Sinkhorn Barycenter via Functional Gradient Descent

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Abstract

In this paper, we consider the problem of computing the barycenter of a set of probability distributions under the Sinkhorn divergence. This problem has recently found applications across various domains, including graphics, learning, and vision, as it provides a meaningful mechanism to aggregate knowledge. Unlike previous approaches which directly operate in the space of probability measures, we recast the Sinkhorn barycenter problem as an instance of unconstrained functional optimization and develop a novel functional gradient descent method named Sinkhorn Descent (SD). We prove that SD converges to a stationary point at a sublinear rate, and under reasonable assumptions, we further show that it asymptotically finds a global minimizer of the Sinkhorn barycenter problem. Moreover, by providing a mean-field analysis, we show that SD preserves the weak convergence of empirical measures. Importantly, the computational complexity of SD scales linearly in the dimension \(d\) and we demonstrate its scalability by solving a 100-dimensional Sinkhorn barycenter problem.

1 Introduction

Computing a nonlinear interpolation between a set of probability measures is a foundational task across many disciplines. This problem is typically referred as the barycenter problem and, as it provides a meaningful metric to aggregate knowledge, it has found numerous applications. Examples include distribution clustering [Ye et al., 2017], Bayesian inference [Srivastava et al., 2015], texture mixing [Rabin et al., 2011], and graphics [Solomon et al., 2015], etc. The barycenter problem can be naturally cast as minimization of the average distance between the target measure (barycenter) and the source measures; and the choice of the distance metric can significantly impact the quality of the barycenter [Feydy et al., 2019]. In this regard, the Optimal Transport (OT) distance (a.k.a. the Wasserstein distance) and its entropy regularized variant (a.k.a. the Sinkhorn divergence) are the most suitable geometrically-faithful metrics, while the latter is more computational friendly. In this paper, we provide efficient and provable methods for the Sinkhorn barycenter problem.

The prior work in this domain has mainly focused on finding the barycenter by optimizing directly in the space of (discrete) probability measures. We can divide these previous methods into three broad classes depending on how the support of the barycenter is determined:

(i) The first class assumes a fixed and prespecified support set for the barycenter and only optimizes the corresponding weights [Stab et al., 2017] [Dvurechenskii et al., 2018] [Kroshnin et al., 2019]. Accordingly, the problem reduces to minimizing a convex objective subject to a simplex constraint. However, fixing the support without any prior knowledge creates undesired bias and affects the quality of the final solution. While increasing the support size (possibly exponentially in the dimension \(d\)) can help to mitigate the bias, it renders the procedure computationally prohibitive as \(d\) grows.

(ii) To reduce the bias, the second class considers optimizing the support and the weights through an alternating procedure [Cuturi and Doucet, 2014] [Claici et al., 2018]. Since the barycenter objective is...
We note that the computation complexity of SD we say a vector function $F$ Additionally, for a functional (iii) Unlike the aforementioned classes, Luise et al. [2019] recently proposed a conditional gradient SD validate the scalability of DF be written in the form

$$DF = \sum_{i=1}^{d} \left[ f \right]_{i}$$

Further, we show the efficiency and efficacy of SD by comparing it with prior art on several problems. We note that the computation complexity of SD depends linearly on the dimension $d$. We hence validate the scalability of SD by solving a 100-dimensional barycenter problem, which cannot be handled by previous methods due to their exponential dependence on the problem dimension.

**Notations.** Let $X \subseteq \mathbb{R}^d$ be a compact ground set, endowed with a symmetric metric $d$ space of probability measures and continuous functions on $X$. We denote the support for a probability measure $\alpha \in M(X)$ by $\text{supp}(\alpha)$ and use $\alpha - a.e.$ to denote "almost everywhere" w.r.t. $\alpha$.

For a vector $a \in \mathbb{R}^d$, we denote its $\ell_2$ norm by $\|a\|$. For a function $f : X \rightarrow \mathbb{R}$, we denote its $L^\infty$ norm by $\|f\|_{\infty} := \max_{x \in X} |f(x)|$ and denote its gradient by $\nabla f : X \rightarrow \mathbb{R}^d$. For a vector function $f : X \rightarrow \mathbb{R}^d$, we denote its $(2, \infty)$ norm by $\|f\|_{2, \infty} := \max_{x \in X} \|f(x)\|$. For an integer $n$, denote $[n] := \{1, \ldots, n\}$.

Given an RKHS $\mathcal{H}$ with a kernel function $k : X \times X \rightarrow \mathbb{R}$, we say a vector function $\psi = ([\psi]_1, \ldots, [\psi]_d) \in \mathcal{H}^d$ if each component $[\psi]_i$ is in $\mathcal{H}$. The space $\mathcal{H}$ has a natural inner product structure and an induced norm, and so does $\mathcal{H}^d$, i.e., $\langle f, g \rangle_{\mathcal{H}^d} = \sum_{i=1}^{d} \langle [f]_i, [g]_i \rangle_{\mathcal{H}}$, $\forall f, g \in \mathcal{H}^d$ and the norm $\|f\|_{\mathcal{H}^d} = \langle f, f \rangle_{\mathcal{H}^d}^{1/2}$. The reproducing property of the RKHS $\mathcal{H}$ reads that given $f \in \mathcal{H}^d$, one has $[f]_i(x) = \langle [f]_i, k_x \rangle_{\mathcal{H}}$ with $k_x(y) = k(x, y)$, which by Cauchy-Schwarz inequality implies that there exists some constant $M_\mathcal{H} > 0$ such that

$$\|f\|_{2, \infty} \leq M_\mathcal{H} \|f\|_{\mathcal{H}^d}, \forall f \in \mathcal{H}^d. \quad (1)$$

Additionally, for a functional $F : \mathcal{H}^d \rightarrow \mathbb{R}$, the Fréchet derivative of $F$ is defined as follows.

**Definition 1.1** (Fréchet derivative in RKHS). For a functional $F : \mathcal{H}^d \rightarrow \mathbb{R}$, its Fréchet derivative $DF[\psi]$ at $\psi \in \mathcal{H}^d$ is a function in $\mathcal{H}^d$ satisfying the following: For any $\xi \in \mathcal{H}^d$ with $\|\xi\|_{\mathcal{H}^d} < \infty$,

$$\lim_{\epsilon \to 0} \frac{F[\psi + \epsilon \xi] - F[\psi]}{\epsilon} = \langle DF[\psi], \xi \rangle_{\mathcal{H}^d}.$$

Note that the Fréchet derivative at $\psi$, i.e., $DF[\psi]$, is a bounded linear operator from $\mathcal{H}^d$ to $\mathbb{R}$. It can be written in the form $DF[\psi](\xi) = \langle DF[\psi], \xi \rangle_{\mathcal{H}^d}$ due to the Riesz–Fréchet representation theorem.
1.1 Related Work on Functional Gradient Descent

A related functional gradient descent type method is the Stein Variation Gradient Descent (SVGD) method by [Liu and Wang, 2016]. SVGD considers the problem of minimizing the Kullback–Leibler (KL) divergence between a variable distribution and a posterior p. Note that SVGD updates the positions of a set of N particles using the score function of the posterior p, i.e. \( \nabla \log p \). Consequently, it requires the access to the target distribution function. Later, [Liu, 2017] prove that SVGD has convergence guarantee in its continuous-time limit (taking infinitesimal step size) using infinite number of particles (\( N \to \infty \)). In comparison, SD is designed to solve the significantly more complicated Sinkhorn barycenter problem and has a stronger convergence guarantee. More precisely, while SD updates the measure using only a sampling machinery of the target measures (no score functions), it is guaranteed to converge sub-linearly to a stationary point when \( \alpha \) is a discrete measure using discrete time steps. This is in sharp contrast to the results for SVGD.

In another work, [Mroueh et al., 2019] considers minimizing the Maximum Mean Discrepancy (MMD) between a source measure and a variable measure. They solve this problem by incrementally following a Sobolev critic function and propose the Sobolev Descent (SD) method. To show the global convergence of the measure sequence generated by SD, [Mroueh et al., 2019] assumes the entire sequence satisfies certain spectral properties, which is in general difficult to verify. Later, [Arbel et al., 2019] consider the same MMD minimization problem from a gradient flow perspective. They propose two assumptions that if either one holds, the MMD gradient flow converges to the entire global solution. However, similar to [Mroueh et al., 2019], these assumptions have to be satisfied for the entire measure sequence. We note that the Sinkhorn barycenter is a strict generalization of the above MMD minimization problem and is hence much more challenging: By setting the number of source measures \( n = 1 \) and setting the entropy regularization parameter \( \gamma = \infty \), problem (4) degenerates to the special case of MMD. Further, the MMD between two probability measures has a closed form expression while the Sinkhorn Divergence can only be described via a set of optimization problems. Consequently, the Sinkhorn barycenter is significantly more challenging. To guarantee global convergence, the proposed SD algorithm only requires one of accumulation points of the measure sequence to be fully supported on \( \mathcal{X} \) with no restriction on the entire sequence.

2 Sinkhorn Barycenter

We first introduce the entropy-regularized optimal transport distance and its debiased version, a.k.a. the Sinkhorn divergence. Given two probability measures \( \alpha, \beta \in \mathcal{M}^1_\text{KL}(\mathcal{X}) \), use \( \Pi(\alpha, \beta) \) to denote the set of joint distributions over \( \mathcal{X}^2 \) with marginals \( \alpha \) and \( \beta \). For \( \pi \in \Pi(\alpha, \beta) \), use \( \langle c, \pi \rangle \) to denote the integral \( \int_{\mathcal{X}^2} c(x,y) d\pi(x,y) \) and use \( \text{KL}(\pi||\alpha \otimes \beta) \) to denote the Kullback-Leibler divergence between the candidate transport plan \( \pi \) and the product measure \( \alpha \otimes \beta \). The entropy-regularized optimal transport distance \( \text{OT}_\gamma(\alpha, \beta) : \mathcal{M}^1_\text{KL}(\mathcal{X}) \times \mathcal{M}^1_\text{KL}(\mathcal{X}) \to \mathbb{R}_+ \) is defined as

\[
\text{OT}_\gamma(\alpha, \beta) = \min_{\pi \in \Pi(\alpha, \beta)} \langle c, \pi \rangle + \gamma \text{KL}(\pi||\alpha \otimes \beta). \tag{2}
\]

Here, \( \gamma > 0 \) is a regularization parameter. Note that \( \text{OT}_\gamma(\alpha, \beta) \) is not a valid metric as there exists \( \alpha \in \mathcal{M}^1_\text{KL}(\mathcal{X}) \) such that \( \text{OT}_\gamma(\alpha, \alpha) \neq 0 \) when \( \gamma \neq 0 \). To remove this bias, [Peyré et al., 2019] introduced the Sinkhorn divergence \( \mathcal{S}_\gamma(\alpha, \beta) : \mathcal{M}^1_\text{KL}(\mathcal{X}) \times \mathcal{M}^1_\text{KL}(\mathcal{X}) \to \mathbb{R}_+ \):

\[
\mathcal{S}_\gamma(\alpha, \beta) := \text{OT}_\gamma(\alpha, \beta) - \frac{1}{2} \text{OT}_\gamma(\alpha, \alpha) - \frac{1}{2} \text{OT}_\gamma(\beta, \beta), \tag{3}
\]

which is a debiased version of \( \text{OT}_\gamma(\alpha, \beta) \). It is further proved that \( \mathcal{S}_\gamma(\alpha, \beta) \) is nonnegative, biconvex and metrizes the convergence in law when the ground set \( \mathcal{X} \) is compact and the metric \( c \) is Lipschitz. Now given a set of probability measures \( \{\beta_i\}_{i=1}^n \), the Sinkhorn barycenter is the measure \( \alpha \in \mathcal{M}^1_\text{KL}(\mathcal{X}) \) that minimizes the average of Sinkhorn divergences

\[
\min_{\alpha \in \mathcal{M}^1_\text{KL}(\mathcal{X})} \left( \mathcal{S}_\gamma(\alpha) := \frac{1}{n} \sum_{i=1}^n \mathcal{S}_\gamma(\alpha, \beta_i) \right). \tag{4}
\]

We will next focus on the properties of \( \text{OT}_\gamma \) since \( \mathcal{S}_\gamma(\alpha) \) is the linear combination of these terms.
We present the with appropriate initialization.

