Breaking the curse: a dimension free computational upper-bound for smooth optimal transport estimation

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Abstract

It is well-known that plug-in statistical estimation of optimal transport suffers from the curse of dimension. Despite recent efforts to improve the rate of estimation with the smoothness of the problem, the computational complexities of these recently proposed methods still degrade exponentially with the dimension. In this paper, thanks to a representation theorem, we derive a statistical estimator of smooth optimal transport which achieves in average a precision $\epsilon$ for a computational cost of $\tilde{O}(\epsilon^{-2})$, where $\gamma$ is the complexity of a semidefinite program mixed with a second order cone program, hence yielding a dimension free rate. Even though our result is theoretical in nature due to the large constants involved in our estimation, it settles the question of whether the smoothness of optimal solutions can be taken advantage of from a computational and statistical point of view.

1 Introduction

The comparison between probability distributions is a fundamental task and has been extensively used in machine learning. For this purpose, optimal transport has recently gained traction in different subfields of machine learning, such as natural language processing (NLP) [35, 4], generative modeling [28], structure prediction [9], domain adaptation [25], clustering [12] and has impact in other areas such as imaging sciences [7, 3]. Indeed, OT is a tool to compare data distributions which has arguably many more geometric properties than other available divergences [23, 30]. In practice, the optimal transport cost is often computed for the squared distance (Wasserstein squared distance) on sampled distributions and it is well-known that optimal transport suffers from the curse of dimensionality [8]: the plug-in strategy, which is simply the Wasserstein distance between the sampled distributions, yields an estimation of the Wasserstein squared distance between a density and its sampled version in $O(1/n^{2/d})$, which degrades rapidly in high dimensions; similar rates hold in the general case of two different distributions. However, high-dimension is the usual setting in machine learning, e.g. NLP, and even if the intrinsic dimensionality of data can be leveraged [32], poor theoretical rates of convergence are a distinguished feature of OT. This problem can be alleviated when the underlying optimal map is smooth [15] where it is shown that theoretical rates are close to $O(1/\sqrt{n})$ rates which increasing smoothness. Such results are applicable when the

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source and target distributions satisfy smoothness assumptions and geometric assumptions on their support since deep analytical results guarantee the smoothness of the optimal map in Euclidean space [24].

**State of the art.** A current research direction consists in developing estimators of the Wasserstein distance that have better performances for particular class of distributions.

Another OT like model is the entropic regularization of OT which has been first advocated as a way to numerically approximate and to make it differentiable [6]. Known rates on the sample complexity of entropic optimal transport can be found in [10, 20] and are of the order $O\left(\frac{1}{\sqrt{n}}\right)$, for small values of $\varepsilon$; while still being in $1/\sqrt{n}$, the constant degrades as expected since it is an approximation of optimal transport. Estimation of optimal transport distance via entropic OT or Sinkhorn divergences naturally exhibits an exponential degradation in high-dimensions. The most advanced results in this direction can be found in [5] where, with few assumptions on the regularity of the optimal map, for an $\epsilon$ accuracy, the squared Wasserstein distance can be estimated using $O(\epsilon^{-d/2+2})$ samples and $\tilde{O}(\epsilon^{-(d+5.5)})$ (with $d' = 2\lfloor\frac{d}{2}\rfloor$) operations with high probability.

In [15] minimax rates leveraging the smoothness of the OT map have been proven. While statistically almost optimal, these rates are not proven to be computationally feasible in their paper. More precisely, under a regularity assumption, the authors propose an estimator of the optimal maps which necessitates, for an $L^2$ error on the map of order $\epsilon$, $O(\epsilon^{-\frac{2s+1+d/2}{2s}})$ samples. However, the authors do not provide any numerical algorithm to achieve these rates. In particular, they use a projection on the space of smooth convex functions.

Weed et al. propose in [33] an estimator of the Wasserstein distance under smoothness of the optimal potentials, which require $O(\epsilon^{-(2d+d/2)})$ samples and using a resampling strategy on the estimated densities can be calculated in $O(\epsilon^{-(2d+d/2)})$. Here again, the resampling is not numerically accessible.

**Contributions.** In all the above contributions, the computational bounds do take advantage of the smoothness of the optimal potentials. In fact, the computational bounds have been much less studied. For instance, in [22, Theorem 12], the authors show, in their framework of "spike model" that a low-dimensional hypothesis of the support of the distribution can be leveraged in order to define statistically efficient estimators that do not suffer from the curse of dimensionality. However, they also give evidence that there is a statistical-computational gap and that these efficient estimators cannot be achieved computationally.

In this paper, we provide a positive answer to the question whether smoothness of the optimal potentials can be computationally beneficial to an efficient statistical estimator. More precisely, we propose an algorithm which, for a given accuracy $\epsilon$, needs $O(\epsilon^{-2})$ samples and a computational time which improves with the regularity of the optimal maps and is at best in $\tilde{O}(\epsilon^{-2\gamma})$, where $\gamma$ is the complexity of a semidefinite program mixed with a second order cone program and independent of the dimension $d$. To the best of our knowledge, it is the first result showing that smoothness can be leveraged in the computational estimation of optimal transport.

The second key contribution of this paper is to provide a new representation theorem for solutions of smooth optimal transport. The inequality constraint in OT can be replaced with an equality constraint involving a finite sum-of-squares in Sobolev space. In comparison with [26], it is a non-trivial extension of their representation result to the case of a continuous set of global minimizers instead of a finite set.
**Strategy of proof.** Optimal transport is formulated as a constrained optimization problem on a space of functions. It is a linear optimization problem under an inequality constraint on these functions. Therefore, it can be interpreted as learning a function which has a particular structure, non-negativity among others. Recent works address this problem. In [1], it is proposed to represent a positive function in a Reproducing Kernel Hilbert Space as a sum-of-squares, following the ideas in the optimization literature via the sum-of-square relaxation [18]. These ideas were further developed in [36, 19] and exploited for non-convex optimization in [26] where the authors recast the problem of minimization of a function $f : D \subset \mathbb{R}^d \to \mathbb{R}$ defined on a domain $D$ as a convex optimization problem, max $c$ under the inequality constraint $c \leq f(x)$ for every $x \in D$. Obviously, this problem is computationally intractable in general and they propose to solve it under structural assumptions on $f(x) - c = \frac{1}{2}\langle \phi(x), A\phi(x) \rangle$ for a positive self-adjoint operator $A : \mathcal{H} \to \mathcal{H}$ where $\mathcal{H}$ is a Reproducing Kernel Hilbert Space (RKHS). The value of this new optimization problem is a priori less than the minimum value of $f$ but it does coincide under the assumption that

$$f = \text{cste} + \frac{1}{2}\langle \phi(x), A\phi(x) \rangle, \quad (1)$$

for some $A\phi$. The key point here is a representation result stating that a fairly large space of smooth functions (to be considered for optimization) can be represented as Equation (1) a sum of squares in RKHS space. Indeed, they show that it is the case if the function $f$ has at least one global minimizer and there is a finite number of global minimizers which all have a non-singular Hessian.

In this paper, we use the same strategy than [26]. Their result is however not directly applicable to the optimal transport problem. Optimal transport in its dual formulation for the quadratic cost also optimize on a subset of non-negative functions. Under smoothness assumption of the optimizer, one is tempted to formulate a result on the computational-statistical efficiency of the problem. However, while leveraging regularity can be done using sampling inequalities for a given smooth function, see [34], it is not possible in general for functions for which only inequality constraints are available. As shown in [26], it is possible though when more structure on the minimizers is available. Therefore, the key issue is the representation formula of the minimizers with the additional sum-of-squares structure. In the dual formulation of OT, the minimizers do not define a finite number of saturation points for the inequality constraint, on the contrary to the hypothesis in [26]. Rather the saturation set of the constraint defined by the optimizers is a continuous set of points, the graph of the optimal transport map. Based on the Morse lemma with parameter, we prove a representation result on the optimizer for smooth OT. This allows to formulate an (infinite dimensional) SDP-SOCP formulation for OT which is tight. By a standard "kernel trick", this problem admits a finite dimensional representation which can be solved by convex optimization algorithms, leading to polynomial computational bounds which are independent of the dimension of the ambient space.

