_{\mathcal{P}_2(\mathbb{R}^d)}$, respectively.

Proof of Proposition 2. To verify the first bullet, we first establish the existence of such a v_t. Let μ_t be the constant speed geodesic and define the set of functions

$$A_\mu := \left\{ z \in L^2([0,1]) : \mathcal{W}(\mu_t, \mu_s) \le \int_s^t z(r)\, dr \ \ \forall\ 0 \le s \le t \le 1 \right\}$$

It is clear that the function $m(r) := \mathcal{W}(\mu_0, \mu_1)$ is in A and satisfies

$$m = \arg\min_{z \in A} \int_0^1 z^p(r)\, dr \tag{30}$$

for any $p \ge 1$. Hence, the metric derivative $|\mu'|$ of μ_t fulfills

$$|\mu'|(t) = d(\mu_0, \mu_1) \qquad \text{Lebesgue almost everywhere for } t \in [0,1]$$

By Theorem 8.3.1 in [1], there exists Borel vector field $v_t : [0,1] \times \mathbb{R}^d \to \mathbb{R}^d$ satisfying the continuity equation (27) such that

$$\|v_t\|_{L^2(\mu_t)} = |\mu'|(t) = \mathcal{W}(\mu_0, \mu_1) \qquad \text{Lebesgue almost everywhere for } t \in [0,1] \tag{31}$$

Combined with (30), this implies that v_t is a solution of (26). Uniqueness of v_t follows directly from the second bullet.

For a constant-speed geodesic μ_t from μ to ν. Theorem 2.4 in [2] gives that, for any $\sigma \in \mathcal{P}_2(\mathbb{R}^d)$,

$$\frac{d}{dt}\frac{1}{2}\mathcal{W}^2(\mu_t, \sigma) = \int \langle v_t(x), x - y \rangle \, d\bar{\gamma}(x,y) \qquad \forall\ \bar{\gamma} \in \Pi_o(\mu_t, \sigma) \tag{32}$$

where $\Pi_o(\mu_t, \sigma) \subseteq \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)$ is the set of optimal transport plans between μ_t and σ. Setting $\sigma = \nu$, the fact that μ_t is a geodesic implies that there is a unique optimal coupling $\gamma \in \mathcal{P}\left(\mathbb{R}^d \times \mathbb{R}^d\right)$ between μ and ν such that

$$((1-t)x + ty, y)_{\#}\, \gamma \ \in \ \Pi_o(\mu_t, \sigma)$$

Hence, (32) gives

$$-(1-t)\mathcal{W}^2(\mu,\nu) = \int \langle v_t(x), x-y\rangle \; d\bar{\gamma}(x,y) = -(1-t)\int \langle v_t((1-t)x+ty), y-x\rangle \; d\gamma(x,y) \tag{33}$$

$$\Rightarrow \quad \mathcal{W}^2(\mu,\nu) = \int \langle v_t((1-t)x+ty), y-x\rangle \; d\gamma(x,y) \tag{34}$$

For t satisfying (31), the fact that $\|v_t\|_{L^2(\mu_t)} = \mathcal{W}(\mu,\nu)$ and $\|y-x\|_{L^2(\gamma)} = \mathcal{W}(\mu,\nu)$ means that (34) gives equality for Cauchy-Schwarz. Thus, $v_t((1-t)x+ty) = y-x$, γ-almost surely and (28) follows for Lebesgue almost every $t \in [0,1]$.

The final bullet is a direct restatement of the results of Section 8.4 in [1]. □

B Proof of iteration complexity (17)

In this section, we provide a proof of Theorem 1. Consider the following lemma which quantifies the stability of the sub-problems that are used in Algorithm 1.

Lemma 2. *Let $\gamma \in \Pi(\mu,\nu)$ be an optimal transport plan between $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ and $\nu \in \mathcal{P}_2(\mathbb{R}^d)$. If $\phi_\mu \in C^1(\mathbb{R}^d)$ is L-smooth*

$$\|\nabla\phi_\mu(x) - \nabla\phi_\mu(y)\| \leq L\,\|x-y\| \tag{35}$$

then

$$\left|\int_{\mathbb{R}^d} \langle \nabla\phi_\mu(x), y-x\rangle \; d\gamma(x,y) - \left(\int_{\mathbb{R}^d} \phi_\mu \, d\nu - \int_{\mathbb{R}^d} \phi_\mu \, d\mu\right)\right| \leq \frac{L}{2}\mathcal{W}^2(\nu,\mu) \tag{36}$$

Proof. First, it will be shown that

$$\left|\int_{\mathbb{R}^d} \langle \nabla\phi_\mu(x), y-x\rangle \; d\gamma(x,y) - \int_0^1 \langle \nabla\phi_\mu, v_t\rangle_{\mu_t} \; dt\right| \leq \frac{L}{2}\mathcal{W}^2(\nu,\mu) \tag{37}$$

for μ_t and v_t which correspond (26) to the unique-constant speed geodesic given by $\gamma \in \Pi(\mu,\nu)$ (9). Notice that, since $\nabla\phi_\mu$ has at most linear growth, therefore both terms in the left-hand side of (37) are finite. Moreover, by (28), one has

$$\int_0^1 \langle \nabla\phi_\mu, v_t\rangle_{\mu_t} \; dt = \int_0^1 \int_{\mathbb{R}^d\times\mathbb{R}^d} \langle \nabla\phi_\mu((1-t)x+ty), y-x\rangle \; d\gamma(x,y)\, dt \tag{38}$$

Thus, Cauchy-Schwarz and (35) give

$$\begin{aligned}
&\left|\int_0^1 \langle \phi_\mu, v_t\rangle_{\mu_t} \; dt - \int_{\mathbb{R}^d\times\mathbb{R}^d} \langle \nabla\phi_\mu(x), y-x\rangle \; d\gamma(x,y)\right| = \\
&\left|\int_0^1 \int_{\mathbb{R}^d\times\mathbb{R}^d} \langle \nabla\phi_\mu((1-t)x+ty) - \nabla\phi_\mu(x), y-x\rangle \; d\gamma(x,y)\, dt\right| \leq \\
&\int_0^1 \int_{\mathbb{R}^d} tL\,\|x-y\|^2 \; d\gamma(x,y)\, dt = \frac{L}{2}\mathcal{W}^2(\nu,\mu)
\end{aligned}$$

To obtain (36), it only remains to show that

$$\int_0^1 \langle \nabla\phi_\mu, v_t\rangle_{\mu_t} \; dt = \int \phi_\mu \, d\nu - \int \phi_\mu \, d\mu \tag{39}$$

Moreover, since v_t satisfies (27), Lemma 8.1.2 in [1] gives

$$\int_0^1 \langle \nabla\psi, v_t\rangle_{\mu_t} \; dt = \int \psi \, d\nu - \int \psi \, d\mu \tag{40}$$

for every $\psi \in C_c^1(\mathbb{R}^d)$– where $C_c^1(\mathbb{R}^d)$ denotes the space of continuously differentiable functions on $\mathbb{R}^d$ with compact support. Hence, (39) will be obtained from (40) by the following approximation argument.