Algorithm 1 Sinkhorn Descent (SD)

Input: measures \( \{\beta_i\}_{i=1}^n \), a discrete initial measure \( \alpha^0 \), a step size \( \eta \), and number of iterations \( S \);
Output: A measure \( \alpha^S \) that approximates the Sinkhorn barycenter of \( \{\beta_i\}_{i=1}^n \);

for \( t = 0 \) to \( S - 1 \) do
    \( \alpha^{t+1} := \tau[\alpha^t] \alpha^t \), with \( \tau[\alpha^t] \) defined in (11);
end for

The Dual Formulation of \( \text{OT}_{\gamma} \). As a convex program, the entropy-regularized optimal transport problem \( \text{OT}_{\gamma} \) has a equivalent dual formulation, which is given as follows:

\[
\text{OT}_{\gamma}(\alpha, \beta) = \max_{f, g \in \mathcal{C}(X)} (f, \alpha) + (g, \beta) - \gamma \langle \exp((f \otimes g - c)/\gamma) - 1, \alpha \otimes \beta \rangle,
\]

where we denote \( [f \otimes g](x, y) = f(x) + g(y) \). The maximizers \( f_{\alpha, \beta} \) and \( g_{\alpha, \beta} \) of (5) are called the \textit{Sinkhorn potentials} of \( \text{OT}_{\gamma}(\alpha, \beta) \). Define the Sinkhorn mapping \( \mathcal{A} : \mathcal{C}(X) \times \mathcal{M}_1^+(X) \rightarrow \mathcal{C}(X) \) by

\[
\mathcal{A}(f, \alpha)(y) = -\gamma \log \int_X \exp \left( (f(x) - c(x, y))/\gamma \right) d\alpha(x).
\]

The following lemma states the optimality condition for the Sinkhorn potentials \( f_{\alpha, \beta} \) and \( g_{\alpha, \beta} \).

Lemma 2.1 (Optimality [Peyré et al., 2019]). The pair \((f, g)\) are the Sinkhorn potentials of the entropy-regularized optimal transport problem (5) if they satisfy

\[
f = \mathcal{A}(g, \beta), \alpha - a.e. \quad \text{and} \quad g = \mathcal{A}(f, \alpha), \beta - a.e.\tag{7}
\]

The Sinkhorn potential is the cornerstone of the entropy regularized OT problem. In the discrete case, it can be computed by a standard method in Genevay et al. [2016]. In particular, when \( \alpha \) is discrete, \( f \) can be simply represented by a finite dimensional vector since only its values on \( \text{supp}(\alpha) \) matter. We describe such method in Appendix A.1 for completeness. In the following, we treat the computation of Sinkhorn potentials as a blackbox, and refer to it as \( \mathcal{SP}_{\gamma}(\alpha, \beta) \).

3 Methodology

We present the Sinkhorn Descent (SD) algorithm for the Sinkhorn barycenter problem ([1]) in two steps: We first reformulate ([1]) as an unconstrained functional minimization problem and then derive the descent direction as the negative functional gradient over a RKHS \( \mathcal{H}^d \). Operating in RKHS allows us to measure the quality of the iterates using a so-called kernelized discrepancy which we introduce in Definition 4.1. This quantity will be crucial for our convergence analysis. The restriction of a functional optimization problem to RKHS is common in the literature as discussed in Remark 3.1.

Alternative Formulation. Instead of directly solving the Sinkhorn barycenter problem in the probability space \( \mathcal{M}_1^+(X) \), we reformulate it as a functional minimization over all mappings on \( X \):

\[
\min_{\mathcal{P}} \left( \mathcal{S}_\gamma(\mathcal{P}_2\alpha_0) := -\frac{1}{n} \sum_{i=1}^n \mathcal{S}_\gamma(\mathcal{P}_2\alpha_0, \beta_i) \right),
\]

where \( \alpha_0 \in \mathcal{M}_1^+(X) \) is some given initial measure, and \( \mathcal{P}_2\alpha \) is the push-forward measure of \( \alpha \in \mathcal{M}_1^+(X) \) under the mapping \( \mathcal{P} : X \rightarrow X \). When \( \alpha_0 \) is sufficiently regular, e.g. absolutely continuous, for any \( \alpha \in \mathcal{M}_1^+(X) \) there always exists a mapping \( \mathcal{P} \) such that \( \alpha = \mathcal{P}\alpha_0 \) (see Theorem 1.33 of [Ambrosio and Gigli, 2013]). Consequently, problems (8) and (3) are equivalent with appropriate initialization.

Algorithm Derivation. For a probability measure \( \alpha \), define the functional \( \mathcal{S}_\alpha : \mathcal{H}^d \rightarrow \mathbb{R} \)

\[
\mathcal{S}_\alpha[\psi] = \mathcal{S}_\gamma ((I + \psi_\gamma)\alpha), \psi \in \mathcal{H}^d.
\]

Here \( I \) is the identity mapping and \( \mathcal{S}_\gamma \) is defined in (1). Let \( \alpha^t \) be the estimation of the Sinkhorn barycenter in the \( t^{th} \) iteration. Sinkhorn Descent (SD) iteratively updates the measure \( \alpha^{t+1} \) as

\[
\alpha^{t+1} = \tau[\alpha^t] \alpha^t,
\]

(10)
via the push-forward mapping (with \(\eta > 0\) being a step-size)

\[
\mathcal{T}[\alpha](x) = x - \eta \cdot DS_\alpha[0](x).
\]  

(11)

Recall that \(DS_\alpha[0]\) is the Fréchet derivative of \(S_\alpha\) at \(\psi = 0\) (see Definition 1.1). Note that \((I + \psi)\alpha = \alpha\) when \(\psi = 0\). Our choice of the negative Fréchet derivative in \(\mathcal{T}[\alpha]\) allows the objective \(S_\alpha(\alpha)\) to have the fastest descent at the current measure \(\alpha = \alpha^t\). We now line the details of SD in Algorithm 1.

Consequently, a solution of (8) will be found by finite-step compositions and then formally passing to the limit \(P = \lim_{t \to \infty} (\mathcal{T}[\alpha^t] \circ \cdots \circ \mathcal{T}[\alpha^0])\).

**Remark 3.1.** We restrict \(\psi\) in (9) to the space \(H^d\) to avoid the inherent difficulty when the perturbation of Sinkhorn potentials introduced by the mapping \((I + \psi)\) can no longer be properly bounded (for \(\psi \in H^d\), we always have the upper bound (1) which is necessary in our convergence analysis). This restriction will potentially introduce error to the minimization of (8). However, this restriction is a common practice for general functional optimization problems: Both SVGD [Liu and Wang, 2016] and SD [Mroueh et al., 2019] explicitly make such RKHS restriction on their transport mappings. [Arbel et al., 2019] constructs the transport mapping using the witness function of the Maximum Mean Discrepancy (MMD) which also lies in an RKHS.

In what follows, we first derive a formula for the Fréchet derivative \(DS_\alpha[0]\) (see (13)) and then explain how it is efficiently computed. The proof of the next proposition requires additional continuity study of the Sinkhorn potentials and is deferred to Appendix C.5.

**Proposition 3.1.** Recall the Fréchet derivative in Definition 1.1. Given \(\alpha, \beta \in \mathcal{M}^+_1(\mathcal{X})\), for \(\psi \in H^d\) denote \(F_1[\psi] = OT_\gamma((I + \psi)\alpha, \beta)\) and \(F_2[\psi] = OT_\gamma((I + \psi)^2\alpha, (I + \psi)\beta)\). Under Assumptions 4.1 and 4.2 (described below), we can compute

\[
DF_1[0](y) = \int_{\mathcal{X}} \nabla f_{\alpha,\beta}(x)k(x, y)d\alpha(x), \quad DF_2[0](y) = 2 \int_{\mathcal{X}} \nabla f_{\alpha,\beta}(x)k(x, y)d\alpha(x),
\]  

(12)

where \(\nabla f_{\alpha,\beta}\) and \(\nabla f_{\alpha,\alpha}\) are the gradients of the Sinkhorn potentials of \(OT_\gamma(\alpha, \beta)\) and \(OT_\gamma(\alpha, \alpha)\) respectively, and \(k\) is the kernel function of the RKHS \(H\).

Consequently the Fréchet derivative of the Sinkhorn Barycenter problem (9) can be computed by

\[
DS_\alpha[0](y) = \int_{\mathcal{X}} \frac{1}{n} \left( \sum_{i=1}^n \nabla f_{\alpha,\beta_i}(x) - \nabla f_{\alpha,\alpha}(x) \right)k(x, y)d\alpha(x).
\]  

(13)

This quantity can be computed efficiently when \(\alpha\) is discrete: Consider an individual term \(\nabla f_{\alpha,\beta}\).

Define \(h(x, y) := \exp \left( \frac{1}{\gamma} (f_{\alpha,\beta}(x) + \mathcal{A}[f_{\alpha,\beta}, \alpha](y) - c(x, y)) \right)\). Lemma 2.1 implies

\[
\int h(x, y)d\beta(y) = 1.
\]

Taking derivative with respect to \(x\) on both sides and rearranging terms, we have

\[
\nabla f_{\alpha,\beta}(x) = \frac{\int_{\mathcal{X}} h(x, y)\nabla_x c(x, y)d\beta(y)}{\int_{\mathcal{X}} h(x, y)d\beta(y)} = \int_{\mathcal{X}} h(x, y)\nabla_x c(x, y)d\beta(y),
\]  

(14)

which itself is an expectation. Note that to evaluate (13), we only need \(\nabla f_{\alpha,\beta}(x)\) on \(\text{supp}(\alpha)\). Using \(\mathcal{SP}_\gamma(\alpha, \beta)\) (see the end of Section 2), the function value of \(f_{\alpha,\beta}\) on \(\text{supp}(\alpha)\) can be efficiently computed. Together with the expression in (14), the gradients \(\nabla f_{\alpha,\beta}(x)\) at \(x \in \text{supp}(\alpha)\) can also be obtained by a simple Monte-Carlo integration with respect to \(\beta\).

**4 Analysis**

In this section, we analyze the finite time convergence and the mean field limit of SD under the following assumptions on the ground cost function \(c\) and the kernel function \(k\) of the RKHS \(H^d\).

**Assumption 4.1.** The ground cost function \(c(x, y)\) is bounded, i.e. \(\forall x, y \in \mathcal{X}, c(x, y) \leq M_c; c(x, y)\) is Lipschitz continuous, i.e. \(\forall x, x', y \in \mathcal{X}, |c(x, y) - c(x', y)| \leq G_c||x - x'||\); and \(c(x, y)\) is continuous, i.e. \(\forall x, x', y \in \mathcal{X}, |c(x, y) - c(x', y)| \leq G_c||x - x'||\).

**Assumption 4.2.** The kernel function \(k(x, y)\) is bounded, i.e. \(\forall x, y \in \mathcal{X}, k(x, y) \leq D_k; k(x, y)\) is Lipschitz continuous, i.e. \(\forall x, x', y \in \mathcal{X}, |k(x, y) - k(x', y)| \leq G_k||x - x'||\).
4.1 Finite Time Convergence Analysis

In this section, we prove that Sinkhorn Descent converges to a stationary point of problem (4) at the rate of \(O(\frac{1}{t})\), where \(t\) is the number of iterations. We first introduce a discrepancy quantity.

**Definition 4.1.** Recall the definition of the functional \(S_\alpha\) in (9) and the definition of Fréchet derivative in Definition 4.1. Given a probability measure \(\alpha \in \mathcal{M}_c^+(\mathcal{X})\), the Kernelized Sinkhorn Barycenter Discrepancy (KSBD) for the Sinkhorn barycenter problem is defined as

\[
S(\alpha, \{\beta_i\}_{i=1}^n):=\|DS_\alpha[0]\|_{L_c}^2.
\]  

(15)

Note that in each round \(t\), \(S(\alpha^t, \{\beta_i\}_i)\) metrizes the stationarity of SD, which can be used to quantify the per-iteration improvement.