### 2 Notations and background

In the following, we consider the optimal transport problem for the quadratic cost on a closed ball $B$, with radius $R > 0$, in the Euclidean space $\mathbb{R}^d$. The set of probability measures on $B$ is denoted by $\mathcal{P}(B)$. The optimal transport problem can be stated in its dual formulation as

$$\text{OT}(\mu, \nu) = \sup_{u, v} \langle u, \mu \rangle + \langle v, \nu \rangle + \iota_{C(\mu, \nu)}(u, v), \quad (2)$$
where $C(\mu, \nu) \overset{\text{def}}{=} \{(u, v) \in C^0(B) \times C^0(B); u(x) + v(y) \leq c(x, y) \text{ for } (x, y) \in \text{Supp}(\mu \otimes \nu)\}$ and $\iota_C$ is the convex indicator function of the convex set $C$. As a standard result in optimal transport theory, under mild conditions on the cost $c(x, y)$ the supremum is attained and the functions $f_*, g_*$ satisfying the so-called potentials, are $c$-convex functions, see [29]. In what follows, we focus on the usual quadratic case $c(x, y) = \frac{1}{2}\|x - y\|^2$ for which Equation (2) can be equivalently rewritten as

$$\text{OT}(\mu, \nu) = \frac{1}{2}(m_2(\mu) + m_2(\nu)) - \inf_{f, g} \langle f, \mu \rangle + \langle g, \nu \rangle + \iota_{C'(\mu, \nu)}(u, v),$$

where $C'(\mu, \nu) \overset{\text{def}}{=} \{(f, g) \in C^0(B) \times C^0(B); \langle x, y \rangle \leq f(x) + g(y) \text{ for } (x, y) \in \text{Supp}(\mu \otimes \nu)\}$ and $m_2(\eta) \overset{\text{def}}{=} \langle \|x\|^2, \eta \rangle$ is the second moment of the measure $\eta$. The moment terms of $\mu$ and $\nu$ can be estimated statistically in $1/\sqrt{n}$ where $n$ is the number of samples and the difficulty lies estimating the infimum. Hence, we shall only focus on this term in the rest of the paper and by a slight abuse of notation, we shall denote

$$\text{OT}(\mu, \nu) = \inf_{f, g} \langle f, \mu \rangle + \langle g, \nu \rangle + \iota_{C'(\mu, \nu)}(u, v).$$

Formulation (4) shows that the optimal potentials can be chosen as convex functions. In the following, we will assume that the optimal potentials $f_*, g_*$ satisfy the following assumption

**Assumption 1.** There exists $s > d + 1$ such that $f_*, g_* \in H^{s+2}(B)$ where $H^s(B)$ is the Sobolev space

$$H^s(B) = \left\{ f \in L^2(B), \sum_{|\beta| \leq k} \int_B \left( \frac{\partial^\beta f}{\partial x^\beta}(x) \right)^2 dx < \infty \right\},$$

where $s > d/2 + k$ with $k \geq 0$. $H^s(B)$ is continuously embedded in $C^k(B)$ (the space of $k$-times differentiable and continuous functions on $B$) endowed with the sup norm and it is a reproducing kernel Hilbert space if $s > d/2$. Another important property used in the representation result is that $H^s$ is a Hilbert algebra when $s > d/2$, i.e. the multiplication is a bounded bilinear operator on $H^s$. Since we apply these properties on $H^s(B \times B)$, it requires at least $s > d$. Therefore, Assumption 1 implies that the potentials belong to $C^{(d/2)+3}(B)$.

Let us discuss the range of validity of this assumption and its consequences. First, regularity of minimizers of optimal transport for the quadratic cost is a deeply studied problem in mathematical analysis. The work of [24] gives sufficient conditions on the distributions $(\mu, \nu)$ that ensure smoothness of the optimal potentials, as follows:

**Theorem 2.1.** Let $X, Y$ be two bounded open subsets of $\mathbb{R}^d$, let $c$ be the quadratic cost $c(x, y) = \frac{\|x - y\|^2}{2}$ and $k \geq 0$. If $(\mu, \nu)$ admit densities $(f, g) \in C^k(X) \times C^k(Y)$, bounded away from zero and infinity, and $Y$ is convex, then the optimal map $T = \nabla u$ sending $\mu$ onto $\nu$ is $C^{k+1}$.

Note that we will use the notation $T$ for the optimal map sending $\mu$ to $\nu$. Second, the $C^2$ regularity of $f_*$ is implied by the fact that $s > d + 3 > d/2 + 2$ and as a consequence, $g_*$ is strongly convex as stated in the next lemma.

**Lemma 2.2.** If $f_*, g_*$ are in $H^{r+2}(B)$ for $r > d/2$, then $g_* = f_*^*$, the Legendre transform of $f_*$ is $\frac{1}{\kappa}$-strongly convex if $\kappa$ is a uniform bound on the Hessian of $f_*$. The proof of the lemma is standard and is postponed in Appendix B.
3 Representation theorem and tight reformulation

We start with the following representation result on the structure of the optimal potentials, which is one of our main contributions in this paper.

**Theorem 3.1.** Let \( \mu, \nu \in \mathcal{P}(B) \) be two probability measures. Under Assumption 1, there exists \( A_* \) a positive, self-adjoint and finite rank operator \( A_* : H^*(B \times B) \to H^*(B \times B) \), such that

\[
f_*(x) + g_*(y) - \langle x, y \rangle = \langle \phi((x, y)), A_* \phi((x, y)) \rangle, \tag{6}
\]

where \( \phi((x, y)) = k((x, y), \cdot) \) with \( k \) the reproducing kernel associated with the Sobolev space \( H^s(B \times B) \).

This result relies on the use of the Morse lemma with parameters, whose proof is standard [13] and recalled in Appendix A.1. However, taking care of the smoothness of the functions introduced in the Morse lemma requires some additional work, done in the following corollary.

**Corollary 3.2.** Let \( f : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R} \) defined by \( f(x, y) \overset{\text{def.}}{=} u(x) + v(y) - \langle x, y \rangle \geq 0 \) and \( (x_0, y_0) \in B \times B \) such that \( f(x_0, y_0) = 0 \). Assuming \( u, v \in H^{s+2}(B) \) and \( v \) is strongly convex in neighborhood of \( y_0 \), it holds in a neighborhood \( V \) of \( (x_0, y_0) \)

\[
f(x, y) = \frac{1}{2} (z(x, y), \partial_{yy} v(0) z(x, y)), \tag{7}
\]

where \( z(x, y) \in H^s(V) \).

**Proof.** Since \( v \) is strongly convex, the Hessian of \( f \) w.r.t \( y \) is non-singular for every \( y \) in a neighborhood of \( y_0 \) and in particular at \( y_0 \). Then, \( f \) being \( C^2 \) (in fact at least \( C^3 \)), the Morse lemma can be applied. Using the proof of the Morse lemma A.1, we have that

\[
a_{ij}(x, y) = 2 \int_0^1 (1 - t) \partial_{ij} v(t(0 - Y(x)) + Y(x)) dt. \tag{8}
\]

It remains to prove that \( a_{ij} \) is indeed in \( H^s(B \times B) \). The first remark is that \( \varphi : (x, y) \to (x, y - Y(x)) \) is a local \( C^1 \) diffeomorphism which belongs to \( H^{s+1}(B \times B) \). Now, we use the fact that for \( r > d+1 \), the composition map \( H^r(B \times B) \times \text{Diff}^r(B \times B) \to H^s(B \times B) \) defined by \( (g, \psi) \mapsto g \circ \psi \) is a \( C^0 \) map, as proven in [16, Theorem 1.1], on \( \psi(x, y) \overset{\text{def.}}{=} (Y(x), y - Y(x)) \) and \( g(x, y) = \partial_{ij} v(ty + x) \). Note that the map \( g \) is \( H^s \) by direct computation and the map \( \psi \) is an \( H^s \) local diffeomorphism. Since \( s > d + 1 \), the hypothesis in [16, Theorem 1.1] on \( r \) is satisfied. Then, Bochner integration implies that \( a_{ij} \) is bounded in \( H^s \).