Define the functions:

$$\beta_-(x) := \left(\sqrt{\|x\|^2+1} - \sqrt{2}\right)^{-1} \quad \text{and} \quad \beta_+(x) := \left(\sqrt{5} - \sqrt{\|x\|^2+1}\right)^{-1}$$

and

$$\eta(x) := \begin{cases} 1 & \text{if } \|x\| \le 1 \\ \frac{e^{\beta_-(x)}}{e^{\beta_-(x)}+e^{\beta_+(x)}} & \text{if } 1 < \|x\| < 2 \\ 0 & \text{if } \|x\| \ge 2 \end{cases}$$

It is easy to verify that $\eta \in C_c^\infty\left(\mathbb{R}^d\right)$ and $\|\nabla\eta(x)\| \le B$ for all $x \in \mathbb{R}^d$ and some constant B. Moreover, η provides a sequence of mollified approximations of ϕ_μ

$$\psi_k(x) := \phi_\mu(x)\eta_k(x) \quad \text{for} \quad \eta_k(x) := \eta\left(\frac{x}{k}\right)$$

where $\psi_k \in C_c^1(\mathbb{R}^d)$. Clearly, (40) holds for all such ψ_k. Thus, if

$$\lim_{k\to\infty} \int \psi_k \, d\nu - \int \psi_k \, d\mu = \int \phi_\mu \, d\nu - \int \phi_\mu \, d\mu \tag{41}$$

and

$$\lim_{k\to\infty} \int_0^1 \langle \nabla\psi_k, v_t\rangle_{\mu_t} \, dt = \int_0^1 \langle \nabla\phi_\mu, v_t\rangle_{\mu_t} \, dt \tag{42}$$

then (39) will follow directly from (40).

The relations (41) and (42) are straight-forward consequences of dominated convergence. Indeed, as $\eta_k \to 1$ and $\nabla\eta_k \to 0$ (pointwise), clearly

$$\psi_k \to \phi_\mu \quad \text{and} \quad \nabla\psi_k \to \nabla\phi_\mu \tag{43}$$

Quadratic growth of ϕ_μ yields $\phi_\mu \in L^2(\mu) \cap L^2(\nu)$ and combined with

$$|\psi_k(x)| \le |\phi_\mu(x)| \quad \forall x \in \mathbb{R}^d$$

(41) clearly holds via dominated convergence. One also has

$$\|\nabla\psi_k(x)\| \le \|\nabla\phi_\mu(x)\| + \frac{B|\phi_\mu(x)|}{k}\mathbf{1}_{\{\|x\|<2k\}} \tag{44}$$

Using the quadratic growth of ϕ_μ, linear growth of $\|\nabla\phi_\mu\|$, and the bound $\|x\|\,\mathbf{1}_{\{\|x\|<2k\}}/k \le 2$, (44) yields

$$\|\nabla\psi_k(x)\| \le \|\nabla\phi_\mu(x)\| + C\,\|x\|\,\mathbf{1}_{\{\|x\|<2k\}} + D \le E\,\|x\| + F \tag{45}$$

for some constants $C, D, E \in \mathbb{R}_+$. Recalling (38), (45) provides

$$\begin{aligned} \int_{\mathbb{R}^d\times\mathbb{R}^d} |\langle \nabla\psi_k((1-t)x+ty), y-x\rangle| \, d\gamma(x,y) &\le \int_{\mathbb{R}^d\times\mathbb{R}^d} \|\nabla\psi_k((1-t)x+ty)\|\,\|y-x\| \, d\gamma(x,y) \\ &\le \int_{\mathbb{R}^d\times\mathbb{R}^d} (E\,\|(1-t)x+ty\| + F)\,\|y-x\| \, d\gamma(x,y) \\ &\le H \end{aligned} \tag{46}$$

for some $H \in \mathbb{R}_+$; where the last inequality is a result of Cauchy-Schwarz. The combination of pointwise convergence (43) and (46) then immediately yield (42) by dominated convergence and (38). □

We also require the following elementary results regarding the convergence of certain polynomial sequences.

Lemma 3. *Let $r_i \in \mathbb{R}_+$ be a sequence of non-negative numbers satisfying*

$$r_{i+1} \le r_i - \kappa r_i^p \tag{47}$$

for some constants $\kappa > 0$ and $p \ge 0$. Then,

$$r_n \le \begin{cases} e^{-\kappa n / r_0^{1-p}} r_0 & \text{if } p \le 1 \\ \left(\kappa n + r_0^{1-p}\right)^{-1/(p-1)} & \text{if } p > 1 \end{cases} \tag{48}$$

Proof. If $p \leq 1$, then (47) combined with the fact that r_i is a non-increasing sequence implies

$$r_i \leq \left(1 - \frac{\kappa}{r_0^{1-p}}\right) r_{i-1}$$

Iterating this inequality from 1 to n yields the first part of (48). Next, let $p > 1$ and notice that, by taking the reciprocals of both sides of (47) and rearranging, one obtains

$$\frac{\kappa r_{i-1}^{p-2}}{1 - \kappa r_{i-1}^{p-1}} \leq r_i^{-1} - r_{i-1}^{-1}$$

Summing this inequality over i (from 1 to n),

$$\kappa n r_k^{p-2} \leq \sum_{i=1}^{n} \frac{\kappa r_{i-1}^{p-2}}{1 - \kappa r_{i-1}^{p-1}} \leq r_k^{-1} - r_0^{-1}$$

where the first inequality is a result of r_i being non-increasing. Algebraic manipulation then provides

$$r_n \leq \left(\kappa n + r_0^{1-p}\right)^{-1/(p-1)}$$

□

Proof of Theorem 1. Recall the parameters specified in Assumptions 1 and 3 and let ϵ be the desired tolerance with which (16) should hold. Let Algorithm 1 be run with the following parameters:

$$\beta_1 = \min\left(\Delta_1, \Delta_2\right), \quad \beta_2 = \alpha(4L)^{-1}, \quad \beta_3 = (1 - \alpha/2)^{1/\alpha} T^{-1/\alpha} \tag{49}$$

and

$$r = \tau\epsilon^{\theta}/2, \quad \hat{\epsilon} = \left(2\alpha^*\right)^{-1} r, \quad \bar{\epsilon} = \alpha r/2, \quad \widetilde{\epsilon} = \left(4\alpha^*\right)^{-1} r, \quad k = \lceil M \rceil \tag{50}$$

where $\alpha^* = (1+\alpha)/\alpha$ is the dual exponent of $1 + \alpha$ and M is defined in (65). It will be shown that the last iterate, μ_l, computed by Algorithm 1 satisfies (16).

First, we bound the decrease in J at each step of Algorithm 1. Let δ_i be the ith value of δ that is computed by Algorithm 1 and let s_i denote the ith value of s. One has the relation

$$\delta_i = \min\left(\beta_1, \beta_2 s_i, \beta_3 s_i^{\alpha^* - 1}\right) \tag{51}$$

and, since $\delta_i \leq \Delta_2$ for all i, $\mu_0 \in S$ implies $\mu_i \in S$ for all i. Via the smoothness of J on S and $\delta_i \leq \Delta_1$, it follows that

$$J(\mu_i) \leq J(\mu_{i-1}) + \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle F(\mu_{i-1}; x), y - x \rangle \, d\gamma(x, y) + \frac{T}{1+\alpha} \delta_i^{1+\alpha}$$

for any optimal transport plan $\gamma \in \Pi(\mu_i, \mu_{i-1})$ between μ_i and μ_{i-1}. Recognizing (12),

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} \left\langle F(\mu_{i-1}; x) - \nabla \widehat{\phi}_{\mu_{i-1}}(x), y - x \right\rangle \, d\gamma(x, y) \leq \left\| F(\mu_{i-1}; x) - \nabla \widehat{\phi}_{\mu_{i-1}} \right\|_{L^2(\mu_{i-1})} W(\mu_i, \mu_{i-1}) \leq \delta_i \hat{\epsilon}$$

and therefore

$$J(\mu_i) \leq J(\mu_{i-1}) + \int_{\mathbb{R}^d \times \mathbb{R}^d} \nabla \widehat{\phi}_{\mu_{i-1}}(x)^T \, (y - x) \, d\gamma(x, y) + \frac{T}{1+\alpha} \delta_i^{1+\alpha} + \delta_i \hat{\epsilon}$$

Via Lemma 2,

$$J(\mu_i) \leq J(\mu_{i-1}) + \int \widehat{\phi}_{\mu_{i-1}} \, d\mu_i - \int \widehat{\phi}_{\mu_{i-1}} \, d\mu_{i-1} + \frac{T}{1+\alpha} \delta_i^{1+\alpha} + \frac{L}{2} \delta_i^2 + \delta_i \hat{\epsilon} \tag{52}$$