**Lemma 4.1 (Sufficient Descent).** Recall the definition of the Sinkhorn Barycenter problem in (4) and the sequence of measures \(\{\alpha^t\}_{t\geq 0}\) in (10) generated by SD (Algorithm 1). Under Assumption 4.1, if we have \(\eta \leq \min\{1/(8L_f M_{Ht}^2), 1/(8 \sqrt{dL_f} M_{Ht}^2)\}\), the Sinkhorn objective always decreases,

\[
S_\gamma(\alpha_{t+1}) - S_\gamma(\alpha_t) \leq -\eta/2 \cdot S(\alpha^t, \{\beta_i\}_i)\).
\]  

(16)

See \(M_{Ht}\) in (1). \(L_f:=4G_c^2/\gamma + L_c\) and \(L_T:=2G_c^2 \exp(3M_c/\gamma)/\gamma\). The proof of the lemma is given Appendix C.7. Based on this result, we can derive the following convergence result demonstrating that SD converges to a stationary point in a sublinear rate.

**Theorem 4.1 (Convergence).** Suppose SD is initialized with \(\alpha^0 \in \mathcal{M}_c^+(\mathcal{X})\) and outputs \(\alpha^t \in \mathcal{M}_c^+(\mathcal{X})\) after \(t\) iterations. Under Assumption 4.1, we have

\[
\min_t S(\alpha^t, \{\beta_i\}_{i=1}^n) \leq 2S(\alpha^0)/(\eta t),
\]  

(17)

where \(0 < \eta \leq \min\{1/(8L_f M_{Ht}^2), 1/(8 \sqrt{dL_f} M_{Ht}^2)\}\) is the step size.

With a slight change to SD, we can conclude its last term convergence as elaborated in Appendix B.3.

4.2 Mean Field Limit Analysis

While Sinkhorn Descent accepts both discrete and continuous measures as initialization, in practice, we start from a discrete initial measure \(\alpha^0\) with \(|\text{supp}(\alpha^0)| = N\). If \(\alpha^0\) is an empirical measure sampled from an underlying measure \(\alpha^\infty\), we have the weak convergence at time \(t=0\), i.e. \(\alpha^0_N \to \alpha^\infty\) as \(N \to \infty\). The mean field limit analysis demonstrates that Sinkhorn Descent preserves such weak convergence for any finite time \(t\):

\[
\alpha^0_N \to \alpha^\infty \Rightarrow \alpha^t_N = SD^t(\alpha^0_N) \to \alpha^\infty = SD^t(\alpha^0),
\]

where we use \(SD^t\) to denote the output of SD after \(t\) steps and use \(\to\) to denote the weak convergence.

**Lemma 4.2.** Recall the push-forward mapping \(T[\alpha](x)\) in SD from (11) and recall \(L_f\) in Lemma 4.1. Under Assumptions 4.2 and 4.2, for two probability measures \(\alpha\) and \(\alpha'\), we have

\[
d_{bl}(T[\alpha]\alpha, T[\alpha']\alpha') \leq (1 + \eta C)d_{bl}(\alpha, \alpha'),
\]  

(18)

where \(C = G_cG_k + \max\{dL_f D_k + dG_cG_k, D_k L_b\}\) and \(L_b:=8G_c^2 \exp(6M_c/\gamma)\). The proof is presented in Appendix C.9. This is a discrete version of Dobrushin’s estimate (section 1.4 in [Golse 2016]). As a result, we directly have the following large N characterization of \(SD^t(\alpha^0_N)\).

**Theorem 4.2 (Mean Field Limit).** Let \(\alpha^0_N\) be an empirical initial measure with \(|\text{supp}(\alpha^0_N)| = N\) and let \(\alpha^\infty\) be the underlying measure such that \(\alpha^0_N \to \alpha^\infty\). Use \(SD^t(\alpha^0_N)\) and \(SD^t(\alpha^\infty)\) to denote the outputs of SD after \(t\) iterations, under the initializations \(\alpha^0_N\) and \(\alpha^\infty\) respectively. Under Assumptions 4.1 and 4.2, for any finite time \(t\), we have

\[
d_{bl}(SD^t(\alpha^0_N), SD^t(\alpha^\infty)) \leq (1 + \eta C)^td_{bl}(\alpha^0_N, \alpha^\infty),
\]

and hence as \(N \to \infty\) we have

\[
\alpha^t_N = SD^t(\alpha^0_N) \to \alpha^t = SD^t(\alpha^\infty).
\]

(19)

\[\text{We acknowledge the factor } \exp(1/\gamma) \text{ is non-ideal, but such quantity constantly appears in the literature related to the Sinkhorn divergence, e.g. Theorem 5 in [Luise et al. 2019] and Theorem 3 in [Genevay et al. 2019a]. It would be an interesting future work to remove this factor.}\]
4.3 KSBD as Discrepancy Measure

In this section, we show that, under additional assumptions, KSBD is a valid discrepancy measure, i.e. $S_\gamma(\alpha) = 0$ implies that $\alpha$ is a global optimal solution to the Sinkhorn barycenter problem \([4]\). The proof is provided in Appendix D. First, we introduce the following positivity condition.

**Definition 4.2.** A kernel $k(x, x')$ is said to be integrally strictly positive definite (ISPD) w.r.t. a measure $\alpha \in \mathcal{M}_1^+(\mathcal{X})$, if $\forall \xi : \mathcal{X} \to \mathbb{R}^d$ with $0 < \int_{\mathcal{X}} \|\xi(x)\|^2 \, d\alpha(x) < \infty$, it holds that

$$\int_{\mathcal{X}^2} \xi(x) k(x, x') \xi(x') \, d\alpha(x) \, d\alpha(x') > 0.$$  

(20)

**Theorem 4.3.** Recall the Fréchet derivative of the Sinkhorn Barycenter problem in \([13]\) and KSBD in \([15]\). Denote $\xi(x) := \frac{1}{n} \sum_{i=1}^n \left( \nabla f_{\alpha, \beta_i}(x) - \nabla f_{\alpha, \alpha}(x) \right)$. We have $\int_{\mathcal{X}} \|\xi(x)\|^2 \, d\alpha(x) < \infty$.

(i) If the kernel function $k(x, x')$ is ISPD w.r.t. $\alpha \in \mathcal{M}_1^+(\mathcal{X})$ and $\alpha$ is fully supported on $\mathcal{X}$, then the vanishing of KSBD, i.e. $S(\alpha, \{\beta_i\}_{i=1}^n) = 0$, implies that $\alpha$ globally minimizes problem \([4]\).

(ii) Use $\alpha^t$ to denote the output of SD after $t$ iterations. If further one of the accumulation points of the sequence $\{\alpha^t\}$ is fully supported on $\mathcal{X}$, then $\lim_{t \to \infty} S_\gamma(\alpha^t) = S_\gamma(\alpha^{*})$.

We show in Appendix \([D.2]\) under an absolutely continuous (a.c.) and fully supported (f.s.) initialization, $\alpha^t$ remains a.c. and f.s. for any finite $t$. This leads to our assumption in (i): One of the accumulation points of $\{\alpha^t\}$ is f.s.. However, to rigorously analyze the support of $\alpha^t$ in the asymptotic case ($t \to \infty$) requires a separate proof. Establishing the global convergence of the functional gradient descent is known to be difficult in the literature, even for some much easier settings compared to our problem \([4]\). For instance, \([Mroueh et al., 2019, Arbel et al., 2019]\) prove the global convergence of their MMD descent algorithms. Both works require additional assumptions on the entire measure sequence $\{\alpha^t\}$ as detailed in Appendix \([D.3]\). See also the convergence analysis of SVGD in \([Lu et al., 2019]\) under very strong assumptions of the score functions.

5 Experiments

We conduct experimental studies to show the efficiency and efficacy of Sinkhorn Descent by comparing with the recently proposed functional Frank-Wolfe method (FW) from \([Luise et al., 2019]\). Note that in round $t$, FW requires to globally minimize the nonconvex function $Q(x) := \sum_{i=1}^n f_{\alpha^t, \beta_i}(x) - f_{\alpha^t, \alpha^t}(x)$ in order to choose the next Dirac measure to be added to the support. Here, $f_{\alpha^t, \beta_i}$ and $f_{\alpha^t, \alpha^t}$ are the Sinkhorn potentials. Such operation is implemented by an exhaustive grid search so that FW returns a reasonably accurate solution. Consequently, FW is computationally expensive even for low dimensional problems and we only compare SD with FW in the first two image experiments, where $d = 2$. (the grid size used in FW grows exponentially with $d$.) Importantly, the size of the support $N$ affects the computational efficiency as well as the solution quality of both methods. A large support size usually means higher computational complexity but allows a more accurate approximation of the barycenter. However, since SD and FW have different support size patterns, it is hard to compare them directly. The support size of SD is fixed after its initialization while FW starts from an initial small-size support and gradually increases it during the optimization procedure. We hence fix the support size of the output measure from FW and vary the support size of SD for a more comprehensive comparison.

**Barycenter of Concentric Ellipses** We compute the barycenter of 30 randomly generated concentric ellipses similarly as done in \([Cuturi and Doucet, 2014, Luise et al., 2019]\). We run FW for 500 iterations and hence the output measure of FW has support size $N = 600$ (FW increases its support size by 1 in each iteration). SD is initialized with a discrete uniform distribution with support size varying from $N \in \{20, 40, 80\}$. Note that in these experiments the chosen support size for SD is even smaller than the initial support size of FW. The result is reported in Figure \([1a]\). In terms of convergence rate, we observe that SD is much faster than FW. Even 20 iterations are sufficient for SD to find a good solution. More importantly, in terms of the quality of the solution, SD with support size $N = 20$ outperforms FW with final support size $N = 600$. In fact, FW cannot find a solution with better quality even with a larger support size. This phenomenon is due to an inevitable limitation of the FW optimization procedure: Each FW step requires to globally minimize the non-convex function \([32]\) via

\[^{2}Claici et al., 2018\] is not included as it only applies to the Wasserstein barycenter problem ($\gamma = 0$).
Figure 1: $N$ is the support size. $\text{FW}$ is not included in (c) as it is impractical in high-dimensional problems (here, the dimension is 100).

Figure 2: Visual results of the ellipses and sketching problem.

Distribution Sketching We consider a special case of the barycenter problem where we only have one source distribution, similarly as done in [Luise et al. 2019]. This problem can be viewed as approximating a given distribution with a fixed support size budget and is hence called distribution sketching. Specifically, a natural image of a cheetah is used as the source measure in $\mathbb{R}^2$. We run $\text{FW}$ for 20000 iterations and the support size of $\text{SD}$ is $N \in \{2000, 4000\}$. The result is reported in Figure 1(b). Since we only have one source measure, the Sinkhorn barycenter loss is very small and hence we use log-scale in the $y$-axis. We can observe that $\text{SD}$ outperforms $\text{FW}$ in terms of the quality of the solution as well as the convergence rate.

Barycenter of Gaussians To demonstrate the efficiency of $\text{SD}$ on high dimensional problems, we consider the problem of finding the barycenter of multivariate Gaussian distributions. Concretely, we pick 5 isotropic Gaussians in $\mathbb{R}^{100}$ with different means. For each of them, we sample an empirical measure with 50000 points and used the obtained empirical measures as source measures. We initialize $\text{SD}$ with an empirical measure sampled from the uniform distribution with support size $N = 5000$. We did not compare with $\text{FW}$ as the global minimizer of $Q(x)$ can not be computed in $\mathbb{R}^{100}$. The result is reported in Figure 1(c). We can see that just like the previous two experiments, $\text{SD}$ converges in less than 20 iterations.