Last, since the product is a bilinear continuous map in \( H^r(B \times B) \) when \( r > d \), \( C(x, y)(y - Y(x)) \) belongs to \( H^s(B \times B) \).

**Proof of Theorem 3.1.** Corollary 3.2 can be applied at every point of the optimal transport graph \( (x, T(x)) \in \text{Int}(B \times B) \). In order to apply it at a point on the boundary, we apply Whitney’s extension theorem [14] on \( g_* \) to extend it smoothly \( C^2 \) on a neighborhood of \( B \). Therefore, the strong convexity of \( g_* \) still holds on a possibly smaller convex neighborhood of \( B \) and then, taking the Legendre transform of \( g_* \), one defines an extension of \( f_* \) for which \( f_* + g_* - c \geq 0 \). Thus,
one can also apply Corollary 3.2 also on the boundary. Indeed, Assumption 1 also applies to this neighborhood of $B$ and Corollary 3.2 gives at each point $x$ a neighborhood of $(x,T(x))$ on which

$$f_*(x) + g_*(y) - \langle x, y \rangle = \frac{1}{2} \langle z(x,y), \partial_{y} v(0) z(x,y) \rangle,$$

where $z(x,y) \in H^s(B \times B)$ and $\partial_{x} v(0)$ is a SDP matrix whose rank is equal to $d$ due to the strong convexity of $v$.

By compactness of the graph $\{(x,T(x)) : x \in B\}$, there exists a finite covering of balls $(B_i)_{i=1,...,k}$ on which the conclusion of Morse’s lemma applies. By standard arguments recalled in Lemma (B.1), there exists a partition of unity of the form $(\omega_i^2)_{i=1}^k$, i.e. $\sum_{i=1}^k \omega_i(x,y)^2 = 1$ with smooth functions $\omega_i$, we get the following equality on a neighborhood of the optimal transport graph $\{(x,T(x)) \in B \times B\}$, for $A_i$ SDP matrices,

$$f_*(x) + g_*(y) - \langle x, y \rangle = h(x,y)$$

where

$$h(x,y) \overset{\text{def.}}{=} \frac{1}{2} \sum_{i=1}^k \langle \omega_i(x,y) z_i(x,y), A_i(\omega_i(x,y) z_i(x,y)) \rangle.$$  

This formula only holds on a neighborhood $V$ on the optimal transport graph, but again choose a partition of unity $v_0^2(x,y) + v_1^2(x,y) = 1$ such that $v_0^2(x,y) = 0$ if $(x,y) \notin V$. One can now write

$$f_*(x) + g_*(y) - \langle x, y \rangle = h(x,y) \omega_0(x,y)^2 + (\omega_1(x,y) \sqrt{h(x,y)})^2,$$

where $\sqrt{h(x,y)} \overset{\text{def.}}{=} \sqrt{f_*(x) + g_*(y) - \langle x, y \rangle}$. The point is that $\omega_1(x,y) \sqrt{h(x,y)} \in H^s$ since $\sqrt{h(x,y)}$ is in $H^s$ outside $V$ and on $V$, $\omega_1$ vanishes. Since $\omega_i$ are smooth functions and $z_i(x,y) \in H^s$ then $\omega_i(x,y) z_i(x,y) \in H^s$. Therefore, $A_i$ exists and its rank is bounded by $kd + 1$.

It is now possible to solve the optimal transport problem on a set of non-negative functions which can be represented as a sum-of-squares.

**Corollary 3.3.** Under Assumption 1, OT can be solved with a supplementary variable $A$ a trace class positive self-adjoint operator on $H^s(B \times B)$,

$$\text{OT}_{\lambda,\eta_1,\eta_2}(\mu, \nu) = \inf_{f,g,A} \{ f, \mu \} + \{ g, \nu \}$$

s.t.

$$\forall (x,y) \in B \times B, f(x) + g(y) - \langle x, y \rangle = \{ \phi((x,y)), A \phi((x,y)) \},$$

$$\text{tr}(A) \leq \lambda, \| f \|_{H^s(B)} \leq \eta_1, \| g \|_{H^s(B)} \leq \eta_2.$$  

In particular, when $\lambda \geq \text{tr}(A_i), \eta_1 \geq \| f_i \|_{H^s(B)}$ and $\eta_2 \geq \| g_i \|_{H^s(B)}$, we have

$$\text{OT}_{\lambda,\eta_1,\eta_2}(\mu, \nu) = \text{OT}(\mu, \nu).$$

In the rest of the paper, we will denote by $\text{OT}^*(\mu, \nu) = \text{OT}_{\text{tr}(A_i),\| f_i \|_{H^s(B)},\| g_i \|_{H^s(B)}}(\mu, \nu)$. With a little abuse of notations, we will also denote $c(x,y) = \langle x, y \rangle$ to write the inequality constraint as $f \oplus g - c \geq 0$ where $f \oplus g : B \times B \to \mathbb{R}$ is given by $(f \oplus g)(x,y) = f(x) + g(y)$. We conclude this section with a standard lemma needed for the use of sampling inequalities.

**Lemma 3.4.** Let $A$ be a trace class, positive self-adjoint operator on a Hilbert algebra $\mathcal{H}$ which is also a RKHS. Then,

$$\| A(\phi(x,y), \phi(x,y)) \|_{\mathcal{H}} \leq M \text{tr}(A),$$

where $M$ is a constant bounding the multiplication operator in $\mathcal{H}$, i.e. $\| fg \|_{\mathcal{H}} \leq M \| f \|_{\mathcal{H}} \| g \|_{\mathcal{H}}$. 

6
Its proof is postponed in Appendix B. In what follows, the operator $A$ is a trace-class positive self-adjoint operator on the RKHS $H^s(B \times B)$.

## 4 Sampling the equality constraint

Instead of solving the problem with the equality constraint over $B \times B$, we sample this constraint as $(\hat{w}, \hat{z}) \sim \mathcal{U}(B \times B)$, the uniform measure on $B \times B$ and we denote the samples $(\hat{w}_i, \hat{z}_i)_{1 \leq i \leq n}$. Our new approximate problem is

$$\inf_{f: s.t.} \langle f, \mu \rangle + \langle g, \nu \rangle$$

where $\mu$ and $\nu$ are defined on the finite dimensional space.

**Lemma 4.1.** A minimizer $f_*, g_*$ of $\hat{\text{OT}}^s(\mu, \nu)$ exists.

**Proof.** We first show that the optimization can be reduced to a set of self-adjoint operator $A$ that are defined on the finite dimensional space.

Consider the space $H_n \subset H^s(B \times B)$ spanned by the functions $k((\hat{w}_i, \hat{z}_i), \cdot)$ for $i = 1, \ldots, n$: $H_n \overset{\text{def.}}{=} \text{Vect}[k((\hat{w}_i, \hat{z}_i), \cdot)]$. It is possible to define the projected operator $p(A)$ on this finite dimensional space which is given by the self-adjoint operator $p(A)(f, g) \mapsto A(\pi_{H_n}(f), \pi_{H_n}(g))$ with $\pi_{H_n} : H \rightarrow H$ the orthonormal projection on $H_n$. By the definition of the trace, one has $\text{tr}(p(A)) \leq \text{tr}(A)$. Importantly, the set of SDP matrices with finite trace is compact.

Therefore, the optimization problem $\hat{\text{OT}}^s$ can be reduced to a compact set for the self-adjoint operator and using the weak topology on the balls of $H^s(B)$ for which the linear objective is continuous, the existence of a minimizer follows by usual compactness argument.

