On the sample complexity of entropic optimal transport

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Abstract. We study the sample complexity of entropic optimal transport in high dimensions using computationally efficient plug-in estimators. We significantly advance the state of the art by establishing dimension-free, parametric rates for estimating various quantities of interest, including the entropic regression function which is a natural analog to the optimal transport map. As an application, we propose a practical model for transfer learning based on entropic optimal transport and establish parametric rates of convergence for nonparametric regression and classification.

1. Introduction

Thanks to remarkable computational advances [PC19], optimal transport (OT) has recently emerged as an effective tool to tackle a wide range of statistical problems that were out of reach of previous methods. Given two measures $\mu$ and $\nu$ on $\mathbb{R}^d$ and a cost function $c : \mathbb{R}^d \times \mathbb{R}^d \to [0, \infty)$, the OT problem [Vil03, Vil09] is the infinite dimensional linear optimization problem given by

$$\inf_{\pi \in \Pi(\mu, \nu)} \int c(x, y) d\pi(x, y),$$

where the infimum is taken over the set $\Pi(\mu, \nu)$ of couplings between $\mu$ and $\nu$. Recall that $\pi \in \Pi(\mu, \nu)$ is a valid coupling between $\mu$ and $\nu$ if $\pi$ is a probability measure on $\mathbb{R}^d \times \mathbb{R}^d$, such that for any measurable $A \subset \mathbb{R}^d$, it holds that $\pi(A \times \mathbb{R}^d) = \mu(A)$ and $\pi(\mathbb{R}^d \times A) = \nu(A)$. Throughout this paper, we assume that $\mu$ and $\nu$ have bounded support. Moreover, for concreteness we set $c(x, y) = \|x - y\|^2$ as in the majority of applications of OT, but our results readily extend to any cost $c$ that is uniformly bounded on the support of $\mu$ and $\nu$. In that case, (1.1) admits a unique minimizer $\pi_0$, called the OT coupling. Therefore, OT provides a principled way of selecting a non-trivial coupling between probability measures. Furthermore, Brenier’s theorem states that under mild regularity conditions on $\mu$, the OT coupling $\pi_0$ is supported on the graph of a deterministic map $T$ called the Brenier map. In other words, $(X, Y) \sim \pi_0$ if and only if $X \sim \mu$ and $Y = T(X) \sim \nu$.

The OT coupling has the following dynamical interpretation in terms of energy minimization. Consider the position $X_t$ at time $t$ of a particle in $\mathbb{R}^d$ evolving according to a time-varying velocity field $v_t : \mathbb{R}^d \to \mathbb{R}^d$ so that $dX_t = v_t(X_t)dt$. It turns out that the velocity field $\{v_t\}$ that transports a population of particles from $X_0 \sim \mu$ to $X_1 \sim \nu$ while minimizing the (kinetic) energy functional $\int \mathbb{E}\|v_t(X_t)\|^2 dt$ is given simply in terms of the Brenier map: it is the velocity field that transports $x$
to $T(x)$ at constant speed along a straight line. Moreover, the minimum energy value is given by the squared Wasserstein distance which is also the value of the minimum in (1.1). This is the Benamou-Brenier formula [San15, Prop. 5.30]. This argument extends to the case where the Brenier map may not exist and it shows that the OT coupling minimizes the energy needed to evolve a population of particles from an initial to a final distribution. This observation has fueled a conceptual shift from the traditional statistical toolbox in cases where the energy minimization perspective is justified. Indeed, the estimation of couplings between datasets has led to spectacular developments on fundamental questions in many areas including statistics [RW18, RW19], economics [TGR21], computer graphics [SdGP+15], computational biology [SST+19, LZKS21], and machine learning [CFTR17].

A central application of optimal transport is transfer learning, where the goal is to transfer information from one dataset to another using the Brenier map. For example, in [FHN+19], an estimated transport map is constructed from a labeled source dataset to an unlabeled target dataset in order to perform classification on the target dataset despite an absence of labels. This question has received a surge of interest in the context of image classification under the name domain adaptation [CFTR17]. Here, the goal is to automatically adapt image classification under shifting image conditions such as lighting. For this class of problems, optimal transport provides a natural candidate to transfer the points using the Brenier map due to its minimum energy property.