Visual Results on Ellipses and Sketching. To compare $\text{SD}$ with $\text{FW}$ visually, we allow $\text{SD}$ with $\text{FW}$ to have a similar amount of particles in the ellipses and sketching tasks, and report the results in Figure 2. Specifically, in $(a_1)$ $\text{SD}$ has 500 particles while in $(a_2)$ $\text{FW}$ has 511 to 591 particles (recall that the support size of $\text{FW}$ grows over iterations); in $(b_1)$ $\text{SD}$ has 8000 particles while in $(a_2)$ $\text{FW}$ has 10001 to 20001 particles. In all cases $\text{FW}$ has at least as much particles as $\text{SD}$ does while having significantly more steps. However, the visual result produced by $\text{SD}$ is clearly better than $\text{FW}$; in $(a_1)$, the circle is very clear in the last picture while in $(a_2)$ all pictures remain vague; in $(b_1)$, the eyes of cheetah are clear, but in $(b_2)$ the eyes remain gloomy.
6 Broader Impact

This work has the following potential positive impact in the society: We propose the first algorithm for the Sinkhorn barycenter problem that is scalable with respect to the problem dimension $d$ (linear dependence), while existing works all have an exponential dependence on $d$. Further, we expect that this functional gradient descent method can be applied to more general optimization problems involving distribution sampling: In principle, the negative gradient of the dual variables instructs the particles in the measure to search the landscape of the minimizer.

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A Preliminaries on the Sinkhorn Potentials

Lemma A.1 (Lemma A.2 elaborated). For a probability measure \( \alpha \in \mathcal{M}^+_1(X) \), use \( \alpha - a.e. \) to denote “almost everywhere w.r.t. \( \alpha \)”. The pair \((f, g)\) are the Sinkhorn potentials of the entropy-regularized optimal transport problem \((5)\) if they satisfy

\[
f = A(g, \beta), \quad \alpha - a.e. \quad \text{and} \quad g = A(f, \alpha), \quad \beta - a.e.,
\]

or equivalently

\[
\int_X h(x, y) d\beta(y) = 1, \quad \alpha - a.e., \tag{22}
\]

\[
\int_X h(x, y) d\alpha(x) = 1, \quad \beta - a.e., \tag{23}
\]

where \( h(x, y) := \exp \left( \frac{1}{\gamma} (f(x) + g(y) - c(x, y)) \right) \).

One can observe that the Sinkhorn potentials are not unique. In fact, for \( \alpha \neq \beta \), the pair \((f_{\alpha, \beta}, g_{\alpha, \beta})\) remains optimal under a constant shift, i.e. \((f_{\alpha, \beta} + C, g_{\alpha, \beta} - C)\) are still the Sinkhorn potentials of \( \text{OT}_{\gamma}(\alpha, \beta) \) for an arbitrary finite \( C \in \mathbb{R} \). Fortunately, it is proved in [Cuturi 2013] that the Sinkhorn potentials are unique up to such scalar translation.

To reduce the ambiguity, we fix an \( x_o \in X \) and choose \( f_{\alpha, \beta}(x_o) = 0 \), since otherwise we can always shift \( f_{\alpha, \beta} \) and \( g_{\alpha, \beta} \) by the amount of \( f_{\alpha, \beta}(x_o) \). While it is possible that \( x_o \notin \text{supp}(\alpha) \), such choice of \( f_{\alpha, \beta} \) is still feasible. This is because the Sinkhorn potentials can be naturally extended to the entire \( X \) from Lemma 2.1 even though the above optimality condition characterizes the Sinkhorn potentials on \( \text{supp}(\alpha), \text{supp}(\beta) \) only.

Further, this choice of \( f_{\alpha, \beta} \) allows us to bound \( \|f_{\alpha, \beta}\|_\infty \) given that the ground cost function \( c \) is bounded on \( X \).

Assumption A.1. The cost function \( c(x, y) \) is bounded: \( \forall x, y \in X, c(x, y) \leq M_c \).

Lemma A.2 (Boundness of the Sinkhorn Potentials). Let \((f, g)\) be the Sinkhorn potentials of problem \((5)\) and assume that there exists \( x_o \in X \) such that \( f(x_o) = 0 \) (otherwise shift the pair by \( f(x_o) \)). Then, under Assumption A.1, \( \|f\|_\infty \leq 2M_c \) and \( \|g\|_\infty \leq 2M_c \).

Next, we analyze the Lipschitz continuity of the Sinkhorn potential \( f_{\alpha, \beta}(x) \) with respect to \( x \).

Assumption A.2. The cost function \( c(x, y) \) is \( G_c \)-Lipschitz continuous with respect to one of its inputs:

\[
\forall x, x' \in X, |c(x, y) - c(x', y)| \leq G_c \|x - x'\|.
\]

Assumption A.2 implies that \( \nabla_x c(x, y) \) exists and for all \( x, y \in X, \|\nabla_x c(x, y)\| \leq G_c \). It further ensures the Lipschitz-continuity of the Sinkhorn potential.

Lemma A.3 (Proposition 12 of [Feydy et al. 2019]). Under Assumption A.2, for a fixed pair of measures \((\alpha, \beta)\), the Sinkhorn potential \( f_{\alpha, \beta} : X \rightarrow \mathbb{R} \) is \( G_c \)-Lipschitz continuous:

\[
\forall x, x' \in X, |f_{\alpha, \beta}(x) - f_{\alpha, \beta}(x')| \leq G_c \|x - x'\|.
\]

Further, the gradient \( \nabla f_{\alpha, \beta} \) exists at every point \( x \in X \), and \( \|\nabla f_{\alpha, \beta}(x)\| \leq G_c, \forall x \in X \).

Assumption A.3. The gradient of the cost function \( c \) is \( L_c \)-Lipschitz continuous: for all \( x, x' \in X \),

\[
\|\nabla_1 c(x, y) - \nabla_1 c(x', y)\| \leq L_c \|x - x'\|.
\]

Lemma A.4. Assume Assumptions A.2 and A.3, and denote \( L_f := 4G_c^2/\gamma + L_c \). For a pair of measures \((\alpha, \beta)\), the gradient of the corresponding Sinkhorn potential \( f_{\alpha, \beta} : X \rightarrow \mathbb{R} \) is Lipschitz continuous:

\[
\forall x, x' \in X, \|\nabla f_{\alpha, \beta}(x) - \nabla f_{\alpha, \beta}(x')\| \leq L_f \|x - x'\|.
\]

A.1 Computation of Sinkhorn Potentials

The Sinkhorn potential is the cornerstone of the entropy regularized OT problem \( \text{OT}_{\gamma}(\alpha, \beta) \). Hence, a key component of our method is to efficiently compute this quantity. An efficient method is given in [Genevay et al. 2016] when both \( \alpha \) and \( \beta \) are discrete measures (discrete case), as well as when \( \alpha \)
is discrete but $\beta$ is continuous (semi-discrete case). More precisely, by plugging in the optimality condition on $g$ in (7), the dual problem (5) becomes

$$OT_{\gamma}(\alpha, \beta) = \max_{f \in \mathbb{C}} \langle f, \alpha \rangle + \langle A(f, \alpha), \beta \rangle.$$  

(26)

Note that (26) only depends on the values of $f$ on the support of $\alpha$, supp($\alpha$), which can be represented by a finite dimensional vector $f \in \mathbb{R}^{\text{supp}(\alpha)}$. Viewing the discrete measure $\alpha$ as a weight vector $\omega_\alpha$ on supp($\alpha$), we have

$$OT_{\gamma}(\alpha, \beta) = \max_{f \in \mathbb{R}^d} \left\{ F(f) := f^T \omega_\alpha + E_{y \sim \beta} [A(f, \alpha)(y)] \right\},$$

that is, $OT_{\gamma}(\alpha, \beta)$ is equivalent to a standard concave stochastic optimization problem, where randomness of the problem comes from $\beta$ (see Proposition 2.1 in Genevay et al. [2016]). Hence, the problem can be solved using off-the-shelf stochastic optimization methods. In the main body, this method is referred as $SP_{\gamma}(\alpha, \beta)$. 

B Lipschitz Continuity of the Sinkhorn Potential

In this section, we provide several lemmas to show the Lipschitz continuity (w.r.t. the underlying probability measures) of the Sinkhorn potentials and the functional gradients we derived in Proposition 3.1. These lemmas will be used in the convergence analysis and the mean field analysis for SD.

B.1 Lipschitz Continuity Study: Sinkhorn Potentials

We first show the Lipschitz continuity of the Sinkhorn potential w.r.t. the bounded Lipschitz norm of the input measures. The bounded Lipschitz metric of measures $d_{bl} : M_1^+(\mathcal{X}) \times M_1^+(\mathcal{X}) \to \mathbb{R}_+$ with respect to the bounded continuous test functions is defined as

$$d_{bl}(\alpha, \beta) := \sup_{\|\xi\|_{Lip} \leq 1} |\langle \xi, \alpha \rangle - \langle \xi, \beta \rangle|,$$

where, given a function $\xi \in \mathcal{C}(\mathcal{X})$, we denote

$$\|\xi\|_{Lip} := \max \{ \|\xi\|_{\infty}, \|\xi\|_{lip} \}, \quad \text{with} \|\xi\|_{lip} := \max_{x,y \in \mathcal{X}} \frac{|\xi(x) - \xi(y)|}{\|x - y\|}.$$

We note that $d_{bl}$ metrizes the weak convergence of probability measures (see Theorem 1.12.4 in Van Der Vaart and Wellner [1996]), i.e. for a sequence of probability measures $\{\alpha_n\}$,

$$\lim_{n \to \infty} d_{bl}(\alpha_n, \alpha) = 0 \iff \alpha_n \rightharpoonup \alpha.$$

Lemma B.1. (i) Under Assumptions A.1 and A.2, for two given pairs of measures $(\alpha, \beta)$ and $(\alpha', \beta')$, the Sinkhorn potentials are Lipschitz continuous with respect to the bounded Lipschitz metric:

$$\|f_{\alpha,\beta} - f_{\alpha',\beta'}\|_{\infty} \leq G_{bl}[d_{bl}(\alpha', \alpha) + d_{bl}(\beta', \beta)],$$

$$\|g_{\alpha,\beta} - g_{\alpha',\beta'}\|_{\infty} \leq G_{bl}[d_{bl}(\alpha', \alpha) + d_{bl}(\beta', \beta)],$$

where $G_{bl} = 2\gamma \exp(2M_{c}/\gamma)G'^{\prime}_{bl}(1/1 - \lambda^2)$ with $G'^{\prime}_{bl} = \max\{\exp(3M_{c}/\gamma), 2G_{c}\exp(3M_{c}/\gamma)/\gamma\}$ and $\lambda = \exp(M_{c}/\gamma)\sqrt{1/(1 - \lambda^2)}$.

(ii) If $(\alpha', \beta')$ are of the particular form $\alpha' = T_{\phi} \alpha$ and $\beta' = \beta$ where $T_{\phi}(x) = x + \phi(x), \phi \in \mathcal{H}^d$, we further have that the Sinkhorn potentials are Lipschitz continuous with respect to the mapping $\phi$. That is, letting $G_{T} := 2G_{c}\exp(3M_{c}/\gamma)/\gamma$ and $c > 0$, we have

$$\|f_{T_{\phi}\alpha,\beta} - f_{\alpha,\beta}\|_{\infty} \leq G_{T}\|\phi\|_{L^2},$$

$$\|g_{T_{\phi}\alpha,\beta} - g_{\alpha,\beta}\|_{\infty} \leq G_{T}\|\phi\|_{L^2}.$$ 

Please see the proof in Appendix C.3. Importantly, this lemma implies that the weak convergence of $(\alpha, \beta)$ ensures the convergence of the Sinkhorn potential: $(\alpha', \beta') \rightharpoonup (\alpha, \beta) \Rightarrow (f_{\alpha',\beta'} \to f_{\alpha,\beta})$ in terms of the $L^\infty$ norm.
Remark B.1. While we acknowledge that the factor $\exp 1/\gamma$ is non-ideal, such quantity constantly appears in the literature related to the Sinkhorn divergence, e.g. Theorem 5 in [Luise et al., 2019] and Theorem 3 in [Genevay et al., 2019]. It would be an interesting future work to remove this factor.