The optimal potentials $(f_*, g_*)$ of $\text{OT}(\mu, \nu)$ satisfy the constraints of $\hat{\text{OT}}^s(\mu, \nu)$, hence by definition of the infimum

$$\hat{\text{OT}}^s(\mu, \nu) \leq \text{OT}(\mu, \nu).$$

**Proposition 4.3.** Let $(\hat{w}_i, \hat{z}_i)_{1 \leq i \leq n}$ be a collection of samples in $B \times B$. If $\hat{h} < \frac{M c_9}{c_8}$, with $c_9$ a strictly positive universal constant, then

$$\text{OT}(\mu, \nu) \leq \hat{\text{OT}}^s(\mu, \nu) + C_{s,d,R} \hat{h}^{s-d} (M \text{tr}(A_*) + \| f_* \oplus g_* - c \|_{H^s(B \times B)}),$$

where $C_{s,d} > 0$ is a constant that only depends on the smoothness level $s$ and the ambient dimension $d$ and $M$ is the constant of Lemma 3.4.
Proposition 5.1. Conditionally on the sampling of $B \times B$ we have the following behavior

$$
\mathbb{E}||\hat{\text{OT}}^*(\hat{\mu},\hat{\nu}) - \hat{\text{OT}}^*(\mu,\nu)||((\hat{w}, \hat{z})) \leq \frac{C(||f_s||_{H^s(B)} + ||g_s||_{H^s(B)})}{\sqrt{m}},
$$

where $C$ is a positive universal constant only depending on $s, d$ and $B$. 

5 Sampling the measures

We now sample the measures $\hat{\mu} = (\hat{x}_i)_{1 \leq i \leq m}, \hat{\nu} = (\hat{y}_i)_{1 \leq i \leq m}$. We are interested in solving

$$
\hat{\text{OT}}^*(\hat{\mu},\hat{\nu}) = \inf_{f,g,A} \langle f, \hat{\mu} \rangle + \langle g, \hat{\nu} \rangle \\
\text{s.t. } \forall j, (f \oplus g)(\hat{w}_j, \hat{z}_j) - c(\hat{w}_j, \hat{z}_j) = \langle \phi((\hat{w}_j, \hat{z}_j)), A\phi((\hat{w}_j, \hat{z}_j)) \rangle, \\
\text{tr}(A) \leq \text{tr}(A_s), ||f||_{H^s(B)} \leq \frac{\text{tr}(A_s)}{s} ||f_s||_{H^s(B)}, ||g||_{H^s(B)} \leq ||g_s||_{H^s(B)}. 
$$

The following theorem shows that this estimator is statistically efficient.

Proof. By Lemma 4.1, an optimal solution to $\hat{\text{OT}}^*(\mu,\nu)$ exists. We denote by $(\hat{f}_s, \hat{g}_s, \hat{A}_s)$ a solution of $\hat{\text{OT}}(\mu,\nu)$ and $\hat{\gamma}_s = \hat{f}_s \oplus \hat{g}_s - c - \langle \phi, \hat{A}_s \phi \rangle$. We have for all $j \in \{1, \ldots, n\}$

$$
\hat{\gamma}_s((\hat{w}_j, \hat{z}_j)) = 0. 
$$

Since $\hat{\gamma}_s \in H^s(B \times B)$ and $B \times B$ satisfies an interior cone condition with $\theta = 2 \arcsin(\frac{\sqrt{2}}{\sqrt{m}}) > 0$, we can apply [34, Theorem 2.6]: if the fill distance $\hat{h}$ satisfies

$$
\hat{h} < \frac{Rc_\theta}{8s^2},
$$

where $c_\theta$ is a strictly positive constant only depending on $\theta$, then the supremum of $\hat{\gamma}_s$ is upper bounded as

$$
\|\hat{\gamma}_s\|_{\infty} \leq C\hat{h}^{s-d} \|\hat{\gamma}_s\|_{H^s(B \times B)},
$$

where $C$ is a universal constant depending on $s, d$ and $\theta$. Now recall that the norm $\hat{\gamma}_s$ can be bounded as

$$
\|\hat{\gamma}_s\|_{H^s(B \times B)} \leq M \text{tr}(A_s) + \|c - f_s \oplus g_s\|_{H^s(B \times B)}.
$$

Hence denoting $\delta_h = C\hat{h}^{s-d}(M \text{tr}(A_s) + \|f_s \oplus g_s - c\|_{H^s(B \times B)})$, we can write

$$
\hat{f}_s \oplus \hat{g}_s - c \geq -\delta_h.
$$

The candidate potentials $(\hat{f}_s(\cdot) + \frac{\delta_h}{2}, \hat{g}_s(\cdot) + \frac{\delta_h}{2})$ satisfy the inequality constraints of OT in formulation (3). Hence, by definition of the infimum, we have the upper bound

$$
\text{OT}(\mu,\nu) \leq \langle \hat{f}_s(\cdot) + \frac{\delta_h}{2}, \mu \rangle + \langle \hat{g}_s(\cdot) + \frac{\delta_h}{2}, \nu \rangle,
$$

which gives the desired result. \qed
Proof. Let \((\hat{f}, \hat{g})\) a pair of optimal potentials for the problem \(\hat{OT}^* (\mu, \nu)\) and \((\tilde{f}, \tilde{g})\) a pair of optimal potentials for the problem \(\tilde{OT}^* (\mu, \nu)\). Conditionally on the sampling of \(B \times B\), both problems share the same constraints hence we can write

\[
\begin{align*}
\hat{OT}^* (\mu, \nu) &\leq \langle \hat{f}, \mu \rangle + \langle \hat{g}, \nu \rangle \\
\tilde{OT}^* (\hat{\mu}, \hat{\nu}) &\leq \langle \hat{f}, \mu \rangle + \langle \hat{g}, \nu \rangle.
\end{align*}
\]

\(\iff\)

\[
\begin{align*}
\hat{OT}^* (\mu, \nu) &\leq \tilde{OT}^* (\hat{\mu}, \hat{\nu}) + \langle \tilde{f}, \mu - \hat{\mu} \rangle + \langle \tilde{g}, \nu - \hat{\nu} \rangle \\
\hat{OT}^* (\hat{\mu}, \hat{\nu}) &\leq \tilde{OT}^* (\mu, \nu) + \langle \tilde{f}, \mu - \hat{\mu} \rangle + \langle \tilde{g}, \nu - \hat{\nu} \rangle.
\end{align*}
\]

Hence, writing the dual \(H^*(B)\) norm for a Radon measure \(\pi\) as

\[
\| \pi \|_{(H^*(B))^*} = \sup_{\| f \|_{H^*(B)} \leq 1} \langle f, \pi \rangle,
\]

we obtain using this notation

\[
|\hat{OT}^* (\mu, \nu) - \tilde{OT}^* (\hat{\mu}, \hat{\nu})| \leq \| f_s \|_{H^*(B)} \| \mu - \hat{\mu} \|_{(H^*(B))^*} + \| g_s \|_{H^*(B)} \| \nu - \hat{\nu} \|_{(H^*(B))^*}.
\]

Applying [2, Lemma 22], we can bound in average the dual norms above as

\[
\mathbb{E}[\| \mu - \hat{\mu} \|_{(H^*(B))^*} (\hat{\nu}, \hat{\nu})] \leq \frac{4 \sqrt{k_{\infty}}}{\sqrt{m}}.
\]

where \(k_{\infty} = \sup_{x \in B} k(x, x)\), the supremum on the diagonal on \(B \times B\) of the reproducing kernel of \(H^*(B)\). Hence we obtain our final result

\[
\mathbb{E}[|\hat{OT}^* (\hat{\mu}, \hat{\nu}) - \tilde{OT}^* (\mu, \nu)| (\hat{\nu}, \hat{\nu})] \leq \frac{4 \sqrt{k_{\infty}} (\| f_s \|_{H^*(B)} + \| g_s \|_{H^*(B)})}{\sqrt{m}}.
\]

Before removing the conditional average and obtain our final approximation result of optimal transport, we need standard results controlling the behavior of \(\hat{h}\) with high probability. Note the statements below were shown in a more general form in [26]. However, since our setting is simpler, we include a direct proof for self-containedness in Appendix B.