Unfortunately, a line of recent work has provided strong evidence that the OT coupling suffers from a statistical curse of dimensionality. Indeed, without further assumptions, the minimax rate for estimating the OT cost is at least $n^{-1/d}$ [NWR19], and a similar rate is conjectured to hold for the problem of estimating the Brenier map $T$ [HR21]. While recent theoretical effort has been devoted to showing that this inefficiency can be alleviated by making structural assumptions—chiefly smoothness—on the transport map, finding computationally efficient and smoothness-adaptive estimators is a challenging and ongoing research topic [FHN+19, HR21, MBNWW21, MNW21, PNW21, VMR+21, MVB+21, DGS21].

In this work, we study an alternative to the OT coupling that we call the Schrödinger coupling. It arises as the solution to the entropically regularized OT problem given by, for $\eta > 0$,

$$
\inf_{\pi \in \Pi(\mu, \nu)} \left\{ \int \|x - y\|^2 d\pi(x, y) + \frac{1}{\eta} \text{KL}(\pi \| \nu) \right\},
$$

(1.2)

where KL denotes the Kullback-Leibler divergence. This regularized problem dates back to early work of Schrödinger [Sch31, Sch32], and recently has largely eclipsed the OT coupling in applications because it offers significant computational advantages. Indeed, it can be computed extremely quickly using the Sinkhorn algorithm [Sin64, Cut13, AWR17, PC19]. Like the OT coupling, the Schrödinger coupling also arises from a minimum energy paradigm. However, in the Schrödinger coupling, the particles evolve according to a stochastic differential equation $dX_t = v_t(X_t)dt + (2\eta)^{-1/2}dW_t$, where $\{W_t\}$ is a standard Brownian motion over $\mathbb{R}^d$. In that case, it can be shown using the Girsanov formula that the velocity field that minimizes the energy functional $\int E\|v_t(X_t)\|^2 dt$ subject to $X_0 \sim \mu$ and $X_t \sim \nu$ induces the Schrödinger coupling; see, e.g., [Léo13].

Most previous works have studied the Schrödinger coupling in the asymptotic regime $\eta \to \infty$ as a surrogate for the original OT problem [EMR15, Pal19, NW21, BGN21, ANWS22, Del22]. In light of the minimum energy interpretation above, we argue that the Schrödinger coupling is a quantity of interest on its own. As a result, we treat instead $\eta$ as a fixed parameter. Recall that we assume that the probability measures $\mu$ and $\nu$ have bounded support. In this case, the Schrödinger coupling
exists and is unique, and we denote it by

$$\pi_\star := \arg \min_{\pi \in \Pi(\mu, \nu)} \left\{ \int \|x - y\|^2 \, d\pi(x, y) + \frac{1}{\eta} \KL(\pi \| \mu \otimes \nu) \right\}, \quad (1.3)$$

This paper focuses on the estimation of the Schrödinger coupling $\pi_\star$ and quantities that are derived from it.

We work in a standard statistical setting. Assume $X_1, \ldots, X_n \sim \mu$ i.i.d., and $Y_1, \ldots, Y_n \sim \nu$ i.i.d. We denote the sample from $\mu$ by $\mathcal{X} := (X_1, \ldots, X_n)$ and the sample from $\nu$ by $\mathcal{Y} := (Y_1, \ldots, Y_n)$. We assume further that the samples $\mathcal{X}$ and $\mathcal{Y}$ are mutually independent. The associated empirical measures are denoted $\mu_n$ and $\nu_n$ respectively. Recall that they are given by

$$\mu_n := \frac{1}{n} \sum_{i=1}^{n} \delta_{X_i}, \quad \nu_n := \frac{1}{n} \sum_{j=1}^{n} \delta_{Y_j}.$$ 

Given samples $\mathcal{X}$ and $\mathcal{Y}$, the empirical Schrödinger coupling is written

$$\pi_n := \arg \min_{\pi \in \Pi(\mu_n, \nu_n)} \left\{ \int \|x - y\|^2 \, d\pi(x, y) + \frac{1}{\eta} \KL(\pi \| \mu_n \otimes \nu_n) \right\}. \quad (1.4)$$

In addition to the computational and conceptual practicalities of Schrödinger couplings, recent work has shown that they may also avoid the statistical curse of dimensionality endemic to unregularized OT. Indeed, Genevay et. al [GCB+19] (see also [MNW19]) established the remarkable result that the cost of $\pi_n$ in (1.4) converges to that of $\pi_\star$ in (1.3) with the dimension-free statistical rate $1/\sqrt{n}$, in stark contrast to the unregularized analog which has statistical rate $n^{-1/d}$ [NWR19]. Implicit to these works is the parametric convergence of various quantities, including empirical dual potentials that converge to their population counterparts at a $1/\sqrt{n}$ rate [MNW19, LSPC19, dBGSLNW22].