Remark B.2. We note that the Lemma B.1 is strictly stronger than preexisting results: (1) Proposition 13 of [Feydy et al., 2019] only shows that the dual potentials are continuous (not Lipschitz-continuous) with the input measures, which is insufficient for the mean field limit analysis conducted in Section 4.2. (2) Under the infinity norm $\|\cdot\|_\infty$, [Luise et al., 2019] bound the variation of the Sinkhorn potential by the total variation distance of probability measures $(\alpha, \beta)$ and $(\alpha', \beta')$. Such result means that strong convergence of $(\alpha, \beta)$ implies the convergence of the corresponding Sinkhorn potential. This is strictly weaker than (i) of Lemma B.1. (3) Further, to prove the weak convergence of the corresponding Sinkhorn potential, Proposition E.5 of the above work [Luise et al., 2019] requires the cost function $c \in C^{s,1}$ with $s > d/2$, where $d$ is the problem dimension. However, Lemma B.1 only assumes $c \in C^1$, independent of $d$. Hence, Lemma B.1 makes a good contribution over existing results.

The continuity results in Lemma B.1 can be further extended to the gradient of the Sinkhorn potentials.

**Lemma B.2.** (i) Under Assumptions A.1 and A.2, for two given pairs of measures $(\alpha, \beta)$ and $(\alpha', \beta')$, with $G_{bl}[d_{bl}(\alpha', \alpha) + d_{bl}(\beta', \beta)] \leq 1$, the gradient of the Sinkhorn potentials are locally Lipschitz-continuous with respect to the bounded Lipschitz metric: With $L_{bl} = 2G_cG_{bl}$,

\[
\|\nabla f_{\alpha,\beta} - \nabla f_{\alpha',\beta'}\|_\infty \leq L_{bl}[d_{bl}(\alpha', \alpha) + d_{bl}(\beta', \beta)],
\]

\[
\|\nabla g_{\alpha,\beta} - \nabla g_{\alpha',\beta'}\|_\infty \leq L_{bl}[d_{bl}(\alpha', \alpha) + d_{bl}(\beta', \beta)].
\]

(ii) If $(\alpha', \beta')$ are of the particular form $\alpha' = T_\phi \alpha$ and $\beta' = \beta$ where $T_\phi(x) = x + \phi(x)$ for $\phi \in H^d$, we further have that the Sinkhorn potentials are Lipschitz-continuous with respect to the mapping $\phi$: Let $G_T := 2G_c\exp(3M_c/\gamma)$ and assume $2G_T\|\phi\|_{2,\infty} \leq 1$. We have with $L_T = 2G_cG_T$,

\[
\|\nabla f_{T_\phi \alpha,\beta} - \nabla f_{\alpha,\beta}\|_\infty \leq L_T\|\phi\|_{2,\infty},
\]

\[
\|\nabla g_{T_\phi \alpha,\beta} - \nabla g_{\alpha,\beta}\|_\infty \leq L_T\|\phi\|_{2,\infty}.
\]

The proof is given in Appendix C.4. The two lemmas B.1, B.2 are crucial to the analysis of the finite-time convergence and the mean field limit of Sinkhorn Descent.

### B.2 Lipschitz Continuity Study: Fréchet Derivative

From Definition 3.1, the Fréchet derivatives derived in Proposition 3.1 are functions in $H^d$ mapping from $X$ to $\mathbb{R}^d$. They are Lipschitz continuous provided that the kernel function $k$ is Lipschitz.

**Assumption B.1.** The kernel function $k : X \times X \to \mathbb{R}_+$ is Lipschitz continuous on $X$: for any $x$ and $x', x'' \in X$

\[
|k(x, y) - k(x', y)| \leq G_k\|x - x'\|.
\]

**Lemma B.3.** Define the functional on RKHS $F[\psi] := \mathcal{O}_{T,\gamma}((I + \psi)_\alpha, \beta)$. Assume Assumptions A.1, A.2, and B.1. The Fréchet derivative $DF[0] \in H^d$ is Lipschitz continuous: Denote $L_\psi = G_cG_k$.

For any $x, x' \in X$,

\[
\|DF[0](x) - DF[0](x')\| \leq L_\psi\|x - x'\|.
\]

Using the above result, the functional gradient can be shown to be Lipschitz continuous.

**Corollary B.1.** Assume Assumptions A.1, A.2, and B.1. Recall $L_\psi = G_cG_k$ from the above lemma. The Fréchet derivative $DS_\alpha[0] \in H^d$ is Lipschitz continuous: For any $x, x' \in X$,

\[
\|DS_\alpha[0](x) - DS_\alpha[0](x')\| \leq L_\psi\|x - x'\|.
\]

### B.3 Last term convergence of SD

With a slight change to SD, we can claim its last term convergence: In each iteration, check if $S(\alpha_t, \{\beta_i\}_{i=1}^n) \leq \epsilon$. If it holds, then we have already identified an $\epsilon$ approximate stationary point and we terminate SD; otherwise we proceed. The termination happens within $O(1/\epsilon)$ loops as the nonnegative objective is reduced at least $O(\epsilon)$ per-round.
C Proof of Lemmas

C.1 Proof of Lemma [A.3]

For simplicity, we omit the subscript of the Sinkhorn potential \( f_{\alpha, \beta} \) and simply use \( f \). Recall the definition of \( h(x, y) \) in Lemma [A.1]

\[
h(x, y) = \exp \left( \frac{1}{\gamma} \left( f(x) + g(y) - c(x, y) \right) \right).
\]

Subtract the optimality condition (22) at different points \( x \) and \( x' \) to derive

\[
\int_{\mathcal{X}} (h(x, y) - h(x', y)) d\beta(y) = 0 \Rightarrow \int_{\mathcal{X}} h(x', y) \left( \exp \left( \frac{f(x) - f(x') - c(x, y) + c(x', y)}{\gamma} \right) - 1 \right) d\beta(y) = 0
\]

Since \( \int_{\mathcal{X}} h(x', y) d\beta(y) = 1 \) (Lemma [A.1]), we have

\[
\exp \left( \frac{c(x', y) - c(x, y)}{\gamma} \right) \leq \exp \left( \frac{|c(x', y) - c(x, y)|}{\gamma} \right) \leq \exp \left( \frac{G_{c} \|x' - x\|}{\gamma} \right),
\]

we derive

\[
\left| \frac{f(x') - f(x)}{\gamma} \right| \leq \left| \log \left( \int_{\mathcal{X}} h(x', y) \exp \left( \frac{G_{c} \|x' - x\|}{\gamma} \right) d\beta(y) \right) \right| \leq \frac{G_{c} \|x' - x\|}{\gamma},
\]

by using \( \int_{\mathcal{X}} h(x', y) d\beta(y) = 1 \) again, which consequently leads to

\[
|f(x') - f(x)| \leq G_{c} \|x' - x\|.
\]

C.2 Proof of Lemma [A.4]

Recall the expression of \( \nabla f \) in (14):

\[
\nabla f(x) = \int_{\mathcal{X}} h(x, y) \nabla_{x} c(x, y) d\beta(y), \quad (28)
\]

where \( h(x, y) := \exp \left( \frac{1}{\gamma} \left( f_{\alpha, \beta}(x) + A[f_{\alpha, \beta}, \alpha](y) - c(x, y) \right) \right) \). For any \( x, x' \in \mathcal{X} \) such that \( \|x_1 - x_2\| \leq \frac{\gamma}{2G_{c}} \), we bound

\[
\| \nabla f(x) - \nabla f(x') \| = \| \int_{\mathcal{X}} h(x, y) \nabla_{x} c(x, y) - h(x', y) \nabla_{x} c(x', y) d\beta(y) \|
\leq \int_{\mathcal{X}} \| h(x, y) \nabla_{x} c(x, y) - h(x', y) \nabla_{x} c(x', y) \| d\beta(y)
\]

To bound the last integral, observe that

\[
\begin{align*}
h(x, y) \nabla_{x} c(x, y) - h(x', y) \nabla_{x} c(x', y) &= h(x, y) \left( \nabla_{x} c(x, y) - \nabla_{x} c(x', y) \right) + \left( h(x, y) - h(x', y) \right) \nabla_{x} c(x', y),
\end{align*}
\]

and therefore

\[
\begin{align*}
\| h(x, y) \nabla_{x} c(x, y) - h(x', y) \nabla_{x} c(x', y) \| &\leq h(x, y) \| \nabla_{x} c(x, y) - \nabla_{x} c(x', y) \| + |h(x, y) - h(x', y)| \| \nabla_{x} c(x', y) \|.
\end{align*}
\]
For the first term, we use the Lipschitz continuity of \( \nabla_x c \) from Assumption A.3 to bound
\[
h(x, y) \| \nabla_x c(x, y) - \nabla_x c(x', y) \| \leq L_c h(x, y) \| x - x' \|.
\]
For the second term, observe that \( \| \nabla_x c(x', y) \| \leq G_c \) from Assumption A.2 and
\[
|h(x, y) - h(x', y)| = h(x', y) \| \frac{f(x) - f(x') - c(x, y) + c(x', y)}{\gamma} \| - 1| < 2h(x', y) \| \frac{f(x) - f(x') - c(x, y) + c(x', y)}{\gamma} |.
\]
Since \( | \exp(z) - 1 | < 2|z| \) when \( |z| \leq 1 \), we further derive
\[
|h(x, y) - h(x', y)| \leq \frac{2G_c}{\gamma} h(x', y) \| x - x' \| = \frac{4G_c^2}{\gamma} h(x', y) \| x - x' \|.
\]
Using the optimality condition \( \int_X h(x, y) d\beta(y) = 1 \) and \( \int_X h(x, y) d\beta(y) = 1 \) from Lemma 2.1 we derive
\[
\| \nabla f(x) - \nabla f(x') \| \leq \int_X L_c h(x, y) \| x - x' \| + \frac{4G_c^2}{\gamma} h(x', y) \| x - x' \| \| x - x' \| d\beta(y) = (L_c + \frac{4G_c^2}{\gamma}) \| x - x' \|.
\]
This implies that \( \nabla^2 f(x) \) exists and is bounded from above: \( \forall x \in \mathcal{X}, \|\nabla^2 f(x)\| \leq L_f \), which concludes the proof.

### C.3 Proof of Lemma B.1

Let \( (f, g) \) and \( (f', g') \) be the Sinkhorn potentials to OT,\( \gamma(\alpha, \beta) \) and OT,\( \gamma(\alpha', \beta') \) respectively. Denote \( u := \exp(f/\gamma), v := \exp(g/\gamma) \) and \( u' := \exp(f'/\gamma), v' := \exp(g'/\gamma) \). From Lemma A.2, \( u \) is bounded in terms of the \( L^\infty \) norm:
\[
\|u\|_\infty = \max_{x \in \mathcal{X}} |u(x)| = \max_{x \in \mathcal{X}} \exp(f/\gamma) \leq \exp(2M_c/\gamma),
\]
which also holds for \( v, u', v' \). Additionally, from Lemma A.3 \( \nabla u \) exists and \( \|\nabla u\| \) is bounded:
\[
\max_x \|\nabla u(x)\| = \max_x \frac{1}{\gamma} |u(x)| \|\nabla f(x)\| \leq \frac{1}{\gamma} \|u(x)\|_\infty \max_x \|\nabla f(x)\| \leq G_c \exp(2M_c/\gamma)/\gamma.
\]

Define the mapping \( A_\alpha \mu := 1/(L_\alpha \mu) \) with
\[
L_\alpha \mu = \int_X l(x, y) \mu(y) d\alpha(y),
\]
where \( l(x, y) := \exp(-c(x, y)/\gamma) \). From Assumption A.1 we have \( \|l\|_\infty \leq \exp(M_c/\gamma) \) and from Assumption A.2 we have \( \|\nabla l(x, y)\| \leq \exp(M_c/\gamma) \|x\| \). From the optimality condition of \( f \) and \( g \), we have \( \nu = A_\alpha u \) and \( \nu = A_\beta v \). Similarly, \( \nu' = A_{\alpha'} u' \) and \( \nu' = A_{\beta'} v' \). Further use \( d_H : C(\mathcal{X}) \times C(\mathcal{X}) \to \mathbb{R} \) to denote the Hilbert metric of continuous functions,
\[
d_H(\mu, \nu) = \log \max_{x, x' \in \mathcal{X}} \frac{\mu(x) \nu(x')}{\mu(x') \nu(x)}.
\]
Note that \( d_H(\mu, \nu) = d_H(1/\mu, 1/\nu) \) if \( \mu(x) > 0 \) and \( \nu(x) > 0 \) \( \forall x \in \mathcal{X} \) and hence \( d_H(L_\alpha \mu, L_\alpha \nu) = d_H(A_\alpha \mu, A_\nu \nu) \). Under the above notations, we introduce the following existing result.