Now, since $\widehat{\phi}_{\mu_{i-1}}$ is L-smooth, it is a Kantorovich potential [1, Section 6.1] for μ_{i-1}– under the cost function $L \left\| x - y \right\|^2 / 2$. Thus, there exists a geodesic ν_t (Proposition 2) such that: $\nu_0 = \mu_{i-1}$ and the transport plan $\gamma_t \in \Pi(\mu_{i-1}, \nu_t)$ between μ_{i-1} and ν_t satisfies [1, Section 8.3]

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} \left\langle \nabla \phi_{\mu_{i-1}}(x), y - x \right\rangle \, d\gamma_t(x, y) = -\frac{t}{L} \left\| \nabla \widehat{\phi}_{\mu_{i-1}} \right\|^2_{L^2(\mu_{i-1})} \quad \text{and} \quad \mathcal{W}\left(\nu_t, \mu_{i-1}\right) = \frac{t}{L} \left\| \nabla \widehat{\phi}_{\mu_{i-1}} \right\|_{L^2(\mu_{i-1})}$$

for $0 \leq t \leq 1$. For the sake of notation, define $g_{i-1} := \left\| \nabla \widehat{\phi}_{\mu_{i-1}} \right\|_{L^2(\mu_{i-1})}$ and set $t = L\delta_i / g_{i-1}$. Clearly, $t \leq 1$ since $\delta_i \leq \beta_2 s_i \leq \beta_2 g_{i-1}$.

By construction, μ_i also satisfies

$$\int \widehat{\phi}_{\mu_{i-1}} \, d\mu_i - \int \widehat{\phi}_{\mu_{i-1}} \, d\mu_{i-1} \leq \int \widehat{\phi}_{\mu_{i-1}} \, d\nu_t - \int \widehat{\phi}_{\mu_{i-1}} \, d\mu_{i-1} + \zeta_i$$

for $\zeta_i = \delta_i \widetilde{\epsilon}$. Hence, with another application of Lemma 2, one obtains

$$\begin{aligned}
\int \widehat{\phi}_{\mu_{i-1}} \, d\mu_i - \int \widehat{\phi}_{\mu_{i-1}} \, d\mu_{i-1} &\leq \int_0^t \left\langle \nabla \widehat{\phi}_{\mu_{i-1}}, v_s \right\rangle_{\nu_s} \, ds + \zeta_i \\
&\leq \int_{\mathbb{R}^d \times \mathbb{R}^d} \left\langle \nabla \widehat{\phi}_{\mu_{i-1}}(x), y - x \right\rangle \, d\gamma(x,y) + \frac{L}{2} \mathcal{W}(\nu_t, \mu_{i-1})^2 + \zeta_i \\
&= -\frac{t}{L} \left(1 - \frac{t}{2} \right) g_{i-1}^2 + \zeta_i \qquad (53)
\end{aligned}$$

Combining (53) with (52) and recalling $\delta_i = t g_{i-1} / L$ gives

$$J(\mu_i) \leq J(\mu_{i-1}) - \frac{t}{L} \left(C - t - \frac{D}{1+\alpha} t^\alpha \right) g_{i-1} + \zeta_i \qquad (54)$$

for the values

$$C := 1 - \hat{\epsilon} \quad \text{and} \quad D := \frac{T}{L^\alpha g_{i-1}^{1-\alpha}}$$

Rewriting (54) using the residual term

$$r(\nu) := J(\nu) - \inf_{\mu \in S} J(\mu) \qquad (55)$$

one obtains

$$r\left(\mu_i\right) \leq r\left(\mu_{i-1}\right) - \frac{t}{L} \left(C - t - \frac{D}{1+\alpha} t^\alpha \right) g_{i-1} + \zeta_i \qquad (56)$$

This relation will now be used to show that Algorithm 1 makes sufficient progress on J, prior to the termination of it's loop.

Let l be the index of the last iterate μ_i which is computed by Algorithm 1. First, observe that if $s_{l+1} \leq r$, then early termination of the loop in Algorithm 1 has occurred. Using (14) and the definitions (50), it follows that

$$\begin{aligned}
\tau \left(r\left(\mu_l\right) \right)^\theta &\leq \left\| F(\mu_l) \right\|_{L^2(\mu_l)} \leq g_l + \hat{\epsilon} \\
&\leq r + \bar{\epsilon} + \hat{\epsilon} \leq \tau \epsilon^\theta \qquad (57)
\end{aligned}$$

and, hence, sufficient progress on J has been made– μ_l satisfies (16). Thus, we need only analyze the case where early termination in Algorithm 1 does not occur and $l = k$ (50).

If $l = k$, then $s_i > r$ for all $i \leq k$ and, by extension, $g_{i-1} > r$ for all $i \leq k$ since s_i is a lower bound for g_{i-1}. In this case, the definitions of $\hat{\epsilon}$ and r (50) imply $C \geq 1 - \alpha / \left(2(1+\alpha) \right)$ and the choices for β_2 and β_3 (49) provide

$$t \leq \min \left(\frac{\alpha}{2(1+\alpha)}, \frac{(1 - \alpha/2)^{1/\alpha}}{D^{1/\alpha}} \right)$$

This gives

$$C - t - \frac{D}{(1+\alpha)} t^\alpha \geq (2\alpha^*)^{-1}$$

from which substitution into (56) yields

$$\begin{aligned}
r\left(\mu_i\right) &\leq r\left(\mu_{i-1}\right) - \frac{t}{2L\alpha^*} g_{i-1} + \zeta_i \\
&\leq r\left(\mu_{i-1}\right) - \frac{\delta_i}{2\alpha^*} g_{i-1} + \zeta_i \\
&\leq r\left(\mu_{i-1}\right) - \frac{\delta_i}{4\alpha^*} g_{i-1} \qquad (58)
\end{aligned}$$

where the last inequality is a result of the definition of $\widetilde{\epsilon}$ (50), ζ_i, and $g_{i-1} > r$. As δ_i is the minimum of three different terms (51), (58) will be used to analyze the amount of progress, that is made on the objective J, corresponding to each of these three terms. Note, the following identities that will be used in the analysis of each term:

$$\left(1 - \frac{\alpha}{2}\right) g_{i-1} \leq g_{i-1} - \frac{\alpha r}{2} \leq g_{i-1} - \bar{\epsilon} \leq s_i \tag{59}$$

and

$$\begin{aligned} -g_{i-1}^p &\leq -\left(\|F(\mu_{i-1})\|_{L^2(\mu_{i-1})} - \hat{\epsilon}\right)^p \\ &\leq -\left(1 - \frac{\alpha}{2+\alpha}\right)^p \|F(\mu_{i-1})\|_{L^2(\mu_{i-1})}^p \leq -\frac{1}{2e} \|F(\mu_{i-1})\|_{L^2(\mu_{i-1})}^p \end{aligned} \tag{60}$$

for all $1 \leq p \leq \alpha^*$. The relation (59) simply observes that s_i is a multiplicative approximation to g_{i-1} in Algorithm 1, while (60) is a consequence of $r - \hat{\epsilon} \leq \|F(\mu_{i-1})\|_{L^2(\mu_{i-1})}$.