In this work, we study the sample complexity of entropic optimal transport for initial tasks such as cost and density estimation as well as downstream applications like regression. Our first set of results improves upon the previous works for entropic OT cost estimation, and also establishes rates for the map as well as the density of $\pi_\star$ with respect to $\mu \otimes \nu$.

The proofs proceed via an elementary and direct analysis of the empirical dual problem. From this, we study the stochastic process $(\pi_n - \pi_\star)(\varphi)$, indexed by bounded functions $\varphi$ and apply these ideas to yield fast $1/n$ rates for a family of transfer learning problems. A major feature of our proofs is their simplicity; we obtain all of our results without resorting to technical empirical process arguments, in contrast to most of the previous statistical literature on both regularized and unregularized OT.

Central limit theorems for the convergence of $\pi_n$ to $\pi_\star$ have been studied by [KTM20] in the discrete support case and partially in [GX21] for more general cases; see also [GNB21] for general consistency results. Quantitative versions of this result, with differences measured in $W_1$, appeared in both [EN21, DDBD21]. The latter quantitative results are similar to our own but because they measure stability in the $W_1$ distance, they give rates which suffer from the curse of dimensionality. Our proofs, however, are different and notably simpler. Moreover, they do not require any smoothness assumptions on the cost function. This paper is organized as follows. We give an introduction to entropic optimal transport in section 2.1 and define the main quantities of interest. Our main results, namely parametric rates of convergence for the estimation of these quantities are presented in section 3 together with applications to transfer learning. Most proofs are postponed to section 4,
except for some technical proofs, including those of high-probability bounds, which are relegated to the appendix.

**Notation.** For an integer $m$, we set $[m] := \{1, \ldots, m\}$, and let $\Sigma_m$ denote the set of permutations on $[m]$. A norm $\| \cdot \|$ without subscript denotes the standard Euclidean distance. Given a probability measure $\beta$ on $\mathbb{R}^m$, and a $\beta$-integrable function $f: \mathbb{R}^m \to \mathbb{R}^k$, we often abbreviate $\beta(f) := \int f d\beta$ or even $\mathbb{E}[f(X)]$ when $\beta$ is clear from the context. When $\beta$ and $f$ are defined on a product space, we may also write $\beta(f(x,y))$ for $\int f(x,y) d\beta(x,y)$. Moreover, for any $q \geq 1$, we put

$$\|f\|_{L^q(\beta)} := \left( \int \|f(x)\|^q d\beta(x) \right)^{1/q}.$$  

The space $L^2(\beta)$ is the Hilbert space (modulo equivalence under this norm) of $f$ for which the above norm is finite and with inner product written $\langle \cdot, \cdot \rangle_{L^2(\beta)}$. By $\|f\|_{L^\infty(\beta)}$ we mean the essential supremum $\text{ess sup} \|f(X)\|$ for $X \sim \beta$. We denote by $L^\infty(\beta)$ the space of functions $f$ such that $\|f\|_{L^\infty(\beta)} < \infty$.

Given two vectors $a, b \in \mathbb{R}^d$, we denote their concatenation $(a, b) \in \mathbb{R}^{2d}$, which is the vector with first $d$ components equal to $a$ and last $d$ components equal to $b$. Given probability distributions $\beta_0$ on $\mathbb{R}^{m_0}$ and $\beta_1$ on $\mathbb{R}^{m_1}$, we denote the product $\beta_0 \otimes \beta_1$, which is defined, for each Borel set $B \subset \mathbb{R}^{m_0} \times \mathbb{R}^{m_1}$, as

$$(\beta_0 \otimes \beta_1)(B) := \int \beta_0(B^y) d\beta_1(y) = \int \beta_1(B_x) d\beta_0(x),$$

where $B^y := \{x \in \mathbb{R}^{m_0}: (x, y) \in B\}$ and $B_x := \{y \in \mathbb{R}^{m_1}: (x, y) \in B\}$. We denote $k$-fold products as $\beta^\otimes k$.