**Lemma C.1** (Birkhoff-Hopf Theorem [Lemmens and Nussbaum 2012], see Lemma B.4 in Luise et al. 2019). Let \( \lambda = \frac{\exp(M_c/\gamma) - 1}{\exp(M_c/\gamma) + 1} \) and \( \alpha \in M_1(\mathcal{X}) \). Then for every \( u, v \in C(\mathcal{X}) \), such that \( u(x) > 0, v(x) > 0 \) \( \forall x \in \mathcal{X} \), we have
\[
d_H(L_\alpha u, L_\alpha v) \leq \lambda d_H(u, v).
\]
Note that from the definition of $d_H$, one has
\[ \| \log \mu - \log \nu \|_\infty \leq d_H(\mu, \nu) = \max_x [\log \mu(x) - \log \nu(x)] + \max_x [\log \nu(x) - \log \mu(x)] \leq 2 \| \log \mu - \log \nu \|_\infty. \]

In the following, we derive upper bound for $d_H(\mu, \nu)$ and use such bound to analyze the Lipschitz continuity of the Sinkhorn potentials $f$ and $g$.

Construct $\tilde{v} := A_x u'$. Using the triangle inequality (which holds since $v(x)$, $v'(x)$, $\tilde{v}(x) > 0$ for all $x \in X$), we have
\[ d_H(v, v') \leq d_H(v, \tilde{v}) + d_H(\tilde{v}, v') \leq \lambda d_H(u, u') + d_H(\tilde{v}, v'), \]
where the second inequality is due to Lemma C.1. Similarly, Construct $\check{u} := A_y v'$. Apply Lemma C.1 again to obtain
\[ d_H(u, u') \leq d_H(u, \check{u}) + d_H(\check{u}, u') \leq \lambda d_H(v, v') + d_H(\check{u}, u'). \]
Together, we obtain
\[ d_H(v, v') \leq \lambda^2 d_H(v, v') + d_H(\tilde{v}, v') + \lambda d_H(u, u') \leq \lambda^2 d_H(v, v') + d_H(\tilde{v}, v') + d_H(\check{u}, u'), \]
which leads to
\[ d_H(v, v') \leq \frac{1}{1 - \lambda^2} [d_H(\tilde{v}, v') + d_H(\check{u}, u')]. \]

To bound $d_H(\tilde{v}, v')$ and similarly $d_H(\check{u}, u')$, observe the following:
\[ d_H(\tilde{v}, v') = d_H(L_{\alpha'} u', L_{\alpha} u') \leq 2 \| \log L_{\alpha'} u' - \log L_{\alpha} u' \|_\infty \]
\[ = 2 \max_{x \in X} |\nabla \log (a_x)([L_{\alpha'} u'](x) - [L_{\alpha} u'](x))| = 2 \max_{x \in X} \frac{1}{L_{\alpha'} u'(x)} \|L_{\alpha'} u'(x) - [L_{\alpha} u'](x)| \]
\[ \leq 2 \max \{ \|1/L_{\alpha'} u'\|_{\infty}, \|1/L_{\alpha} u'\|_{\infty} \} \|L_{\alpha'} u' - L_{\alpha} u'\|_\infty, \] (29)
where $a_x \in ([L_{\alpha'} u'](x), [L_{\alpha} u'](x))$ in the second line is from the mean value theorem. Further, in the inequality we use $\max \{ \|1/L_{\alpha'} u'\|_{\infty}, \|1/L_{\alpha} u'\|_{\infty} \} = \max \{ \|A_{\alpha'} u'\|_{\infty}, \|A_{\alpha} u'\|_{\infty} \} \leq \exp(2M_c/\gamma)$. Consequently, all we need to bound is the last term $\|L_{\alpha'} u' - L_{\alpha} u'\|_\infty$.

**Result (i)** We first note that $\forall x \in X$, $\|l(x, \cdot) u'(\cdot)\|_{bl} < \infty$: In terms of $\| \cdot \|_\infty$
\[ \| l(x, \cdot) u'(\cdot) \|_\infty \leq \| l(x, \cdot) \|_\infty \| u'(\cdot) \|_{bl} \leq \exp(3M_c/\gamma) < \infty. \]
In terms of $\| \cdot \|_{lip}$, we bound
\[ \| l(x, \cdot) u'(\cdot) \|_{lip} \leq \| l(x, \cdot) \|_\infty \| u'(\cdot) \|_{lip} + \| l(x, \cdot) \|_{lip} \| u'(\cdot) \|_\infty \]
\[ \leq \exp(M_c/\gamma) G_c \exp(2M_c/\gamma)/\gamma + \exp(M_c/\gamma) G_c \exp(2M_c/\gamma)/\gamma \]
\[ = 2G_c \exp(3M_c/\gamma)/\gamma < \infty. \]
Together we have $\| l(x, y) u'(y) \|_{bl} \leq \max \{ \exp(3M_c/\gamma), 2G_c \exp(3M_c/\gamma)/\gamma \}$. From the definition of the operator $L_{\alpha}$, we have
\[ \| L_{\alpha'} u' - L_{\alpha} u' \|_\infty = \max_{x} \left| \int_X l(x, y) u'(y) d\alpha'(y) - \int_X l(x, y) u'(y) d\alpha(y) \right| \]
\[ \leq \| l(x, y) u'(y) \|_{bl} d_{bl}(\alpha', \alpha). \]
All together we derive
\[ d_H(v', v) \leq \frac{2\exp(2M_c/\gamma) \| l(x, y) u'(y) \|_{bl} \| d_{bl}(\alpha', \alpha) + d_{bl}(\beta', \beta) \|}{1 - \lambda^2} (\lambda = \frac{\exp(M_c/\gamma) - 1}{\exp(M_c/\gamma) + 1}). \]
Further, since $d_H(v', v) \geq \| \log v' - \log v \|_\infty = \frac{1}{2} \| f' - f \|_\infty$, we have the result:
\[ \| f' - f \|_\infty \leq \frac{2 \gamma \exp(2M_c/\gamma) \| l(x, y) u'(y) \|_{bl} \| d_{bl}(\alpha', \alpha) + d_{bl}(\beta', \beta) \|}{1 - \lambda^2}. \] (30)
Similar argument can be made for $\| g' - g \|_\infty$. 

We will compute $DF$. We now bound the integrand:

$$h(x)$$

where we use the Lipschitz continuity of $f'$. Result (i): Using (i) of Lemma B.1, we bound

and the rest of the proof. Let $T$

Denote $DF$ bound the term $O_T$.

From the expression (14) of $OT$, we can use results from Lemma B.1 to bound the term $|f(x) + g(y) - f'(x) - g'(y)|$.

Result (i): Using (i) of Lemma B.1, we bound

$$\|\nabla f(x) - \nabla f'(x)\| = \frac{1}{\lambda} \int_{\mathcal{X}} (h(x,y) - h'(x,y)) \nabla_x c(x,y) d\beta(y)$$

where $h'(x,y) := \exp(\frac{1}{2}(f'(x) + g'(y) - c(x,y)))$, the second inequality holds since $|\exp(x) - 1| < 2|x|$ when $|x| \leq 1$ and $|f(x) + g(y) - f'(x) - g'(y)| < 1$. We can use results from Lemma B.1 to bound the term $|f(x) + g(y) - f'(x) - g'(y)|$.

Result (ii): Using (ii) of Lemma B.1, we bound

$$\|\nabla f(x) - \nabla f'(x)\| \leq 2G_cG_b[d\beta |\alpha', \alpha| + d\beta |\beta', \beta|].$$

C.4 Proof of Lemma B.2

From the restriction on $d\beta |\alpha', \alpha| + d\beta |\beta', \beta|$ or the size of the mapping $|\phi|_{\infty}$, we always have $|f(x) + g(y) - f'(x) - g'(y)| < 1$ from Lemma B.1.

Denote the Sinkhorn potentials to $OT_\gamma |\alpha, \alpha|$ and $OT_\gamma |\alpha', \alpha'|$ by $(f, g)$ and $(f', g')$ respectively. From the expression (14) of $\nabla f$ and $\nabla f'$, we have

$$\|\nabla f(x) - \nabla f'(x)\| = \frac{1}{\lambda} \int_{\mathcal{X}} (h(x,y) - h'(x,y)) \nabla_x c(x,y) d\beta(y)$$

where $h'(x,y) := \exp(\frac{1}{2}(f'(x) + g'(y) - c(x,y)))$, the second inequality holds since $|\exp(x) - 1| < 2|x|$ when $|x| \leq 1$ and $|f(x) + g(y) - f'(x) - g'(y)| < 1$. We can use results from Lemma B.1 to bound the term $|f(x) + g(y) - f'(x) - g'(y)|$.

Result (i): Using (i) of Lemma B.1, we bound

$$\|\nabla f(x) - \nabla f'(x)\| \leq 2G_cG_b[d\beta |\alpha', \alpha| + d\beta |\beta', \beta|].$$

Result (ii): Using (ii) of Lemma B.1, we bound

$$\|\nabla f(x) - \nabla f'(x)\| \leq 2G_cG_{T_\gamma} |\phi|_{\infty}.$$
Using the optimality from Lemma A.1, we have \( f_X h(x, y) d\beta(y) = 1 \) and hence \( \langle h - 1, T_x \alpha \otimes \beta \rangle = 0 \). Subtracting the 1st equality from the last inequality,

\[
OT(\gamma T_x \alpha, \beta) - OT(\gamma \alpha, \beta) \geq \langle f, T_x \alpha - \alpha \rangle.
\]

Use the change-of-variables formula of the push-forward measure to obtain

\[
\frac{1}{\epsilon} (f, T_x \alpha - \alpha) = \frac{1}{\epsilon} \int_X \left( (f \circ T)(x) - f(x) \right) d\alpha(x) = \int_X \nabla f(x + \epsilon' \phi(x)) \phi(x) d\alpha(x),
\]

where \( \epsilon' \in [0, \epsilon] \) is from the mean value theorem. Further use the Lipschitz continuity of \( \nabla f \) in Lemma A.4 we have

\[
\lim_{\epsilon \to 0} \frac{1}{\epsilon} (f, T_x \alpha - \alpha) = \int_X \nabla f(x) \phi(x) d\alpha(x).
\]

Since \( \phi \in H^d \), we have \( \phi(x) = \langle \phi, k(x, \cdot) \rangle_{H^d} \) and hence

\[
\lim_{\epsilon \to 0} \frac{1}{\epsilon} (OT(\gamma T_x \alpha, \beta) - OT(\gamma \alpha, \beta)) \geq \langle \int \nabla f(x) k(x, \cdot) d\alpha(x), \phi \rangle_{H^d}.
\]

Similarly, let \( f' \) and \( g' \) be the Sinkhorn potentials to \( OT(\gamma T_x \alpha, \beta) \), using \( f' \to f \) as \( \epsilon \to 0 \), we can have an upper bound

\[
\lim_{\epsilon \to 0} \frac{1}{\epsilon} (OT(\gamma T_x \alpha, \beta) - OT(\gamma \alpha, \beta)) \leq \langle \int \nabla f'(x + \epsilon' \phi(x)) k(x, \cdot) d\alpha(x), \phi \rangle_{H^d}.
\]

Since \( \phi \in H^d \), we have \( \|\phi\|_{2, \infty} \leq M_H \|\phi\|_{H^d} < \infty \) with \( M_H \in \mathbb{R}_+ \) being a constant. Using Lemma B.1 we have that \( \nabla f' \) is Lipschitz continuous with respect to the mapping

\[
\lim_{\epsilon \to 0} \|\nabla f'(x + \epsilon' \phi(x)) - \nabla f(x + \epsilon' \phi(x))\| \leq \lim_{\epsilon \to 0} cG_T \|\phi\|_{2, \infty} = 0.
\]

Besides, using Lemma A.4 we have that \( \nabla f \) is continuous and hence \( \lim_{\epsilon \to 0} \nabla f(x + \epsilon' \phi(x)) = \nabla f(x) \) and consequently we have \( \lim_{\epsilon \to 0} \frac{1}{\epsilon} (OT(\gamma T_x \alpha, \beta) - OT(\gamma \alpha, \beta)) = \langle \int \nabla f(x) k(x, \cdot) d\alpha(x), \phi \rangle_{H^d} \).