**Lemma 5.2.** Let \(B\) a ball of \(\mathbb{R}^d\) of center \(x_B\) and radius \(R\). Then, for a uniform sampling \(\tilde{y} = (\tilde{y}_1, \cdots, \tilde{y}_n)\) of \(B\), the fill distance \(\hat{h} = \sup_{x \in B} \inf_{i} \| x - \tilde{y}_i \|_2\) that, with probability at least \(1 - \delta\), if \(n \geq n_0(R, d)\), then the following upper bound holds

\[
\hat{h} \leq C n^{-1/d} \left[\log \left( \frac{n}{\delta} \right) \right]^{2/d},
\]

where \(C > 0\) is a positive constant depending on \(R, d\).

From this lemma, we can deduce a similar upper bound when the sampling is done uniformly on \(B \times B\). The proof of these two results can be found in Appendix B.

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Corollary 5.3. Denoting the sampling \((\hat{w}, \hat{z}) = ((\hat{w}_i, \hat{z}_i)_{1 \leq i \leq n})\) such that \((\hat{w}, \hat{z}) \sim \mathcal{U}(B \times B)\), if \(n \geq n_0\) where \(n_0 = n_0(R, d)\), then with probability at least \(1 - \delta\),

\[
\hat{h} \leq C n^{-1/(2d)} \left[ \log \left( \frac{n}{\delta} \right) \right]^{1/d},
\]

where \(C > 0\) is a positive constant depending on \(R, d\).

We can now state our approximation result.

Proposition 5.4. Choosing \(n\) such that \(n \log(n)^{-1} \geq C_1(1 + \frac{s}{2d}) s^{2d}\) where \(C_1\) is a strictly positive constant depending on \(d\) and \(R\), we have

\[
\mathbb{E}[\| OT(\mu, \nu) - \hat{OT}^*(\hat{\mu}, \hat{\nu})\|] \leq \left( m^{-1/2} + C_2 \left( \frac{1}{\sqrt{n}} \right)^{(s/d)-1} \log(n)^{s-d} \right),
\]

where \(C_2\) is a strictly positive constant depending on \(s, d, R, \text{tr}(A), \|f_*\|_{H^r(B)}, \|g_*\|_{H^r(B)}\) and \(\hat{OT}(\mu, \nu)\).

Proof. Denoting for \(0 < \delta < 1\), \(\alpha_{n, \delta} = C n^{-1/(2d)} \left[ \log \left( \frac{n}{\delta} \right) \right]^{1/d}\), where \(C\) is the constant in Lemma 5.2, the term \(\mathbb{E}[\| OT(\mu, \nu) - \hat{OT}(\hat{\mu}, \hat{\nu})\|]\) can be decomposed as following

\[
\mathbb{E}[\| OT(\mu, \nu) - \hat{OT}^*(\hat{\mu}, \hat{\nu})\|] = \mathbb{P}(\hat{h} \leq \alpha_{n, \delta}) \mathbb{E}[\| OT(\mu, \nu) - \hat{OT}^*(\hat{\mu}, \hat{\nu})\| | \hat{h} \leq \alpha_{n, \delta}] \]

(43)

\[
+ \mathbb{P}(\hat{h} > \alpha_{n, \delta}) \mathbb{E}[\| OT(\mu, \nu) - \hat{OT}^*(\hat{\mu}, \hat{\nu})\| | \hat{h} > \alpha_{n, \delta}],
\]

(44)

The term (43) can be upper-bounded as

\[
\mathbb{P}(\hat{h} \leq \alpha_{n, \delta}) \mathbb{E}[\| OT(\mu, \nu) - \hat{OT}^*(\hat{\mu}, \hat{\nu})\| | \hat{h} \leq \alpha_{n, \delta}] \leq \mathbb{E}[\| OT(\mu, \nu) - \hat{OT}^*(\hat{\mu}, \hat{\nu})\| | \hat{h} \leq \alpha_{n, \delta}]
\]

(45)

\[
+ \mathbb{E}[\| \hat{OT}^*(\mu, \nu) - \hat{OT}^*(\hat{\mu}, \hat{\nu})\| | \hat{h} \leq \alpha_{n, \delta}].
\]

(46)

Assuming \(\alpha_{n, \delta} \leq \frac{Rc}{s_{\delta s^2}}\), we can apply Proposition 4 and Proposition 5.1, yielding the upper bound

\[
(43) \leq \frac{C}{\sqrt{m}} + C_{s,d,R} \alpha_{n, \delta}^{s/d}(M \text{tr}(A) + \|f_* \oplus g_* - c\|_{H^r(B)}).
\]

(47)

Now, according to Lemma 5.2, we have the upper bound \(\mathbb{P}(\hat{h} > \alpha_{n, \delta}) \leq \delta\). Hence, the term (44) is upper-bounded by

\[
(44) \leq \delta \mathbb{E}[\| OT(\mu, \nu) - \hat{OT}^*(\hat{\mu}, \hat{\nu})\| | \hat{h} > \alpha_{n, \delta}].
\]

(48)

Recalling that almost surely,

\[
\hat{OT}^*(\hat{\mu}, \hat{\nu}) \leq \|f_*\|_{\infty} + \|g_*\|_{\infty} \leq \text{cste}(\|f_*\|_{H^r(B)} + \|g_*\|_{H^r(B)}),
\]

(49)

we can write (44) \(\leq \delta (OT(\mu, \nu) + \text{cste}(\|f_*\|_{H^r(B)} + \|g_*\|_{H^r(B)})).\) Fixing \(\delta = \left( \frac{1}{\sqrt{m}} \right)^{(s/d)-1}\), we obtain
that if \( n^{-1/d} \log(n) \approx (1 + \frac{1}{2d})^{1/d} \leq \frac{R_{\alpha}}{8d} \), then
\[
\mathbb{E}[\|\hat{O}_T(\mu, \nu) - \hat{O}_T^*(\hat{\mu}, \hat{\nu})\|] \leq \frac{C}{\sqrt{m}} \quad (50)
\]
\[+ \text{cste} \left( \frac{1}{\sqrt{n}} \right)^{(s/d)-1} (\log(n))^{\frac{3d}{4}} (M \text{tr}(A_*) + \|f_* \oplus g_* - c\|_{H^*(B)}) \quad (51)
\]
\[+ \left( \hat{O}_T(\mu, \nu) + \text{cste} (\|f_*\|_{H^*(B)} + \|g_*\|_{H^*(B)}) \left( \frac{1}{\sqrt{n}} \right)^{(s/d)-1} \right). \quad (52)
\]

6 Kernel trick and main result

The usual kernel trick can be applied on the minimization of \( \hat{O}_T^* \) in order to obtain a convex optimization algorithm to solve it.

**Proposition 6.1.** The model \( \hat{O}_T^*(\hat{\mu}, \hat{\nu}) \) admits the following finite parametrization
\[
\hat{O}_T^*(\hat{\mu}, \hat{\nu}) = \inf_{(\alpha, \beta) \in \mathbb{R}^m, A \in S^+_m} \frac{1}{m} (1K_\mu \alpha + 1K_\nu \beta)
\]
\[\text{s.t. } \forall j, [K_\mu]_j \alpha + [K_\nu]_j \beta - c(w_j, z_j) = \Phi_j^T A \Phi_j, \quad (54)
\]
\[\alpha^T K_\mu \alpha \leq \|f_*\|_{H^*(B)}^2, \beta^T K_\nu \beta \leq \|g_*\|_{H^*(B)}^2, \text{tr}(A) \leq \text{tr}(A_*) \quad (55)
\]

where \( S^+_m \) is the cone of SDP matrices of size \( n \times n \), \( \Phi_j \) is the \( j \)-th column of the upper triangular cholesky decomposition of the matrix \( K = (k((\hat{w}_i, \hat{z}_j), (\hat{w}_j, \hat{z}_j)))_{ij}, K_\mu = (k_1(\hat{x}_i, \hat{x}_j))_{ij}, K_\nu = (k_1(\tilde{y}_i, \tilde{y}_j))_{ij}, K_{\hat{w}, \hat{\nu}} = (k_1(\hat{w}_i, \tilde{x}_j))_{ij} \) and \( K_{\hat{z}, \hat{\nu}} = (k_1(\tilde{z}_i, \tilde{y}_j))_{ij} \) where \( k \) is the reproducing kernel of \( H^*(B \times B) \) and \( k_1 \) is the reproducing kernel of \( H^*(B) \).