For $\theta \in \mathbb{R}^m$, let $\text{supp}(\theta) \subset [m]$ denote the coordinates on which $\theta$ is non-zero. For each $\theta \in \mathbb{R}^m$ and $S \subset [m]$, let $\theta_S := (\theta_k \mathbb{1}[k \in S])_{k=1}^m$, namely the vector with coordinates not in $S$ set to 0. A continuously differentiable function $\rho: \mathcal{H} \to \mathbb{R}$, where $\mathcal{H}$ is a Hilbert space equipped with norm $\| \cdot \|$ is said to be $\alpha$-strongly convex with respect to the norm $\| \cdot \|$ on a convex set $C \subset \mathcal{H}$ if, for all $u, v \in C$,

$$\rho(v) \geq \rho(u) + \langle \nabla \rho(u), v-u \rangle + \frac{\alpha}{2} \|u-v\|^2.$$

It is said to be $\alpha$-strongly concave on $C$ if $-\rho$ is $\alpha$-strongly convex on $C$.

We frequently use the notation $A \lesssim B$ to write the inequality $A \leq cB$ where $c = c(\eta)$ is a constant depending only on $\eta$. These suppressed constants are typically exponentially large in $\eta$. While the exact dependence of our results in $\eta$ can be easily extracted from our proofs, we have made no attempt to optimize it since we think of $\eta$ as a constant of order 1 throughout. We leave to future work the interesting direction of improving the dependence of our statistical results on $\eta$.

### 2. Preliminaries on entropic optimal transport

As stated in the introduction, we assume throughout that $\mu$ and $\nu$ have bounded support. By re-scaling the entropic OT objective, we make the following assumption.

**Assumption 1.** Assume for $\mu$-almost every $x$ and $\nu$-almost every $y$, $\|x\| \leq 1/2$ and $\|y\| \leq 1/2$. 
Our main results pertain to specific quantities arising in optimal transport. While these are natural and straightforward, their introduction requires a bit of additional notation. In this section, we introduce our main quantities of interest: dual potentials, cost function, density, and a map known as the entropic regression function. Empirical counterparts for these objects are functions defined only data points and this section ends with the description of a canonical way to extend them over the entire space \( \mathbb{R}^d \) (or \( \mathbb{R}^d \times \mathbb{R}^d \)).

We begin in section 2.1 by providing background and notation for the dual entropic optimal transport problem that forms the foundation of our results. Thus equipped, we introduce in section 2.2 the main quantities of interest, as well as their empirical counterparts, which serve as a basis for our estimators. In section 2.3 we introduce the aforementioned canonical extensions.

### 2.1 Duality theory for entropic optimal transport

The following results, as well as a discussion of the literature on duality for the entropic optimal transport problem, can be found in [DMG20].

**Theorem 1 (Strong duality).** Let \( P \) and \( Q \) be distributions on \( \mathbb{R}^d \) with bounded support and fix \( \eta > 0 \). Denote the entropic optimal transport problem

\[
S(P, Q) := \inf_{\pi \in \Pi(P, Q)} \left\{ \pi(\|x - y\|^2) + \frac{1}{\eta} \text{KL}(\pi \| P \otimes Q) \right\}. \tag{2.1}
\]

The infimum is attained by a unique \( \pi_* \in \Pi(P, Q) \) and strong duality holds in the sense that

\[
S(P, Q) = \sup_{(f, g) \in L^\infty(P) \times L^\infty(Q)} \left\{ P(f) + Q(g) - \frac{1}{\eta} (P \otimes Q)(e^{-\eta\|x - y\|^2 + \eta f(x) + \eta g(y)} - 1) \right\}. \tag{2.2}
\]

The supremum above is attained at a pair \((f_0, g_0) \in L^\infty(P) \times L^\infty(Q)\) of dual potentials, which are unique up to the translation \((f_0, g_0) \mapsto (f_0 + c, g_0 - c)\) for \( c \in \mathbb{R} \).

Moreover, primal and dual solutions are linked via the following relationships. For any pair \((f, g) \in L^\infty(P) \times L^\infty(Q)\), let \( \pi \) be the measure with density

\[
\frac{d\pi}{d(P \otimes Q)}(x, y) = e^{-\eta\|x - y\|^2 + \eta f(x) + \eta g(y)}. \tag{2.3}
\]

Then the pair \((f, g)\) is optimal for (2.2) if and only if \( \pi \in \Pi(P, Q) \) and \( \pi \) is optimal for (2.2).