First, consider the case where $\delta_i = \beta_1$. Substitution into (58), coupled with (60), provides

$$r(\mu_i) \leq r(\mu_{i-1}) - \frac{\beta_1}{8e\alpha^*} \|F(\mu_{i-1})\|_{L^2(\mu_{i-1})} \tag{61}$$

Applying (14) to (61) and defining $r_i := r(\mu_i)$ (for the sake of notation) yields

$$r_i \leq r_{i-1} - \kappa^{(1)} r_{i-1}^{\theta} \quad \text{for} \quad \kappa^{(1)} := \omega\beta_1 \tag{62}$$

for the constant $\omega = (8e\alpha^*)^{-1}\tau$. In the cases (51) corresponding to β_2 and β_3, similar applications of the previous identities (along with (59)) give

$$r_i \leq r_{i-1} - \kappa^{(2)} r_{i-1}^{2\theta} \quad \text{for} \quad \kappa^{(2)} := \omega\tau(1-\alpha/2)\beta_2 \tag{63}$$

$$r_i \leq r_{i-1} - \kappa^{(3)} r_{i-1}^{\alpha^*\theta} \quad \text{for} \quad \kappa^{(3)} := \omega\left(\tau(1-\alpha/2)\right)^{1/\alpha}\beta_3 \tag{64}$$

Now, for the sake of notation, define the function

$$z(u,v) := u^{-1}\epsilon^{-(1-v)_-}\left(r_0 \log^{1/(1-v)}(r_0/\epsilon)\right)^{(1-v)_+}$$

where $(\cdot)_+$ and $(\cdot)_-$ denote the positive and negative parts. Using Lemma 3, it follows that, if (62) occurs for more than $\omega^{-1}z(\beta_1,\theta)$ iterations of Algorithm 1, then $r_k \leq \epsilon$, where k is the index of the last loop iteration in Algorithm 1. Similar deductions for (63) and (64) lead to the conclusion that, if

$$k \geq \omega^{-1}\left(z(\beta_1,\theta) + z(\tau(1-\alpha/2)\beta_2, 2\theta) + z((\tau(1-\alpha/2))^{1/\alpha}\beta_3, \alpha^*\theta)\right) := M \tag{65}$$

then either (62), (63), or (64) has occurred sufficiently many times during the execution of Algorithm 1 to guarantee $r_k \leq \epsilon$. As k has been chosen exactly so that $k = \lceil M \rceil$ (50), one obtains that μ_k satisfies (16). The desired complexity bound (17) on M now follows by plugging in for β_1, β_2, and β_3 in (65) and then, taking asymptotic estimates as $\epsilon \to 0$; the term $z((\tau(1-\alpha/2))^{1/\alpha}\beta_3, \alpha^*\theta)$ clearly dominates. □

C Computational solution of the Frank-Wolfe problem (15)

This section provides a concrete, computational procedure and complexity guarantee for the subroutine (15) in Algorithm 1 which, for $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, requires solution of the problem

$$\inf_{\nu \in \mathcal{P}_2(\mathbb{R}^d), \mathcal{W}(\nu,\mu) \leq \delta} \int f \, d\nu \tag{66}$$

The starting point to solve this problem is duality. The dual of (66) is

$$D(f) := \sup_{\lambda \in \mathbb{R}_+} \left[\int_{\mathbb{R}^d} f_\lambda(x)\, d\mu(x) - (\delta^2\lambda)/2\right], \qquad \text{where } f_\lambda(x) := \inf_{y \in \mathbb{R}^d} f(y) + \frac{\lambda}{2}\|x-y\|^2 \tag{67}$$

where f_λ is the Moreau-Yosida envelope [62] for f. The problem (67) permits practical computation since it requires only finite dimensional optimization procedures to calculate f_λ and perform ascent in λ. Moreover, strong duality between (66) and (67) holds under quite general circumstances [6] and, particularly for any of the circumstances in this work where f is assumed to be smooth.

Previous work [6, 54] has noted that, in general, solution of (67) might still be computationally infeasible for smooth f; for arbitrary λ, f_λ could obscure a computationally difficult problem with many local minima. However, for large enough λ, f_λ is quite computable since it's defining minimization problem becomes convex. So long as all relevant λ in (67) are large enough, this means that (67) will be efficiently computable. This is equivalent to ensuring that the trust-region size δ in (66) is not too large.

With the following results, we establish a bound on δ which is simultaneously small enough to achieve computational tractability for (67), but large enough to permit the iterative complexities of Theorem 1. Algorithms 2 and 3 are also provided to leverage these results and yield a computational procedure with concrete complexity for solving (66). For simplicity, rewrite (67) as

$$D(f) = \sup_{\lambda \in \mathbb{R}} \; g(\lambda) - \left(\delta^2 \lambda\right)/2, \qquad \text{where } g(\lambda) := \int_{\mathbb{R}^d} f_\lambda \, d\mu \tag{68}$$

Recall that a function $\phi : \mathbb{R}^d \to \bar{\mathbb{R}}$ is called *semiconvex* if

$$x \longrightarrow \phi(x) + \frac{\lambda}{2} \left\| x - x_0 \right\|^2 \tag{69}$$

is convex for some $\lambda \geq 0$ and some $x_0 \in \mathbb{R}^d$. Further, a continuously differentiable function ϕ is called L-smooth if it has L-Lipschitz gradients:

$$\left\| \nabla \phi(y) - \nabla \phi(x) \right\| \leq L \left\| y - x \right\| \tag{70}$$

Lemma 4. *If f is differentiable and ρ_*-semiconvex* (69)*, the function g* (68) *is differentiable on (ρ_*, ∞) and*

$$g'(\lambda) = \frac{1}{2} \int_{\mathbb{R}^d} \left\| y^*_{\lambda,x} - x \right\|^2 d\mu(x), \quad y^*_{\lambda,x} := \arg\min_{y \in \mathbb{R}^d} f(y) + \frac{\lambda}{2} \left\| y - x \right\|^2 \tag{71}$$

where the unique minimizer $y^*_{\lambda,x}$ satisfies

$$\frac{1}{2} \left\| y^*_{\lambda,x} - x \right\|^2 \leq \frac{2}{\left(\lambda - \rho_*\right)^2} \left\| \nabla f(x) \right\|^2 \tag{72}$$

Additionally, for any $\rho_* < \lambda_1 \leq \lambda_2$ one has

$$\left(1 - 2\sqrt{\frac{\lambda_2 - \lambda_1}{\lambda_2 - \rho_*}} \right) g'(\lambda_1) \leq g'(\lambda_2) \tag{73}$$

That is, for any $t^* > \rho_*$, g' is $1/2$-Holder continuous on $[t^*, \infty)$ with a constant depending only on t^* and ρ_*.

Proof. Define the functions

$$a_\lambda(y; x) := f(y) + \frac{\lambda}{2} \left\| y - x \right\|^2 \qquad \text{and} \qquad z_x(\lambda) := \inf_{y \in \mathbb{R}} a_\lambda(y; x)$$

Since f is ρ_*-semiconvex (69), $a_\lambda(y; x)$ is $\lambda - \rho_*$ strongly convex in y for $\lambda > \rho_*$. Therefore, the minimizer $y_{\lambda,x}$ is unique. Further, semiconvexity and differentiability of f provide the lower bound

$$a_\lambda(y; x) \geq f(x) + l_\lambda(y; x) \qquad \text{where} \qquad l_\lambda(y; x) := \nabla f(x)^T (y - x) + \frac{\lambda - \rho_*}{2} \left\| y - x \right\|^2$$

Noticing $l_\lambda(y; x) > 0$ for any $y \in \mathbb{R}^d$ such that $\left\| y - x \right\| > \left(2 \left\| \nabla f(x) \right\|\right) / \left(\lambda - \rho_*\right)$, one obtains (72).

For open subsets $O \subset (\rho_*, \infty)$ whose closure does not contain ρ_*, (72) implies that the radius of the ball containing $y^*_{\lambda,x}$ is uniformly bounded for all $\lambda \in O$. Danskin's theorem [30] can, therefore, be

applied to the function $z_x(\lambda) := f_\lambda(x)$ (67) to conclude that $z_x(\lambda)$ is differentiable on (ρ_*, ∞) with derivative

$$z_x'(\lambda) = \frac{1}{2}\left\|y_{\lambda,x}^* - x\right\|^2$$

Observing that $g(\lambda) = \mathbb{E}_{x\sim\mu}\left[z_x(\lambda)\right]$, the conclusion (71) then follows from (72) and dominated convergence.