From Definition 1.1 we have the result of \( DF_1[0] \). The result of \( DF_2[0] \) can be obtained similarly.

C.6 Proof of Lemma 4.2

From Proposition 3.1 and (13), we recall the expression of \( DS_\alpha[0] \) by

\[
DS_\alpha[0] = \int_X \frac{1}{n} \sum_{i=1}^n \nabla f_{\alpha, \beta_i}(x) - \nabla f_{\alpha, \alpha}(x) k(x, y) d\alpha(x), \tag{31}
\]

and we have \( T[\alpha](x) = x - \eta DS_\alpha[0](x) \). Consequently, using Corollary B.1 we have

\[
\|T[\alpha]\|_{lip} = \max_{x \neq y} \frac{\|T[\alpha](x) - T[\alpha](y)\|}{\|x - y\|} = \max_{x \neq y} \frac{\|x - y - \eta(DS_\alpha[0](x) - DS_\alpha[0](y))\|}{\|x - y\|} \leq 1 + \eta \|DS_\alpha[0]\|_{lip} \leq 1 + \eta G_c G_k.
\]

The following lemma states that \( T[\alpha] \) is Lipschitz w.r.t. \( \alpha \) in terms of the bounded Lipschitz norm.

Lemma C.2. For any \( x \in X \) and any \( \alpha, \alpha' \in M^+_1(X) \), we have

\[
\|T[\alpha](y) - T[\alpha'](y)\|_{2, \infty} \leq \eta \max\{dL_k D_k + dG_c G_k, D_k L_{bl}, d_{bl}(\alpha', \alpha)\}.
\]

We defer the proof to Appendix C.6.1. Based on such lemma, for any \( h \) with \( \|h\|_{bl} \leq 1 \), we have

\[
\|h, T[\alpha] \alpha\|_h - \langle h, T[\alpha'] \alpha' \rangle \leq \|h \circ T[\alpha], \alpha\| - \langle h \circ T[\alpha], \alpha' \rangle \leq \langle h \circ T[\alpha], \alpha - \alpha' \rangle + \|T[\alpha], \alpha' - \alpha \|.
\]

We now bound these two terms individually: For the first term,

\[
\|h \circ T[\alpha], \alpha\| \leq \|h \circ T[\alpha]\|_{lip} d_{bl}(\alpha, \alpha') \leq \max\{\|h\|_\infty, \|h\|_{lip}\} d_{bl}(\alpha, \alpha') \leq (1 + \eta G_c G_k) d_{bl}(\alpha, \alpha');
\]

and
And for the second term, use Lemma C.2 to derive
\[ |(h \circ T[\alpha], \alpha') - (h \circ T[\alpha'], \alpha')| \leq \|h \circ T[\alpha] - h \circ T[\alpha']\|_{\infty} \leq \|h\|_{lip} \max_{x \in \mathcal{X}} \|T[\alpha](x) - T[\alpha'](x)\| \]
\[ \leq \eta \max\{dL_f D_k + dG_c G_k, D_k L_{bl}\} d_{bl}(\alpha', \alpha). \]
Combining the above inequalities, we have the result
\[ d_{bl}(T[\alpha] \alpha, T[\alpha'] \alpha') \leq (1 + \eta G_c G_k + \eta \max\{dL_f D_k + dG_c G_k, D_k L_{bl}\}) d_{bl}(\alpha', \alpha). \]

C.6.1 Proof of Lemma C.2

Recall the definition of \( T[\alpha](x) = x - \eta D S_{\alpha}[0](x) \), where the functional \( S_{\alpha} \) is defined in (9) and the Fréchet derivative is computed in (13). For any \( y \in \mathcal{X} \), we have
\[ \|T[\alpha](y) - T[\alpha'](y)\| \leq \eta \|D S_{\alpha}[0](y) - D S_{\alpha'}[0](y)\| \]
\[ \leq \eta \left( \int_{\mathcal{X}} \left[ \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha, \beta_i}(x) - \nabla f_{\alpha', \alpha}(x) \right] k(x, y) d\alpha(x) \right) - \int_{\mathcal{X}} \left[ \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta_i}(x) - \nabla f_{\alpha', \alpha}(x) \right] k(x, y) d\alpha'(x) \]
\[ + \eta \left( \int_{\mathcal{X}} \left[ \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta_i}(x) - \nabla f_{\alpha', \alpha}(x) \right] k(x, y) d\alpha(x) \right) - \int_{\mathcal{X}} \left[ \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta_i}(x) - \nabla f_{\alpha', \alpha}(x) \right] k(x, y) d\alpha'(x) \]
\[ = \eta \left( \int_{\mathcal{X}} \left[ \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha, \beta_i}(x) - \nabla f_{\alpha, \alpha}(x) \right] - \left[ \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta_i}(x) - \nabla f_{\alpha', \alpha}(x) \right] \right) k(x, y) d\alpha(x) \]
\[ + \eta \left( \int_{\mathcal{X}} \left[ \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha, \beta_i}(x) - \nabla f_{\alpha, \alpha}(x) \right] k(x, y) d\alpha(x) \right) - \int_{\mathcal{X}} \left[ \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta_i}(x) - \nabla f_{\alpha', \alpha}(x) \right] k(x, y) d\alpha'(x). \]

For the first term, use Lemma B.2 to bound
\[ \| \int_{\mathcal{X}} \left( \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha, \beta_i}(x) - \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta_i}(x) - \nabla f_{\alpha', \alpha}(x) \right) k(x, y) d\alpha(x) \| \]
\[ \leq D_k L_{bd} d_{bl}(\alpha', \alpha). \]

For the second term, we bound
\[ \| \int_{\mathcal{X}} \left[ \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta_i}(x) - \nabla f_{\alpha', \alpha}(x) \right] k(x, y) d\alpha(x) \right) - \int_{\mathcal{X}} \left[ \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta_i}(x) - \nabla f_{\alpha', \alpha}(x) \right] k(x, y) d\alpha'(x) \right) \|
\[ \leq \int_{\mathcal{X}} \left[ \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta_i}(x) - \nabla f_{\alpha', \alpha}(x) \right] k(x, y) d\alpha(x) \right) - \int_{\mathcal{X}} \left[ \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta_i}(x) - \nabla f_{\alpha', \alpha}(x) \right] k(x, y) d\alpha'(x) \right) \|
\[ \leq \sum_{i=1}^{d} \left| \int_{\mathcal{X}} \left[ \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta_i}(x) - \nabla f_{\alpha', \alpha}(x) \right] k(x, y) d\alpha(x) \right) - \int_{\mathcal{X}} \left[ \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta_i}(x) - \nabla f_{\alpha', \alpha}(x) \right] k(x, y) d\alpha'(x) \right) \|
\[ \leq \sum_{i=1}^{d} \left| \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta_i}(\cdot) - \nabla f_{\alpha', \alpha}(\cdot) \right| k(\cdot, y) d\alpha \right) - \int_{\mathcal{X}} \left[ \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta_i}(\cdot) - \nabla f_{\alpha', \alpha}(\cdot) \right] k(\cdot, y) d\alpha'(x) \right) \|
\[ \leq \sum_{i=1}^{d} \| \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta_i}(\cdot) - \nabla f_{\alpha', \alpha}(\cdot) \|_{\mathcal{D}_{bl}(\alpha', \alpha)}. \]
Therefore, we only need to bound \( \sum_{i=1}^{d} \| \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta'}(x) - \nabla f_{\alpha', \alpha'}(x) \|_{\text{lip}} k(x, y) \|_{\text{iip}} \). In terms of \( L^\infty \) norm, we have

\[
\sum_{i=1}^{d} \| \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta'}(\cdot) - \nabla f_{\alpha', \alpha'}(\cdot) \|_{\text{lip}} k(\cdot, y) \|_{\infty} \leq dD_{k} \| \nabla f_{\alpha', \beta'} \|_{\infty} \leq dD_{k} G_{c}.
\]

In terms of \( \| \cdot \|_{\text{iip}} \), denote \( \tilde{\nabla}(x) = \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta'}(x) - \nabla f_{\alpha', \alpha'}(x) \). For all \( x, x' \in \mathcal{X} \), we have

\[
\frac{||\tilde{\nabla}(x)||k(x, y) - |\tilde{\nabla}(x')|k(x', y)|}{||x - x'||} \leq \frac{||\tilde{\nabla}(x)|k(x, y) - |\tilde{\nabla}(x')|k(x', y)| + |\tilde{\nabla}(x')|k(x, y) - |\tilde{\nabla}(x')|k(x', y)|}{||x - x'||} \leq L_{f} D_{k} + G_{c} G_{k},
\]

and hence \( \sum_{i=1}^{d} \| \frac{1}{n} \sum_{i=1}^{n} \nabla f_{\alpha', \beta'}(\cdot) - \nabla f_{\alpha', \alpha'}(\cdot) \|_{\text{iip}} \) \leq dL_{f} D_{k} + dG_{c} G_{k}. All together, we have for any \( y \in \mathcal{X} \)

\[
\| T[\alpha](y) - T[\alpha'](y) \| \leq \eta \max\{dL_{f} D_{k} + dG_{c} G_{k}, D_{k} L_{bl}\} d_{bl}(\alpha', \alpha).
\]

### C.7 Proof of Lemma 4.1

We first recall a proposition from [Feydy et al., 2019], which shows that the dual potentials are the variations of \( \text{OT}_{\gamma} \) w.r.t. the underlying probability measure.

**Definition C.1.** We say \( h \in \mathcal{C}(\mathcal{X}) \) is the first-order variation of a functional \( F : \mathcal{M}_{1}^{+}(\mathcal{X}) \to \mathbb{R} \) at \( \alpha \in \mathcal{M}_{1}^{+}(\mathcal{X}) \) if for any displacement \( \xi = \beta - \alpha \) with \( \beta \in \mathcal{M}_{1}^{+}(\mathcal{X}) \), we have

\[
F(\alpha + t\xi) = F(\alpha) + t(h, \xi) + o(t).
\]

Further we denote \( h = \nabla_{\alpha} F(\alpha) \).

**Lemma C.3.** The first-order variation of \( \text{OT}_{\gamma}(\alpha, \beta)(\alpha \neq \beta) \) with respect to the measures \( \alpha \) and \( \beta \) is the corresponding Sinkhorn potential, i.e. \( \nabla_{(\alpha, \beta)} \text{OT}_{\gamma}(\alpha, \beta) = \langle f_{\alpha, \beta}, y_{\alpha, \beta} \rangle. \) Further, if \( \alpha = \beta \), we have \( \nabla_{\alpha} \text{OT}_{\gamma}(\alpha, \alpha) = 2f_{\alpha, \alpha}. \)

Recall that \( \alpha^{t+1} = T[\alpha^t](\cdot) \) where the push-forward mapping is of the form \( T[\alpha^t](x) = x - \eta DS_{\alpha^t}[0](x) \) with \( DS_{\alpha^t}[0] \) given in (13). Using the convexity of \( S_{\gamma} \) and Lemma C.3, we have

\[
S_{\gamma}(\alpha^{t+1}) - S_{\gamma}(\alpha^t) \leq \langle \nabla_{\alpha} S_{\gamma}(\alpha) |_{\alpha = \alpha^{t+1}}, \alpha^{t+1} - \alpha^t \rangle,
\]

where

\[
= \langle \frac{1}{n} \sum_{i=1}^{n} f_{\alpha^{t+1}, \beta_i} - f_{\alpha^{t+1}, \alpha^{t+1}}, T[\alpha^t] \alpha^t - \alpha^t \rangle.
\]

Further, we have

\[
= \langle \frac{1}{n} \sum_{i=1}^{n} f_{\alpha^{t+1}, \beta_i} - f_{\alpha^{t+1}, \alpha^{t+1}} \circ T[\alpha^t] - \frac{1}{n} \sum_{i=1}^{n} f_{\alpha^{t+1}, \beta_i} - f_{\alpha^{t+1}, \alpha^{t+1}} \rangle, \alpha^t \rangle.
\]