**Proof.** This reduction follows from the two following simple observations. First, \( \hat{O}_T^* \) can be minimized for a fixed operator \( A \) with respect to \( f, g \) which implies that \( f \) can be represented as \( f = k \ast \alpha \) and \( g = k \ast \beta \) where \( k \) is the kernel associated with the RKHS \( H^*(B) \).

The reduction on a finite dimensional subspace for the self-adjoint operator is done in the proof of Lemma 4.1, where we used the orthogonal projection (which is norm decreasing) of \( A \) onto \( H_n \) def. \( \text{Vect}([k((x_i, y_i), \cdot)])) \).

Last, computing the Cholesky decomposition of \( K \), one can choose the corresponding orthonormal basis\(^1\) w.r.t. the RKHS norm to represent \( A \); i.e. \( \text{Id}_n = \Phi^{-T} K \Phi^{-1} \) which implies Formula (54). \( \square \)

There is no straightforward result upper-bounding the complexity of the program (53), since it is a mix of semi-definite and second order cone programs. Fortunately, it can be re-written as a large standard semi-definite problem, optimizing on symmetric positive \((2m + n + 1) \times (2m + n + 1)\) matrices and with \( p(n, m) = (1 + 2n + 2m + 2n \times m + m^2 + (m - 1)^2) \) constraints.

\(^1\)The kernel of \( H^* \) leads to non-singular kernel matrix since it is universal.
Proposition 6.2. The problem \((53)\) can be re-written in a standard semi-definite programming (dual) form as

\[
(53) \iff \begin{cases} 
\max_{X \in S_{2m+n+1}^+} \text{tr}(CX) \\
\text{tr}(A_iX) = b_i, \forall i \in \{1, \ldots, p(m,n)\}
\end{cases}
\]

where \(C\) and the \(A_i\) are symmetric matrices in \(\mathbb{R}^{(2m+n+1)^2}\) such that for \(i \geq n + 2\), the matrix \(A_i\) has at exactly 2 non-zero coefficients.

The proof is left in Appendix B. Because of the large number of constraints, solving naively \((56)\) with a precision \(\epsilon\), using for instance the algorithm described in [21, Section 11.3], has a \(\tilde{\mathcal{O}}((m+n)^{0.5} \log(1/\epsilon))\) worst case complexity, where the notation \(\tilde{\mathcal{O}}\) hides poly-log factors. We believe that this reformulation is very sub-optimal and that problem \((53)\) can be solved with a \(\tilde{\mathcal{O}}((m+n)^{\gamma} \log(1/\epsilon))\) worst case complexity with \(\gamma \leq 4.5\). However, refining this bound is beyond the scope of this study.

We can now state our main result.

Theorem 6.3. Under Assumption 1, setting \(m = \epsilon^{-2}\) and \(n = (\frac{1}{\epsilon})^{2/(s/d-1)} \log(\frac{1}{\epsilon})^2\), the estimator \(\hat{\text{OT}}^*(\hat{\mu}, \hat{\nu})\) can be computed in \(\tilde{\mathcal{O}}((\epsilon^{-2} + \epsilon^{-2/(s/d-1)})^\gamma)\) time and when \(\epsilon\) is sufficiently small, it reads

\[
\mathbb{E}\| \text{OT}(\mu, \nu) - \hat{\text{OT}}^* (\hat{\mu}, \hat{\nu}) \| \leq C \epsilon,
\]

where \(C\) is a constant that depends on \(\text{OT}(\mu, \nu), \|f_*\|_{H^s(B)}, \|g_*\|_{H^s(B)}, s, R\) and \(d\).

In particular, when \(s/d - 1 \geq 1\), i.e. \(s \geq 2d\), the term \(\epsilon^{-2}\) is dominant and the complexity is \(\tilde{\mathcal{O}}(\epsilon^{-2s})\). Otherwise, the complexity scales as \(\tilde{\mathcal{O}}(\epsilon^{-2s/(s/d-1)})\) when \(s < 2d\).

7 Discussion

For readability, we presented this result in a simple setting. (1) The measures are supported on the same Euclidean ball. It is certainly not difficult to adapt the proofs under the assumptions on the support of the measures used in Theorem 2.1. (2) The constrained formulation of OT via semi-infinite programming and its finite dimensional version make use of hard constraint. We expect a soft constraint formulation to work as well, while being more adaptive.

There are a few interesting directions to be explored following our result. First, the rates obtained in this paper are valid in the regime of sampling inequalities and therefore they suffer from large constants. This rather theoretical contribution encourages the design of numerical algorithms that can achieve these rates for a reasonable amount of samples. It would be interesting to check experimentally the behavior of the proposed algorithm in practice for a number of samples out of the regime of application.

Second, it is natural to ask whether it is possible to extend the result to other costs. While it seems possible under smoothness and mild assumptions on the cost and the minimizers, these hypothesis do not transfer directly to hypothesis on the measures themselves unless regularity results hold for this cost. Such results are available in the literature and known under the name of Ma-Trudinger-Wang (MTW) condition which gives guarantees for the optimal map to be smooth.
when the measures are smooth (and other mild assumptions). However, the MTW condition is quite restrictive on the set of costs and the set of geometries [17].

Last, our representation result suggests that the results in [26] could be extended to other settings of interest where the set of global minimizers of the function is not discrete.

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The Morse Lemma with parameters

The Morse Lemma with parameters is proven in [13] and stated in the smooth $C^{\infty}$ case. The following theorem is a rewriting of [13] included here for completeness. The slight difference is that we need this theorem stated with less differentiability assumptions.

**Theorem A.1.** Let $f : \mathbb{R}^d \times \mathbb{R}^n \mapsto \mathbb{R}$ be a $C^2$ function. Assume that $\partial_y f(0, 0) = 0$ and that $\partial_{yy} f(0, 0)$ is non-singular. Then, the equation $\partial_y f(x, y) = 0$ defines a map $Y(x)$ in a neighborhood of $(0, 0)$ such that in a neighborhood of $(0, 0)$, one has

$$f(x, y) = f(x, Y(x)) + \frac{1}{2} \langle z(x, y), \partial_{xx} f(0, 0) z(x, y) \rangle,$$

where $z(x, y)$ is $C^0$. Moreover, the map $\varphi : \mathbb{R}^d \times \mathbb{R}^n \mapsto \mathbb{R}^d \times \mathbb{R}^n$ defined by $\varphi(x, y) = (x, y - Y(x))$ is a local $C^1$ diffeomorphism at $(0, 0)$.

**Proof.** The map $Y(x)$ is obtained by the application of the implicit function theorem to the function $\partial_y f(\cdot, \cdot)$ at point $(0, 0)$. Since the map $Y$ is $C^1$, the map $\varphi$ is a local $C^1$ diffeomorphism. Using Taylor’s formula at every point $(x, Y(x))$ in a neighborhood of $(0, 0)$, we get

$$f(x, y) - f(x, Y(x)) = \frac{1}{2} \sum_{i,j=1}^n a_{ij}(x, y)(y_j - Y_j(x))(y_i - Y_i(x)).$$

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where
\[ a_{ij}(x, y) = 2 \int_0^1 (1 - t) \partial_{ij} f(x, t(y - Y(x)) + Y(x))dt, \]
where the partial derivatives are taken w.r.t. the \( y \) variable. We thus have coefficients \( a_{ij} \) that are \( C^0 \). Thus, the matrix \( A(x, y) := [a_{ij}(x, y)] \) is a symmetric positive definite matrix in a neighborhood of 0 and is continuous w.r.t. \( x, y \). Moreover, \( A(0) = \partial_{yy} f(0, 0) \).