We denote the population dual objective by

\[
\Phi(f, g) := \mu(f) + \nu(g) - \frac{1}{\eta}(\mu \otimes \nu)(e^{-\eta(\|x - y\|^2 - f(x) - g(y))}) + \frac{1}{\eta}. \tag{2.4}
\]

To account for translation invariance of dual potentials, we distinguish the unique optimal dual potentials \((f_*, g_*)\) such that \( \nu(g_*) = 0 \).

Throughout our proofs, we make extensive use of another optimal pair of dual potentials denoted \((\bar{f}_*, \bar{g}_*)\) defined by \( \bar{f}_* = f_* + \nu_n(f_*) \) and \( \bar{g}_* = g_* - \nu_n(g_*) \) so that \( \nu_n(\bar{g}_*) = 0 \).

The empirical dual objective \( \Phi_n \) is defined by

\[
\Phi_n(f, g) := \mu_n(f) + \nu_n(g) - \frac{1}{\eta}(\mu_n \otimes \nu_n)(e^{-\eta(\|x - y\|^2 - f(x) - g(y))}) + \frac{1}{\eta}. \tag{2.5}
\]
As in the population case, we distinguish the unique optimizers \((f_n, g_n)\) such that \(\nu_n(g_n) = 0\).

In the sequel, we will be using the gradient of \(\Phi_n\) that are defined as elements of (the dual of) \(L^2(\mu_n) \times L^2(\nu_n)\) and given by

\[
\langle \nabla \Phi_n(f, g), (\varphi, \psi) \rangle_{L^2(\mu_n) \times L^2(\nu_n)} = (\mu_n \otimes \nu_n)((\varphi(x) + \psi(y))(1 - e^{-\eta(\|x-y\|^2 - f(x) - g(y)))})
\]

(2.6)

In particular, we readily get the following expression for the norm of the above gradient:

\[
\|\nabla \Phi_n(f, g)\|_{L^2(\mu_n) \times L^2(\nu_n)}^2 = \frac{1}{n} \sum_{i=1}^{n} \left(1 - \frac{1}{n} \sum_{j=1}^{n} p(X_i, Y_j)\right)^2 + \frac{1}{n} \sum_{j=1}^{n} \left(1 - \frac{1}{n} \sum_{i=1}^{n} p(X_i, Y_j)\right)^2
\]

(2.7)

where \(p\) is the density defined in (2.3) and is given by \(p(x, y) = e^{-\eta\|x-y\|^2 + \eta f(x) + \eta g(y)}\).

**Remark 2.** Throughout this paper we make extensive use of the fact that \(\Phi, \Phi_n, \text{ and } \nabla \Phi_n\) enjoy the following translation invariance property: For any constant \(c \in \mathbb{R}\), it holds

\[
\Phi(f, g) = \Phi(f + c, g - c), \quad \Phi_n(f, g) = \Phi_n(f + c, g - c), \quad \text{and} \quad \nabla \Phi_n(f, g) = \nabla \Phi_n(f + c, g - c).
\]

**2.2 Quantities of interest**

Beyond the couplings \(\pi_*\) and \(\pi_n\) that have already been defined, we now introduce important quantities associated to entropic optimal transport: cost, density, and map.

**Cost.** Using (2.1), define the population entropic OT cost as \(S := S(\mu, \nu)\) and its plug-in estimator \(S_n := S(\mu_n, \nu_n)\).

**Density.** Define the density of the optimal coupling \(\pi_*\) with respect to the product measure \(\mu \otimes \nu\) as

\[
p_*(x, y) := \frac{d\pi_*}{d(\mu \otimes \nu)}(x, y) = e^{-\eta(\|x-y\|^2 - f_*(x) - g_*(y))}.
\]

(2.8)

The statement \(\pi_* \in \Pi(\mu, \nu)\) can then be written in the following succinct manner. For \(\mu\)-almost every \(x\) and \(\nu\)-almost every \(y\),

\[
\nu(p_*(x, \cdot)) = \mu(p_*(\cdot, y)) = 1.
\]

(2.9)