Finally, let $\rho_* < \lambda_1 \leq \lambda_2$. Since $z_x(\lambda)$ is concave in λ

$$|z_x'(\lambda_1) - z_x'(\lambda_2)| = z_x'(\lambda_1) - z_x'(\lambda_2)$$

and it is enough to show a one-sided bound on the quantity $z_x'(\lambda_1) - z_x'(\lambda_2)$. To this end, observe

$$z_x'(\lambda_1) - z_x'(\lambda_2) \leq \left\|y_{\lambda_1,x}^* - x\right\| \left\|y_{\lambda_2,x}^* - y_{\lambda_1,x}^*\right\| \tag{74}$$

Hence, (73) can be provided by producing a bound on $\left\|y_{\lambda_2,x}^* - y_{\lambda_1,x}^*\right\|$. Strong convexity of $a_\lambda(y;x)$ in y yields the identity

$$a_{\lambda_2}(y_{\lambda_2,x}^*;x)+\frac{\lambda_2-\rho_*}{2}\left\|y_{\lambda_2,x}^* - y_{\lambda_1,x}^*\right\|^2 \leq a_{\lambda_2}(y_{\lambda_1,x}^*;x) = a_{\lambda_1}(y_{\lambda_1,x}^*;x)+\frac{\lambda_2-\lambda_1}{2}\left\|y_{\lambda_1,x}^* - x\right\|^2$$

which, when combined with the fact that $a_{\lambda_1}(y_{\lambda_1,x}^*;x) \leq a_{\lambda_2}(y_{\lambda_1,x}^*;x)$ ($z_x(\lambda)$ is non-decreasing in λ), gives

$$\left\|y_{\lambda_2,x}^* - y_{\lambda_1,x}^*\right\| \leq \sqrt{\frac{\lambda_2-\lambda_1}{\lambda_2-\rho_*}}\left\|y_{\lambda_1,x}^* - x\right\| \tag{75}$$

Applying (75) to (74) and rearranging produces

$$\left(1 - 2\sqrt{\frac{\lambda_2-\lambda_1}{\lambda_2-\rho_*}}\right) z_x'(\lambda_1) \leq z_x'(\lambda_2) \tag{76}$$

Taking the expectation with respect to x on both sides of (76) yields (73). □

Lemma 5. *If f is L-smooth* (70) *and $L < \lambda$ then any optimizer*

$$f(y^*) + \frac{\lambda}{2}\left\|y^* - x\right\|^2 = \inf_{y\in\mathbb{R}^d} f(y) + \frac{\lambda}{2}\left\|y - x\right\|^2$$

satisfies $\left\|y^* - x\right\| \geq \frac{\left\|\nabla f(x)\right\|}{2\lambda}$.

Proof. From L-smoothness and the fact $\lambda > L$, the function

$$v(y) := f(y) + \frac{\lambda}{2}\left\|y - x\right\|^2$$

is $(\lambda - L)$-strongly convex. To show $\left\|\nabla f(x)\right\| / (2\lambda) \leq \left\|y^* - x\right\|$ notice

$$\nabla f(y^*) + \lambda(y^* - x) = 0 \tag{77}$$

by first-order optimality conditions for y^*. Combining (77) with the L-smoothness of f, one obtains

$$\begin{aligned}&\left\|\nabla f(x) - \nabla f(y^*)\right\|^2 \leq L^2\left\|x - y^*\right\|^2\\ \Rightarrow\ &\left\|\nabla f(x)\right\|^2 + \left(\lambda^2 - L^2\right)\left\|x - y^*\right\|^2 \leq 2\lambda\nabla f(x)^T(x - y^*) \leq 2\lambda\left\|\nabla f(x)\right\|\left\|x - y^*\right\|\end{aligned} \tag{78}$$

Using the fact that $\lambda > L$, the desired result then follows directly from (78). □

The properties provided by Lemma 4 and Lemma 5 now enable establishment of a relationship between trust region size δ (66) and the decision variables in (67).

Proposition 3. *If f is differentiable and ρ_*-semiconvex then, for any $\epsilon > 0$, there exists a $\lambda_\epsilon \leq \rho_* + \left\|\nabla f(x)\right\|_{L^2(\mu)}^2 / (2\epsilon)$ such that*

$$\left(\sup_{\lambda\in\mathbb{R}} g(\lambda) - \left(\delta^2\lambda\right)/2\right) - \left(g(\lambda_\epsilon) - \left(\delta^2\lambda_\epsilon\right)/2\right) \leq \epsilon \tag{79}$$

Further, if f is L-smooth (70) *and $\delta = \left\|\nabla f(x)\right\|_{L^2(\mu)} / C$ for $C \geq 2L$, then λ_ϵ can be chosen in the interval $[l, u] \subseteq \mathbb{R}$ for*

$$l = \rho_* \quad \text{and} \quad u = \min\left(\beta, \rho_* + C\right) \tag{80}$$

where $\beta = \rho_* + \left\|\nabla f(x)\right\|_{L^2(\mu)}^2 / (2\epsilon)$

Proof. For any $\hat{\lambda} \geq \rho_*$, ρ_*-semiconvexity of f and the definition of g (68) provide the lower and upper bounds

$$g(\hat{\lambda}) = \int_{\mathbb{R}^d} f_{\hat{\lambda}} \, d\mu \geq \int_{\mathbb{R}^d} f \, d\mu - \frac{\|\nabla f(x)\|^2_{L^2(\mu)}}{2(\hat{\lambda} - \rho_*)} \qquad \text{and} \qquad g(\lambda) \leq \int f \, d\mu, \;\; \forall \lambda \in \mathbb{R}$$

These allow one to obtain the identity

$$g(\hat{\lambda}) - \left(\delta^2 \hat{\lambda}\right)/2 \geq \left(g(\lambda) - \left(\delta^2 \lambda\right)/2\right) - \frac{\|\nabla f(x)\|^2_{L^2(\mu)}}{2(\hat{\lambda} - \rho_*)} + \frac{\delta^2\left(\lambda - \hat{\lambda}\right)}{2} \tag{81}$$

for any $\hat{\lambda} \geq \rho_* \geq 0$. Via (81), Proposition 3 can be easily established; indeed let us first show (79).

Define $\lambda_n \in \mathbb{R}$ to be an optimizing sequence for (68)

$$\lim_{n\to\infty} g(\lambda_n) - \left(\delta^2 \lambda_n\right)/2 = D(f)$$

and set $\beta := \rho_* + \|\nabla f(x)\|^2_{L^2(\mu)}/(2\epsilon)$. Since g is upper-semicontinuous, it is sufficient to show that there exists a $\lambda_\epsilon \leq \beta$ satisfying (79) if $\beta < \liminf\limits_{n\to\infty} \lambda_n$. Since $\beta < \liminf_{n\to\infty} \lambda_n$, one can assume without loss of generality that $\beta < \lambda_n$ for all $n \in \mathbb{N}$. Substituting $\hat{\lambda} = \beta$ and $\lambda = \lambda_n$ in (81) simplifying provides

$$g(\beta) - \left(\delta^2 \beta\right)/2 \geq g(\lambda_n) - \left(\delta^2 \lambda_n\right)/2 - \epsilon \tag{82}$$

Taking the limit in (82) and setting $\lambda_\epsilon = \beta$ gives the desired result (79).

To show the second half of Proposition 3, observe that the previous result implies one can assume $\liminf_{n\to\infty} \lambda_n \leq \beta$ for an optimizing sequence λ_n– otherwise, β is ϵ-optimal. The immediate consequence of this assumption is that an optimizer λ^* of (68) exists. Indeed, L-smoothness of f provides $g(\lambda) = -\infty$ for any $\lambda < -L$ and, combined with $\liminf_{n\to\infty} \lambda_n \leq \beta$, the optimizing sequence λ_n can be assumed to be bounded. Via Bolzano-Weierstrauss, the sequence is therefore convergent to some $\lambda^* \leq \beta$ and upper-semicontinuity of g along with lower-semicontinuity of ψ^* then imply that λ^* is an optimizer of (68).