We are now looking for a solution \( C(x, y) \) of the following equation,
\[ C^\top(x, y)A(0, 0)C(x, y) = A(x, y), \]
where \( C \) is a symmetric matrix. This equation is satisfied at \( x, y = 0 \) for \( C = \text{Id} \). The map \( \Psi : S_n(\mathbb{R}) \to S_n(\mathbb{R}), \Psi(C) = C^\top A(0)C \) is locally invertible and smooth at \( C = \text{Id} \), therefore \( C(x, y) = \Psi^{-1}(A(x, y)) \).

Since one can now write \( A(x, y) = C^\top(x, y)A(0)C(x, y) \) as a continuous function of \( x, y \), the result is proven,
\[ f(x, y) - f(x, Y(x)) = \frac{1}{2} (C(x, y)(y - Y(x)), \partial_{xx} f(0, 0)C(x, y)(y - Y(x))). \]

We recall hereafter the classical version of the implicit function theorem in order to highlight the regularity involved, used in Corollary 3.2.

**Theorem A.2.** Let \( g : \mathbb{R}^d \times \mathbb{R}^n \to \mathbb{R}^n \) be a continuously differentiable map in a neighborhood of \((0, 0)\) such that \( g(0, 0) = 0 \) and such that \( \partial_x g \) is non-singular. Then, the equation \( g(p, x) = 0 \) has a unique solution \( X(p) \) for all \( p \) in a neighborhood of \((0, 0)\). The map \( X(p) \) is \( C^1 \) in a neighborhood of 0 and one has
\[ \partial_p X(p) = -(\partial_x g)^{-1}(\partial_p g(p, X(p))). \]

As an immediate consequence of formula (63), the regularity of \( g \) is transferred to \( X \). For instance if \( g \) is \( C^k \) for \( k \geq 1 \), then so is \( X \). Similarly, for \( r \geq 1 \) and \( D \) a ball containing \((0, 0)\) in the neighborhood of definition of \( X \), if \( g \in H^r(D) \cap C^1(D) \), then so is \( X \).

**B Other proofs**

**Proof of Lemma 2.2.** Since \( f_* \) is \( C^2 \), its Hessian \( \nabla^2 f \) can be bounded in operator norm by \( \kappa \) uniformly on the domain \( B \). It implies that the gradient \( \nabla f_* \) is a \( \kappa \)-Lipschitz map, that is
\[ \|\nabla f_*(y) - \nabla f_*(x)\| \leq \kappa\|y - x\|, \]
Since \( \nabla f_* \circ \nabla g_* = \text{Id} \) on \( B \), we get,
\[ \|y - x\| \leq \kappa\|\nabla g_*(y) - \nabla g_*(x)\|, \]
which implies, since \( g_* \) is also \( C^2 \), that \( g_* \) is \( \frac{1}{\kappa} \)-strongly convex.

The following lemma is elementary and included here for completeness.
Lemma B.1. Let $D \subset \mathbb{R}^d$ be an compact domain and a finite open cover $(V_k)_{k \in I}$ of $D$. There exists a ("squashed") partition of unity $\omega_k$ subordinate to $(V_k)_{k \in I}$ such that

$$\sum_{k \in I} \omega_k^2 = 1,$$

where $\omega_k$ are smooth functions.

Proof. Consider the smooth bump function $\text{bump}(x) = \beta(||x||+2)\beta(2-||x||)$ with $\beta(r) = \frac{\alpha(r)}{\alpha(0)}$ for $r > 0$ with $\alpha(r) = e^{-\frac{1}{r^2}}$ if $r > 0$ and 0 if $r \leq 0$. The function $\alpha$ is smooth and flat at 0, more importantly it is also the case for $\sqrt{\alpha}$. Therefore, $\sqrt{\text{bump}(x)}$ is a smooth function, as well as $\sqrt{\sum_{i=1}^k \text{bump}(\lambda_i(x-c_i))}$ with $c_i \in \mathbb{R}^d$ and $\lambda > 0$. As is standard, for each $x \in V_k$, take $\text{bump}_{x,k}$ a dilation-translation of the bump such that $\text{Supp}(\text{bump}_{x,k}) \subset V_k$ and $\text{bump}_{x,k} = 1$ on a ball $B_{x,k}$. By compactness of $D$, extract a finite cover $(B_{x,k})_{x \in I,k \in I}$ and define $\rho_k = \sum_{x \in V_k} \text{bump}_{x,k}$, then

$$\omega_k(x) = \sqrt{\sum_{i=1}^k \rho_i}$$

satisfy the requirements since $\sum_k \rho_k$ is smooth and positive everywhere on $D$. □

Proof of Lemma 3.4. Since $A$ is a positive self-adjoint operator, there exists an orthonormal basis $(e_i)_{i \in \mathbb{N}}$ of $\mathcal{H}$ such that

$$A = \sum_{i=0}^\infty \lambda_i e_i \otimes e_i,$$

Therefore, $A(\varphi(x,y), \varphi(x,y)) = \sum_{i=0}^\infty \lambda_i e_i(x,y)^2$ and its norm is bounded as follows,

$$\|A(\varphi(x,y), \varphi(x,y))\| \leq \sum_{i=0}^\infty \lambda_i \|e_i^2\| \| \leq \text{tr}(A) M.$$

Proof of Lemma 5.2. For $\alpha > 0$, we want to upper bound the probability of the event

$$A_\alpha = (\sup_{x \in B_{1,\|\cdot\|_2}} \inf_{1 \leq j \leq n} \|x - y_j\|_2 > \alpha).$$

Let $(z_1, \cdots, z_{p_\alpha})$ be a $\frac{\alpha}{2}$ covering of $(B_{1,\|\cdot\|_2})$. The covering $z$ can be chosen such that

$$p_\alpha \leq (1 + \frac{AR}{\alpha})^d,$$

see for instance [31, Proposition 1.1]. The following upper-bound holds

$$\sup_{x \in B_{1,\|\cdot\|_2}} \inf_{1 \leq k \leq p_\alpha} \|x - y_j\|_2 \leq \sup_{1 \leq k \leq p_\alpha} \inf_{1 \leq j \leq n} \|z_k - y_j\|_2 + \frac{\alpha}{2}.$$

Hence denoting the event $B_\alpha = (\sup_{1 \leq k \leq p_\alpha} \inf_{1 \leq j \leq n} \|z_k - y_j\|_2 > \frac{\alpha}{2})$, we have $A_\alpha \subset B_\alpha$. The event $B_\alpha$ can be re-written as

$$B_\alpha = \bigcup_{1 \leq k \leq p_\alpha} \left( \inf_{1 \leq j \leq n} \|z_k - y_j\|_2 > \frac{\alpha}{2} \right),$$

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and using the union bound, we have

\[ \mathbb{P}(B_n) \leq \sum_{1 \leq k \leq p_n} \mathbb{P}\left( \inf_{1 \leq j \leq n} \|z_k - y_j\|_2 > \frac{\alpha}{2} \right). \]  

(73)

Denoting, for \( x \in B, F_x \) the cumulative density function of the (independent) random variables \( \|x - y_i\|_2 \), we have

\[ \mathbb{P}(B_n) \leq \sum_{1 \leq k \leq p_n} \left[ 1 - F_{x_k}(\frac{\alpha}{2}) \right]^n \]  

(74)

\[ \leq p_n \sup_{x \in B} \left[ 1 - F_x(\frac{\alpha}{2}) \right]^n. \]  

(75)

Now recall that for fixed \( \alpha \leq 2R \), the quantity \( F_x(\frac{\alpha}{2}) \) is proportional to the volume the intersection of the intersection \( B(x, \frac{\alpha}{2}) \cap B \). When \( \|x\| + \frac{\alpha}{2} \leq R \), the ball \( B(x, \frac{\alpha}{2}) \) is contained in \( B \). When \( \|x\| \) increases and \( \|x\| + \frac{\alpha}{2} > R \), the volume of the intersection decreases and is minimal at for \( x \) on the boundary. For such \( x \), a direct application of [27, Equation (3)] shows that this volume that we denote \( \mathcal{V} \) is lower bounded as

\[ \mathcal{V}(B(x, \frac{\alpha}{2}) \cap B) \geq C_2 \alpha^d I_{1-\frac{2}{3\pi}} (\frac{d+1}{2}, \frac{1}{2}), \]  