For succinctness, denote \( \xi^t = \frac{1}{n} \sum_{i=1}^{n} f_{\alpha^{t+1}, \beta_i} - f_{\alpha^{t+1}, \alpha^t} \). Hence, we have

\[
S_{\gamma}(\alpha^{t+1}) - S_{\gamma}(\alpha^t) \leq \langle \xi^t + \eta \nabla[\xi^t](x - \eta DS_{\alpha^t}[0](x)) - \xi^{t+1} \alpha^t \rangle
\]

\[
= -\eta \int \langle \nabla[\xi^t](x - \eta DS_{\alpha^t}[0](x)), DS_{\alpha^t}[0](x) \rangle d\alpha^t(x),
\]

20
where the last equality is from the mean value theorem with $\eta \in [0, \eta]$. We now bound the integral by splitting it into three terms and analyze them one by one.

\[
\int_X \langle \nabla \xi^{t+1}(x - \eta' DS_{\alpha^t}[0](x)), DS_{\alpha^t}[0](x) \rangle d\alpha^t(x) \\
= \int_X \langle \nabla \xi^t(x), DS_{\alpha^t}[0](x) \rangle d\alpha^t(x) \tag{1} \\
+ \int_X \langle \nabla \xi^t(x - \eta' DS_{\alpha^t}[0](x)) - \nabla \xi^t(x), DS_{\alpha^t}[0](x) \rangle d\alpha^t(x) \tag{2} \\
+ \int_X \langle \nabla \xi^{t+1}(x - \eta' DS_{\alpha^t}[0](x)) - \nabla \xi^t(x - \eta' DS_{\alpha^t}[0](x)), DS_{\alpha^t}[0](x) \rangle d\alpha^t(x). \tag{3}
\]

For (1), since $DS_{\alpha^t}[0] \in H^d$, we have $DS_{\alpha^t}[0](x) = \langle DS_{\alpha^t}[0], k(x, \cdot) \rangle$ and hence

\[
\int_X \langle \nabla \xi^t(x), DS_{\alpha^t}[0](x) \rangle d\alpha^t(x) = \int \langle \nabla \xi^t(x)k(x, \cdot), DS_{\alpha^t}[0] \rangle_{H^d} d\alpha^t(x) \\
= \|DS_{\alpha^t}[0]\|_{H^d}^2 = S(\alpha^t, \{\beta_i^t\}_{i=1}^n),
\]

where the last equality is from the Definition 4.1 and the expression of $DS_{\alpha^t}[0]$ in (13).

For (2), note that the summands of $\nabla \xi^t$ are of the form $\nabla f_{\alpha, \beta}$ (or $\nabla f_{\alpha, \beta}$) which is proved to be Lipschitz in Lemma A.4. Consequently, we bound

\[
\left| \int \langle \nabla \xi^t(x - \eta' DS_{\alpha^t}[0](x)) - \nabla \xi^t(x), DS_{\alpha^t}[0](x) \rangle d\alpha^t(x) \right| \\
\leq \int \| \nabla \xi^t(x - \eta' DS_{\alpha^t}[0](x)) - \nabla \xi^t(x) \| \|DS_{\alpha^t}[0](x)\| d\alpha^t(x) \\
\leq \int 2L_f \eta \|DS_{\alpha^t}[0](x)\|^2 d\alpha^t(x) \quad \# \text{Lemma A.4} \\
\leq 2\eta L_f M_H^2 \|DS_{\alpha^t}[0]\|_{H^d}^2 = 2\eta L_f M_H^2 S(\alpha^t, \{\beta_i^t\}_{i=1}^n). \quad \# \text{see (1)}
\]

where we use $\forall f \in H^d$, $\exists M_H > 0 \text{ s.t. } \|f(x)\| \leq M_H \|f\|_{H^d}, \forall x \in X$ in the third inequality.

For (3), similar to (2), the summands of $\nabla \xi^t$ are proved to be Lipschitz in (ii) of Lemma B.2 and hence we bound

\[
\left| \int \langle \nabla \xi^{t+1}(x - \eta' DS_{\alpha^t}[0](x)) - \nabla \xi^t(x - \eta' DS_{\alpha^t}[0](x)), DS_{\alpha^t}[0](x) \rangle d\alpha^t(x) \right| \\
\leq \| \| \nabla \xi^{t+1}(x - \eta' DS_{\alpha^t}[0](x)) - \nabla \xi^t(x - \eta' DS_{\alpha^t}[0](x)) \| \|DS_{\alpha^t}[0](x)\| \|d\alpha^t(x) \| \\
\leq \int \sqrt{\eta} L_T \|DS_{\alpha^t}[0]\|_{2,\infty} \|DS_{\alpha^t}[0]\| d\alpha^t(x) \quad \# \text{Lemma B.2} \\
\leq 2\eta \sqrt{\eta} L_T M_{H^\alpha}^2 \|DS_{\alpha^t}[0]\|_{H^d}^2 = 2\eta \sqrt{\eta} L_T M_{H^\alpha}^2 S(\alpha^t, \{\beta_i^t\}_{i=1}^n) \quad \# \text{see (1)}
\]

Combining the bounds on (1), (2), (3), we have:

\[
\mathcal{S}_f(\alpha^{t+1}) - \mathcal{S}_f(\alpha^t) \leq -\eta(1 - 2\eta L_f M_H^2 - 2\eta \sqrt{\eta} L_T M_{H^\alpha}^2) S(\alpha^t, \{\beta_i^t\}_{i=1}^n),
\]

which leads to the result when we set $\eta \leq \min\{\frac{1}{8L_T M_{H^\alpha}^2}, \frac{1}{8\sqrt{\eta} L_T M_{H^\alpha}^2}\}$. 

21
D A Discussion on the Global Optimality

D.1 Proof of Theorem 4.3

We first show \( \int_X \| \xi(x) \|^2 \, d\alpha(x) < \infty \):

\[
\int_X \| \xi(x) \|^2 \, d\alpha(x) = \int_X \left\| \frac{1}{n} \sum_{i=1}^n \nabla f_{\alpha, \beta_i}(x) - \nabla f_{\alpha, \alpha}(x) \right\|^2 \, d\alpha(x)
\]

= \int_X \left\| \frac{1}{n} \sum_{i=1}^n \nabla f_{\alpha, \beta_i}(x) \right\|^2 + 2\| \nabla f_{\alpha, \alpha}(x) \|^2 \, d\alpha(x) \leq 4G_f < \infty

(i) \( S(\alpha, \{ \beta_i \}_{i=1}^n) = 0 \) \& \( \text{supp}(\alpha) = X \Rightarrow \max_{\beta \in M^+_1(X)} \langle -\nabla \alpha S_\alpha(\alpha), \beta - \alpha \rangle \leq 0 \):

From the integrally strictly positive definiteness of the kernel function \( k(x, x') \), we have that \( \int_X \| \xi(x) \|^2 \, d\alpha(x) = 0 \) which implies \( \nabla \xi = \frac{1}{n} \sum_{i=1}^n \nabla f_{\alpha, \beta_i} - \nabla f_{\alpha, \alpha}(x) = 0 \) for all \( x \in \text{supp}(\alpha) \). Further, we have that \( \xi \) is a constant function on \( X \) by \( \text{supp}(\alpha) = X \). Since we can shift the Sinkhorn potential by a constant amount without losing its optimality, we can always ensure that \( \xi \) is exactly a zero function. This implies the optimality condition of the Sinkhorn barycenter problem: \( \max_{\beta \in M^+_1(X)} \langle -\nabla \alpha S_\alpha(\alpha), \beta - \alpha \rangle \leq 0 \).

(ii) Using Theorem 4.1 and (i), one directly has the result.

D.2 Fully Supported Property of \( S \)D at Finite Time

WLOG, suppose that \( c(x, y) = \infty \) if \( x \notin X \). From the monotonicity of Lemma 4.1, the support of \( \alpha^t \) will not grow beyond \( X \). Let \( p^t \) be the density function of \( \alpha^t \). The density \( p^{t+1} \) is given by \( p^{t+1}(x) = p^t(T[\alpha^t]^{-1}(x)) \), where \( T[\alpha^t] \) is the mapping defined in (11). For a sufficiently small step size, the determinant is always positive. Consequently, \( p^{t+1}(x) = 0 \) implies \( p^t(T[\alpha^t]^{-1}(x)) = 0 \) which is impossible since \( p^t \) is f.s. Therefore, \( p^{t+1} \) is also a.c. and f.s.

D.3 Review the Assumptions for Global Convergence in Previous Works

We briefly describe the assumptions required by previous works [Arbel et al. 2019, Mroueh et al. 2019] to guarantee the global convergence to the MMD minimization problem. We emphasize that both of these works make assumptions on the ENTIRE measure sequence. In the following, we use \( \nu_p \) to denote the target measure.

In [Mroueh et al. 2019], given \( \nu \in M^+_1(X) \), Mroueh et al. [2019] define the Kernel Derivative Gramian Embedding (KDGE) of \( \nu \) by

\[
D(\nu) := E_{x \sim \nu} \left( [\Phi(x)]^\top J\Phi(x) \right),
\]

where \( \Phi \) is the feature map of a given RKHS and \( J\Phi \) denotes its Jacobian matrix. Further denote the classic Kernel Mean Embedding (KME) by

\[
\mu(\nu) := E_{x \sim \nu} \Phi(x).
\]

SoD requires the entire variable measure sequence \( \{ \nu_q \} \), \( q \geq 0 \) to satisfy for any measure \( \nu_q \) such that \( \delta_{p,q} := \mu(\nu_q) - \mu(\nu_p) \neq 0 \)

\[
D(\nu) \delta_{p,q} \neq 0.
\]

In [Arbel et al. 2019, Arbel et al. 2019] proposed two types of assumptions such that either of them leads to the global convergence of their (noisy) gradient flow algorithm. Specifically, denote the squared weighted Sobolev semi-norm of a function \( f \) in an RKHS with respect to a measure \( \nu \) by \( \| f \|_{H(\nu)}^2 = \int_X \| \nabla f(x) \|^2 \, d\nu(x) \). Given two probability measures on \( X \), \( \nu_p \) and \( \nu_q \), define the weighted negative Sobolev distance \( \| \nu_p - \nu_q \|_{H(\nu)^{-1}(\nu)} \) by

\[
\| \nu_p - \nu_q \|_{H(\nu)^{-1}(\nu)} = \sup_{f \in L^2(\nu), \| f \|_2 \leq 1} \left| \int_X f(x) \nu_p(x) - \int_X f(x) \nu_q(x) \right|.
\]

In Proposition 7 of [Arbel et al. 2019], if for the entire variable measure sequence \( \{ \nu_q \} \) generated by their gradient flow algorithm, \( \| \nu_p - \nu_q \|_{H(\nu)^{-1}(\nu)} \) is always bounded, then \( \nu_q \) weakly converges to
Further, the authors also propose another noisy gradient flow algorithm and provide its global convergence guarantee under a different assumption: Let $f_{\nu_p, \nu_q}$ be the unnormalized witness function to $\text{MMD}(\nu_p, \nu_q)$. Let $\mu$ be the standard gaussian distribution and let $\beta > 0$ be a noise level. Denote $D_{\beta}(\nu_q) := \mathbb{E}_{x \sim \nu_q, \mu}[\|\nabla f_{\nu_p, \nu_q}(x + \beta \mu)\|^2]$. The noisy gradient flow algorithm globally converges if for all $n$ there exists a noise level $\beta_n$ such that
\[
8\lambda^2 \beta_n^2 \text{MMD}(\nu_p, \nu_n) \leq D_{\beta_n}(\nu_n),
\]
and $\sum_{i=0}^{n} \beta_i^2 \to \infty$. Here $\lambda$ is some problem dependent constant.

E Implementation

The code to reproducing the experimental results can be found in the following link: [https://github.com/shenzebang/Sinkhorn_Descent](https://github.com/shenzebang/Sinkhorn_Descent). Our implementation is based on Pytorch and geomloss.

[https://www.kernel-operations.io/geomloss/](https://www.kernel-operations.io/geomloss/)