The main consequence of the existence of λ^* is that, in combination with (81), one has the upper bound

$$\begin{aligned}
\frac{\delta^2(\lambda^* - \lambda)}{2} - \frac{1}{2(\lambda - \rho_*)_+}\|\nabla f(x)\|^2_{L_2(\mu)} + g(\lambda^*) - \left(\delta^2 \lambda^*\right)/2 \leq g(\lambda) - \left(\delta^2 \lambda\right)/2 \\
\Rightarrow \quad \frac{\delta^2\left(\lambda^* - \lambda\right)}{2} \leq \frac{\|\nabla f(x)\|^2_{L_2(\mu)}}{2(\lambda - \rho_*)_+} \\
\Rightarrow \quad \delta^2(\lambda - \rho_*)_+\left(\lambda^* - \lambda\right) \leq \|\nabla f(x)\|^2_{L_2(\mu)}
\end{aligned} \tag{83}$$

if $\lambda \leq \lambda^*$. Taking $\lambda = (\lambda^* + \rho_*)/2$ above will lead to the desired conclusion of Proposition 3– so long as $\rho_* \leq \lambda^*$. To show that $C \geq 4L$ implies $\rho_* \leq \lambda^*$, observe that Lemma 5, in combination with Lemma 4, implies

$$\frac{1}{8\lambda^2}\|\nabla f(x)\|^2_{L^2(\mu)} \leq \partial_+ g(\lambda), \quad \lambda \geq L \tag{84}$$

where $\partial_+(\cdot)$ denotes the derivative of g from the right. Under $C \geq 4L$, (84) produces the relation

$$\frac{\delta^2}{2} \leq \frac{1}{8L^2}\|\nabla f(x)\|^2_{L^2(\mu)} \leq \partial_+ g(L) \leq \partial_+ g(\rho_*) \tag{85}$$

since $\rho_* \leq L$. As g is concave, (85) immediately gives $g(\rho_*) - \left(\delta^2 \rho_*\right)/2 \geq g(\lambda) - \left(\delta^2 \lambda\right)/2$ for all $\lambda < \rho_*$. Hence, λ^* can be chosen so that $\rho_* \leq \lambda^*$. Finally, using the fact that $\rho_* \leq \lambda^*$ and substituting $\lambda = (\lambda^* + \rho_*)/2$ into (83), one obtains

$$\lambda^* \leq \rho_* + \left(\frac{4\|\nabla f(x)\|^2_{L^2(\mu)}}{\delta^2}\right)^{1/2} \leq \rho_* + C \tag{86}$$

After combining (86) with the bounds $\rho_* \leq \lambda^*$ and $\lambda^* \leq \beta$, the final conclusion of Proposition 3 follows. □

With the bounds of Proposition 3 in hand, a suitable gradient oracle for g (68) can be provided.

Definition 5 (Gradient oracle with high probability)**.** A function $\theta_g : \mathbb{R} \to \mathbb{R}$ is called a (ϵ, γ)-gradient oracle *with high probability* for g if, when queried with a λ, it returns an independent random sample $\theta_g(\lambda)$ satisfying

$$\mathbb{P}\left(\left[|\theta_g(\lambda) - g'(\lambda)| \geq \frac{\epsilon}{\max(\lambda - l, 1)}\right]\right) \leq \gamma \tag{87}$$

Algorithm 2 Gradient oracle for g (68)

Input: Distribution μ, point λ, semi-convexity parameter ρ_*, smoothness parameter L, error tolerance ϵ

Sample $x \sim \mu$

$y_0 \leftarrow x$, $\kappa \leftarrow \sqrt{(\lambda + L)/(\lambda - \rho_*)}$

$k \leftarrow \max\left(\lceil 4\kappa \log(12\kappa \left\|\nabla f(x)\right\| / \epsilon)\rceil, 0\right)$

for $1 \leq i \leq k$ **do**

$z_i = y_{i-1} - \frac{1}{\kappa}\left(\nabla f(y_{i-1}) + \lambda(y_{i-1} - x)\right)$

$y_i = z_i + \frac{\kappa - 1}{\kappa + 1}\left(z_i - z_{i-1}\right)$

return $\theta = \frac{1}{2}\left\|y_k - x\right\|^2$

Proposition 4. *For a ρ_*-semiconvex function $f : \mathbb{R}^d \to \mathbb{R}$, which is also $L \geq \rho_*$ smooth* (70)*, the mean of*

$$K \geq \frac{64\left\|\nabla f(x)\right\|_{L^4(\mu)}^4}{(\lambda - \rho_*)^2 \min\left((\lambda - \rho_*)^2, 1\right)\gamma\tilde{\epsilon}^2} \tag{88}$$

independent calls to Algorithm 2 with inputs $\lambda > \rho_*$ and $\epsilon = \tilde{\epsilon}/(2\max(\lambda - \rho_*, 1))$, provides a $(\tilde{\epsilon}, \gamma)$-gradient oracle with high probability (5) *on the interval (ρ_*, ∞).*

Proof. Consider the sample x which is computed by Algorithm 2. In light of Lemma 4, it is clear that

$$\theta^* := \frac{1}{2}\left\|y_{\lambda,x}^* - x\right\|^2$$

is an unbiased estimate of $g'(\lambda)$. Hence, to prove establish Proposition 4, it will first be shown that the output of Algorithm 2, θ, satisfies

$$|\theta - \theta^*| \leq \epsilon \quad \text{and} \quad \theta \leq \left(\frac{4\left\|\nabla f(x)\right\|}{\lambda - \rho_*}\right)^2 \tag{89}$$

when $\lambda \in (\rho_*, \infty)$.

To this end, notice that Algorithm 2 performs Nesterov's accelerated gradient descent [48] on the $\lambda - \rho_*$-strongly convex and $\lambda + L$-smooth function $a_\lambda(y; x)$. Strong convexity yields the identity

$$\frac{\lambda - \rho_*}{2}\left\|y_{\lambda,x}^* - y\right\|^2 \leq a_\lambda(y; x) - a_\lambda(y_{\lambda,x}^*; x) \tag{90}$$

while the convergence guarantees of accelerated gradient descent [48, Theorem 2.2.3] give

$$a_\lambda(y_k; x) - a_\lambda(y_{\lambda,x}^*; x) \leq \left(1 - \kappa^{-1}\right)^k (\lambda + L)\left\|y_{\lambda,x}^* - x\right\|^2 \tag{91}$$

for $\kappa = \sqrt{(\lambda + L)/(\lambda - \rho_*)}$. Combining these relations and setting $C = 2\left\|\nabla f(x)\right\|/(\lambda - \rho_*)$

$$\left\|y_{\lambda,x}^* - y_k\right\|^2 \leq \frac{2\left(a_\lambda(y_k; x) - a_\lambda(y_{\lambda,x}^*; x)\right)}{\lambda - \rho_*} \leq 2\left(1 - \kappa^{-1}\right)^k \kappa^2\left\|y_{\lambda,x}^* - x\right\|^2 \leq 2\left(\frac{\epsilon}{6C}\right)^2 \tag{92}$$

since $k \geq 4\kappa \log(6\kappa C/\epsilon)$ and $\left\|y_{\lambda,x}^* - x\right\| \leq C$ via (72). Completing the analysis,

$$|\theta - \theta^*| = \frac{1}{2}\left|\left\|y_k - x\right\|^2 - \left\|y_{\lambda,x}^* - x\right\|^2\right| \leq \frac{1}{2}\left\|y_k - y_{\lambda,x}^*\right\|\left(\left\|y_k - x\right\| + \left\|y_{\lambda,x}^* - x\right\|\right) \tag{93}$$

$$\leq \frac{3}{2}\left\|y_k - y_{\lambda,x}^*\right\|\left\|y_{\lambda,x}^* - x\right\| \leq \epsilon \tag{94}$$

where triangle inequality provides both (93) and

$$\|y_k - x\| \leq 2 \left\|y^*_{\lambda,x} - x\right\| \leq 2C \tag{95}$$

Moreover, (94) is the desired left-hand inequality of (89) while (95) contains the desired right-hand inequality.