(76)

where \( C_2 \) is a constant independent of \( \alpha \) and \( I_r(a, b) \) is the regularized incomplete beta function given by

\[ I_r(a, b) = \int_0^r t^{a-1} (1 - t)^{b-1} dt. \]  

(77)

Since \( I_r(a, b) \) increases from 0 to 1 at point \( r = 1 \), for \( \alpha \leq R \), there exists \( C'_2 \) independent of \( \alpha \) such that

\[ \mathcal{V}(B(x, \frac{\alpha}{2}) \cap B) \geq C'_2 \alpha^d \]  

(78)

leading to the upper-bound

\[ \mathbb{P}(A_n) \leq (1 + (\frac{4R}{\alpha})^d)(1 - C \alpha^d)^n. \]  

(79)

Since we assumed \( \alpha \leq R \), we have \( (1 + (\frac{4R}{\alpha})^d) \leq 2(\frac{4R}{\alpha})^d \) and taking the logarithm, we have

\[ \log(\mathbb{P}(A_n)) \leq C_1 - C_2 \log(\alpha) + n \log(1 - C \alpha^d) \]

(80)

\[ \leq C_1 - C_2 \log(\alpha) - n C \alpha^d, \]  

(81)

where \( C_1, C_2 \) are constants depending on \( R, d \) and \( C_2 > 0 \). Taking \( \alpha \) of the form \( \alpha = C_3 n^{-1/d} \log(\frac{n}{\delta})^{2/d} \), for \( 0 < \delta < 1 \) we obtain the upper bound

\[ \log(\mathbb{P}(A_n)) \leq C_1 - C_2 [-\frac{1}{d} \log(n) + \log(\frac{2}{d} \log(\frac{n}{\delta})) + \log(C_3)] - C C_3 \log(\frac{n}{\delta}))^2 \]  

(82)

\[ \leq C'_1 + C'_2 \log(n) - C''_2 \log(\log(n)) + C C'_3 (\log(\delta) - \log(n))^2. \]  

(83)

Hence, for \( n \geq n_0 \) where \( n_0 \) is a constant depending on \( R, d \), we have

\[ \log(\mathbb{P}(A_n)) \leq C C'_3 \log(\delta). \]  

(84)
Choosing $C_3 = C^{-1/d}$, we obtain that if $n \geq n_0$ then with probability at least $1 - \delta$
\[
\hat{h} \leq C n^{-1/d} \log \left( \frac{n}{\delta} \right)^{2/d},
\]for some constant $C$ solely depending on $R, d$.

\textbf{Proof of Corollary 5.3.} The proof relies on the existence of bi-lipschitz map from the unit ball of $\mathbb{R}^d$ to the unit cube of $\mathbb{R}^d$ (see [11, Corollary]) that preserves the volume. We will denote this application $\Phi^d$. Since $\Phi^d$ preserves the volume, $(\Phi^d(\hat{w} - CB), \Phi^d(\hat{z} - CB))$ is a uniform sampling of the unit cube $C^d \times C^d = C^{2d}$. Conversely, the random variable
\[
\hat{\zeta} = (\Phi^{2d})^{-1}(\Phi^d(\hat{w} - CB), \Phi^d(\hat{z} - CB))
\]is a uniform sampling of the unit sphere of $\mathbb{R}^{2d}$. Defining
\[
\hat{h}(\hat{\zeta}) = \sup_{x \in B(\mathbb{R}^{2d})} \inf \|x - \zeta_i\|_2,
\]
since the $\Phi^k$ are bi-lipschitz, there exists $L \geq 0$ such that
\[
\hat{h}(\hat{\zeta}) \geq L \hat{h}(\hat{w}, \hat{z}),
\]
where we define $\hat{h}(\hat{w}, \hat{z})$ as
\[
\hat{h}(\hat{w}, \hat{z}) = \sup_{x_1, x_2 \in B \times B} \inf \|x_1, x_2 - (\hat{w}_i, \hat{z}_i)\|_2.
\]
In particular, applying Lemma 5.2, there exists $C$ such that for $0 < \delta < 1$,
\[
P \left( \hat{h}(\hat{w}, \hat{z}) \leq C n^{-1/(2d)} \log \left( \frac{n}{\delta} \right)^{1/d} \right) \geq 1 - \delta
\]
\textbf{Proof of Proposition 5.3.} Start by making the change of variables
\[
\begin{align*}
\alpha' &= K_{\mu}^{1/2} \alpha \\
\beta' &= K_{\nu}^{1/2} \beta \\
c_1 &= \frac{1}{m} 1 K_{\mu}^{1/2} \\
c_2 &= \frac{1}{m} 1 K_{\nu}^{1/2} \\
\zeta_i &= -[K_{\hat{w}, \hat{\mu}} K_{\hat{z}, \hat{\mu}}^{-1/2}]_i \\
k_i &= -[K_{\hat{z}, \hat{\nu}} K_{\hat{z}, \hat{\nu}}^{-1/2}]_i \\
b_i &= c(\hat{w}_i, \hat{z}_i)
\end{align*}
\]
With these notations, the problem to solve becomes
\[
\sup_{\alpha, \beta, A \in S_n^*} c_1^\top \alpha + c_2^\top \beta
\]
\text{ s.t. } \forall i \in \{1, \cdots, n\}, c_1^\top \alpha + \alpha_i^\top \beta + \Phi_i^\top A \Phi_i = b_i
\]
\[
\text{tr}(A) \leq \text{tr}(A_*) , \|A\|^2_2 \leq \|f_*\|^2_2, \|\beta\|^2_2 \leq \|g_*\|^2_2.
\]
Now, let us remark that the cone constraint $\|\alpha\|^2 \leq \|f_*\|^2_{\mathcal{H}_s(B)}$ can be replaced by a semi-definite constraint $A(\alpha, \|f_*\|_{\mathcal{H}_s(B)}) \geq 0$, where

$$C(\alpha, \|f_*\|_{\mathcal{H}_s(B)}) = \left( \begin{array}{ccc} \frac{\|f_*\|_{\mathcal{H}_s(B)}}{\alpha} & \alpha^\top & \alpha \\ \alpha & \|f_*\|_{\mathcal{H}_s(B)} \times \text{Id} \end{array} \right) \quad (95)$$

Using this result, we can re-write our optimization problem as

$$\sup_{\alpha, \beta, A, \eta} \text{tr}(CX(\alpha, \beta, A, \eta)) \quad (96)$$

$$\text{s.t. } \forall i \in \{1, \cdots, n+1\}, \text{tr}(C_i X(\alpha, \beta, A, \eta)) = b_i, X(\alpha, \beta, A, \eta) \geq 0, \quad (97)$$

where for $i \leq n$

$$C_i = \left( \begin{array}{ccccc} C(\zeta_i^2, 0) & 0 & 0 & 0 \\ 0 & C(\eta_i^2, 0) & 0 & 0 \\ 0 & 0 & \Phi_i & 0 \\ 0 & 0 & 0 & 0 \end{array} \right), \quad (98)$$

and where $b_{n+1} = \text{tr}(A_*)$ and

$$C_{n+1} = \left( \begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \text{Id} & 0 \\ 0 & 0 & 0 & 1 \end{array} \right), \quad (99)$$

and where we optimize over symmetric positive matrices $X(\alpha, \beta, A, \eta)$ of the form

$$X(\alpha, \beta, A, \eta) = \left( \begin{array}{cccc} C(\alpha, \|f_*\|_{\mathcal{H}_s(B)}) & 0 & 0 & 0 \\ 0 & C(\beta, \|g_*\|_{\mathcal{H}_s(B)}) & 0 & 0 \\ 0 & 0 & A & 0 \\ 0 & 0 & 0 & \eta \end{array} \right) \quad (100)$$

To enforce this structure, we simply have to add $(n+2m+2n \times m + m^2 + (m-1)^2)$ constraints of the form $\text{tr}(C_i X) = 0$, where the $C_i$ are symmetric matrices with exactly 2 non-zeros components.