Establishing Proposition 4 is now a straightforward consequence of Chebyshev's inequality using (89). Indeed, one has

$$\left|\mathbb{E}\left[\theta\right] - g'(\lambda)\right| \leq \frac{\tilde{\epsilon}}{2\max\left(\lambda - \rho_*, 1\right)} \quad \text{and} \quad \theta \leq \frac{16}{(\lambda - \rho_*)^2} \left\|\nabla f(x)\right\|^2 \tag{96}$$

when $\epsilon = \tilde{\epsilon}/\left(2\max\left(\lambda - \rho_*, 1\right)\right)$. Letting $\bar{\theta}$ be the average of K independent calls to Algorithm 2, Chebyshev's inequality gives

$$\mathbb{P}\left(\left|\bar{\theta} - \mathbb{E}\left[\theta\right]\right| \geq \frac{\tilde{\epsilon}}{2\max(\lambda - \rho_*, 1)}\right) \leq \frac{64 \ \left\|\nabla f(x)\right\|^4_{L^4(\mu)}}{(\lambda - \rho_*)^2 \min\left(\left(\lambda - \rho_*\right)^2, 1\right) \tilde{\epsilon}^2 K} \leq \gamma \tag{97}$$

□

The supergradient oracle of Proposition 4 provides a mechanism to perform ascent steps in λ to solve (68). Indeed, one can now perform bisection ascent for this problem. For the sake of our Frank-Wolfe procedure, it is of importance that this ascent procedure implicitly maintains a primal-feasible iterate for

$$\inf_{\pi \in \Pi(\mu)} \int f \, d\pi + \psi\left(\int \frac{1}{2} \left\|y - x\right\|^2 \, d\pi\right) \tag{98}$$

and makes progress on the primal-dual gap between (98) and (67). For this reason, we title the algorithm a "primal-dual" algorithm.

Algorithm 3 Primal-dual, bisection ascent for (68)

Input: Supergradient oracle θ_g, error tolerance ϵ, termination width B
  $\eta \leftarrow \infty$, $b \leftarrow l$
  while $u - l > \epsilon/B$ **do**
    $\lambda \leftarrow (l + u)/2$
    $\eta \leftarrow \theta_g(\lambda)$, $\eta \leftarrow \left(\eta - \left(\psi^*\right)'(\lambda)\right)$
    if $\eta < -\epsilon/\max\left(\lambda - b, 1\right)$ **then** $u \leftarrow \lambda$
    else $l \leftarrow \lambda$
  return u

Remark 7. The primal iterate that this algorithm maintains can be clarified by recalling that the conditions of Proposition 3 guarantee that $\lambda^* > \rho_*$ for any ρ_*-semiconvex f and optimal λ^* in (67). Since the function $y \mapsto f(y) + \lambda/2 \left\|x - y\right\|^2$ is strictly convex for $\lambda > \rho_*$, the distribution given by

$$(X, m(X)) \sim \pi_{\lambda,\mu}, \qquad X \sim \mu, \quad m_\lambda(x) = \arg\min_{y \in \mathbb{R}^d} f(y) + \frac{\lambda}{2} \left\|y - x\right\|^2 \tag{99}$$

provide the unique coupling such that

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} f(y) + \frac{\lambda^*}{2} \left\|y - x\right\|^2 \, d\pi_{\lambda,\mu}(x, y) = \int_{\mathbb{R}^d} \min_{y \in \mathbb{R}^d} \left(f(y) + \frac{\lambda^*}{2} \left\|y - x\right\|^2\right) d\mu(x) \tag{100}$$

Through λ, Algorithm 3 implicitly maintains $\pi_{\lambda,\mu}$ and the criterion used for bisection of an interval in Algorithm 3 is designed to make progress on the primal-dual gap between the current dual iterate λ_i and $\pi_{\lambda_i,\mu}$:

$$G(\lambda_i) := \int f \, d\pi_{\lambda_i,\mu} + \infty \mathbf{1}_{(\delta,\infty)}\left(\int \left\|y - x\right\|^2 \, d\pi_{\lambda_i,\mu}\right) - \left(g(\lambda_i) - \left(\delta^2 \lambda_i\right)/2\right) \tag{101}$$

This stands contrary to other approaches [54] for solving (67) where the computed dual feasible iterate λ_i need not provide a primal feasible iterate.

Theorem 6. *If $\mu \in \mathcal{P}_2\left(\mathbb{R}^d\right)$, f is L-smooth* (70)*, and $\delta \leq \|\nabla f\|_{L^2(\mu)} / (2L)$, there exists a stochastic algorithm which (for any probability $\gamma < 1$) computes a λ^* such that $\mathcal{W}\left(\nu_{\lambda^*}, \mu\right) \leq \delta$ and*

$$\int f \, d\nu_{\lambda^*} - \inf_{\mathcal{W}(\nu,\mu)\leq\delta} \int f \, d\nu \leq \epsilon \tag{102}$$

where ν_{λ^*} is second marginal of $\pi_{\lambda^*,\mu}$ in (99)*. This algorithm requires at most $\widetilde{O}(L^2 \|\nabla f\|^4_{L^4(\mu)} / ((1-\gamma)\epsilon^2))$ independent samples from μ and executes $\widetilde{O}(L^{5/2} \|\nabla f\|^4_{L^4(\mu)} / ((1-\gamma)\epsilon^2))$ gradient evaluations of f in expectation.*

Lemma 7. *Under the assumptions of Theorem 6, let Algorithm 3 be run with a (ϵ, τ)-gradient oracle (Definition 5) and $B = 4(g'(l))^2$ on the interval $[l, u]$. Recalling* (99)*, if $1 \leq l - L$ and $g'(u) - \delta^2/2 \leq 0 \leq g'(l) - \delta^2/2$, the output λ^* of Algorithm 3 satisfies (recall* (101)*)*

$$G(\lambda^*) \leq (4 + l)\epsilon \tag{103}$$

with probability at least $1 - \tau\left(\log_2\left(B(u-l)/\epsilon\right) + 1\right)$.

Proof. Let λ_i, u_i, l_i and η_i denote the ith values of λ, u, l and η which are computed by Algorithm 3– the indexes l_0, u_0 denote the initial values of these variables. Let k denote the total number of iterations performed by the loop of Algorithm 3. Since $u_i - l_i = (u_{i-1} - l_{i-1})/2$, it is clear that $k \leq \log_2\left(B(u_0 - l_0)/\epsilon\right) + 1$. Thus, using (87) and the fact that λ_i depends only on $\theta_g(\lambda_j)$ for $j < i$, one obtains the union bound

$$\mathbb{P}\left(\bigcup_{i\leq k}\left[|\theta_g(\lambda_i) - g'(\lambda_i)| \geq \frac{\epsilon}{\max(\lambda_i - l_0, 1)}\right]\right) \leq \tau\left(\log_2\left(B(u_0 - l_0)/\epsilon\right) + 1\right) \tag{104}$$

Hence, it need only be shown that (103) holds when

$$|\theta_g(\lambda_i) - g'(\lambda_i)| \leq \frac{\epsilon}{\max\left(\lambda_i - l_0, 1\right)} \qquad \forall\, i \leq k \tag{105}$$

For brevity, set $\epsilon_{\lambda_i} = \epsilon / \max(\lambda_i - l_0, 1)$ and recall $\eta_i = \theta_g(\lambda_i) - \delta^2/2$. Define $\eta_i^* := g'(\lambda_i) - \delta^2/2$ to be the true supergradient of (68) which η_i approximates. From (105)

$$\eta_i \eta_i^* \leq 0 \qquad \Rightarrow \qquad \max\left(|\eta_i|, |\eta_i^*|\right) \leq \epsilon_{\lambda_i} \tag{106}$$

Hence, at all iterations prior to the last iteration (iteration k), η_i and η_i^* have the same sign. Since $\lambda \mapsto \left(g(\lambda) - \left(\delta^2\lambda\right)/2\right)$ is concave, this gives

$$\sup_{\lambda\in[l_i,u_i]} g(\lambda) - \left(\delta^2\lambda\right)/2 = \sup_{\lambda\in[l_{i-1},u_{i-1}]} g(\lambda) - \left(\delta^2\lambda\right)/2 \tag{107}$$

for all $1 < i < k$. Additionally, if $\eta_k \eta_k^* > 0$ then (107) also holds for $i = k$.

From Algorithm 3, it is clear that either $u_k = \lambda_i$ for some $i > 0$ such that $\eta_i < -\epsilon_{\lambda_i}$ or $u_k = u_0$. Similarly, $l_k = \lambda_j$ for some $j > 0$ such that $\eta_j \geq -\epsilon_{\lambda_j}$ or $l_k = l_0$. One can assume, without loss of generality, that $l_k = \lambda_j$ for some $j > 0$ and, in combination with (106) and $g'(u_0) - \delta^2/2 \leq 0 \leq g'(l_0) - \delta^2/2$, this gives

$$-\epsilon_{\lambda_j} \leq g'(l_k) - \delta^2/2 \quad \text{and} \quad g'(u_k) - \delta^2/2 \leq 0 \tag{108}$$

Thus,

$$G(u_k) = \int f \, d\pi_{u_k,\mu} - \left(g(u_k) - \left(\delta^2 u_k\right)/2\right) = u_k\left(\delta^2/2 - g'(u_k)\right)$$

and using (73), one obtains

$$\begin{aligned} G(u_k) &\leq u_k\left(\delta^2/2 - \left(1 - \frac{2}{\sqrt{u_k - \rho_*}}(u_k - l_k)^{1/2}\right) g'(l_k)\right) \\ &\leq u_k\epsilon_{\lambda_j} + \frac{2u_k(u_k - l_k)^{1/2}}{\sqrt{u_k - \rho_*}} g'(l_k) \end{aligned} \tag{109}$$

where the last inequality is a result of (108). To bound the first term on the left side of (109), notice that $l_k \neq l_0$ implies there exists a minimal $t > 0$ such that $l_t \neq l_0$. Clearly,

$$u_k \epsilon_{\lambda_j} = \frac{u_k \epsilon}{\max(\lambda_j - l_0, 1)} \leq \frac{u_k \epsilon}{\max(\lambda_t - l_0, 1)} \leq \epsilon \frac{u_t - l_0}{\max(\lambda_t - l_0, 1)} + l_0 \epsilon \leq (2 + l_0)\epsilon$$

Combining this with the termination condition

$$u_k - l_k \leq \frac{\epsilon}{B} \leq \frac{\epsilon}{4g(l_0)^2} \leq \frac{\epsilon}{4g(l_k)^2}$$

to bound the second term of (109), one obtains

$$T \leq (4 + l_0)\epsilon$$

□

Proof of Theorem 6. Let $l = L + 1$ and $u = L + 1 + 4L$ and apply Algorithm 3 to the interval $[l, u]$ with the supergradient oracle given by Proposition 4. Set the error tolerance used by Algorithm 3 to $\epsilon / (4 + L + 1)$ and the termination width to $B := 16 \|\nabla f(x)\|^4_{L^2(\mu)}$. Likewise, the error tolerance used in Proposition 4 should be be $\epsilon / (4 + L + 1)$ and the error probability should be $(1 - \gamma)/(\log_2 (B(u - l) (4 + L + 1) / \epsilon) + 1)$.

Under this setting of parameters, Lemma 7 establishes that the output of λ^* of Algorithm 3 satisfies

$$G(\lambda^*) \leq \epsilon \tag{110}$$

with probability γ so long as

$$g'(u) - \delta^2/2 \leq 0 \leq g'(l) - \delta^2/2 \tag{111}$$

To see that (111) is fulfilled for the chosen l and u, notice that the conditions of Theorem 6 guarantee that Lemma 4 holds. Hence, (85) gives

$$g'(l) - \delta^2/2 \geq 0$$

Similarly, (72) provides

$$g'(u) - \delta^2/2 \leq 2 \|\nabla f(x)\|^2_{L^2(\mu)} / (u - L)^2 - \delta^2/2 \leq \|\nabla f(x)\|^2_{L^2(\mu)} / \left(16L^2\right) - \delta^2/2 \leq 0$$

Hence, (111) holds and the output λ^* of Algorithm 3 obeys (110) with probability γ.

It remains to compute a bound on the number of samples from μ which are required by this procedure. Clearly, by the definition of Algorithm 3, at most $\lceil \log_2 (B(u - l) (4 + L + 1) / \epsilon) \rceil$ calls are made to the supergradient oracle given by Proposition 4. Via (88), this yields that at most

$$\frac{(8(4 + L + 1)(\log_2 (B(u - l) (4 + L + 1) / \epsilon) + 1))^2 \|\nabla f(x)\|^4_{L^4(\mu)}}{(1 - \gamma)\epsilon^2} \tag{112}$$

invocations of Algorithm 2 are performed with an error parameter which is at least $\epsilon / (2 (4 + L + 1) (\max (u - L, 1)))$. Since each invocation of Algorithm 2 requires a single sample of μ, it follows from (112) that

$$\widetilde{O}\left(\frac{L^2 \|\nabla f(x)\|^4_{L^4(\mu)}}{(1 - \gamma)\epsilon^2}\right)$$

samples are used by Algorithm 3– where $\widetilde{O}$ suppresses logarithmic factors in $L, C, M, \|\nabla f(x)\|^2_{L^2(\mu)}$, and ϵ.

Finally, to compute a bound on the expected number of gradient evaluations of f that are performed notice that, for an error parameter of ϵ, each of the k calls to Algorithm 2 (with error tolerance $\epsilon/(4(u - l))$) executes at most

$$t = \max\left(\left\lceil 4\kappa \log\left(\frac{48\kappa \|\nabla f(x)\| (u - l)}{\epsilon}\right)\right\rceil, 0\right)$$

gradient evaluations of f; x and κ are the random sample and condition number, respectively, which are used in Algorithm 2. Both x and κ are random variables, but $\kappa = ((\lambda + L)/(\lambda - \rho_*))^{1/2} \leq (1 + 2L)^{1/2}$ and (due to Jensen)

$$\mathbb{E}\left[\max\left(\log\left(z\right), 0\right)\right] \leq \log \mathbb{E}\left[\max\left(z, 1\right)\right]$$

for any non-negative random variable z. Hence, the expected number of gradient evaluations performed by Algorithm 2 obeys the bound

$$\mathbb{E}_\mu\left[t\right] \leq 4\left(1 + 2L\right)^{1/2} \log \mathbb{E}_\mu\left[\left(\max\left(\frac{48(1 + 2L)^{1/2}\left\|\nabla f(x)\right\|\left(u - l\right)}{\epsilon}, 1\right)\right]\right) \tag{113}$$

Summing over the k calls to Algorithm 2 and using the identity $u \leq l + 4L$, one obtains

$$\mathbb{E}_\mu\left[t\right] = \widetilde{O}\left(\frac{L^{5/2}\left\|\nabla f(x)\right\|_{L^4(\mu)}^4}{(1 - \gamma)\epsilon^2}\right)$$

□