Equivalently,

\[
f_*(x) = -\frac{1}{\eta} \ln \left(\int e^{-\eta\|x-y\|^2 + \eta g_*(y)} d\nu(y)\right)
\]

(2.10)

\[
g_*(y) = -\frac{1}{\eta} \ln \left(\int e^{-\eta\|x-y\|^2 + \eta f_*(x)} d\nu(x)\right)
\]

(2.11)

Its empirical counterpart is the density of \(\pi_n\) with respect to the product measure \(\mu_n \otimes \nu_n\). It is defined for all \(x \in \mathcal{X}\) and \(y \in \mathcal{Y}\), as

\[
p_n(x, y) := \frac{d\pi_n}{d(\mu_n \otimes \nu_n)}(x, y) = e^{-\eta(\|x-y\|^2 - f_n(x) - g_n(y))}.
\]

(2.12)

The marginal constraints then become, for all \(x \in \mathcal{X}\) and \(y \in \mathcal{Y}\), the equalities

\[
\nu_n(p_n(x, \cdot)) = \mu_n(p_n(\cdot, y)) = 1.
\]

(2.13)
**Map.** Finally, we consider the entropic analog of the optimal transport map, namely the *entropic regression function*—sometimes called “barycentric projection”—defined as the map

\[
b_*(x) := \mathbb{E}_{\pi_*}[Y \mid X = x]. \tag{2.14}
\]

Its empirical counterpart is the plug-in estimator

\[
b_n(x) := \mathbb{E}_{\pi_n}[Y \mid X = x]. \tag{2.15}
\]

The estimator \( b_n \) was recently proposed in [PNW21] as a computationally efficient surrogate for a smooth Brenier map, and rates of estimation were established, albeit suboptimal ones.

### 2.3 Canonical extensions

The marginal constraints in (2.13) induce a canonical extension of the optimal dual potentials \((f_n, g_n)\) to maps defined on all of \( \mathbb{R}^d \) [Ber20, PNW21]. For example, the marginal constraint for \( x \in \mathcal{X} \) implies

\[
e^{-\eta f_n(x)} = \frac{1}{n} \sum_{j=1}^{n} e^{-\eta \|x - Y_j\|^2 + \eta g_n(Y_j)}. \tag{2.16}
\]

Since the right-hand side makes sense for any \( x \in \mathbb{R}^d \), we thus abuse notation and define \( f_n(x) \), for any \( x \in \mathbb{R}^d \), to satisfy this equation. We similarly define \( g_n(y) \), for any \( y \in \mathbb{R}^d \), to satisfy

\[
e^{-\eta g_n(y)} = \frac{1}{n} \sum_{i=1}^{n} e^{-\eta \|X_i - y\|^2 + \eta f_n(X_i)}. \tag{2.17}
\]

In turn, this canonical extension also applies to the density \( p_n \) in a straightforward manner as well as to the entropic regression function estimator \( b_n \). From now on, we employ the definition

\[
b_n(x) = \frac{\sum_{i=1}^{n} Y_i p_n(x,Y_i)}{\sum_{i=1}^{n} p_n(x,Y_i)} = \frac{1}{n} \sum_{i=1}^{n} Y_i p_n(x,Y_i), \quad x \in \mathbb{R}^d. \tag{2.18}
\]

### 3. Main results

In this section, we state our main results on the rates of estimation of the quantities introduced in section 2.2. We also present our main application to transfer learning.

#### 3.1 Sample complexity

In this section we give our main results on rates of estimation for various quantities arising from entropic optimal transport: the cost, the density of the coupling, the entropic regression function, as well as the coupling itself.
Cost. Our first result concerns the rate of convergence of $S_n$ to $S$. We emphasize that the unregularized analog of this quantity ($\eta \to \infty$) is generically of order at least $n^{-2/d}$, and, in fact, it is known that no estimator for the unregularized cost can beat the rate $n^{-1/d}$ in general [NWR19]. For the entropic problem, existing results imply $\mathbb{E}|S_n - S| \lesssim 1/\sqrt{n}$ under mild assumptions on $\mu$ and $\nu$ [GCB+19, LSPC19, MNW19, dBGSLNW22]. Our techniques yield a commensurate bound in a stronger sense: a $1/n$ rate both for the mean squared error and the bias using a different proof. The result stating that the bias is an order of magnitude smaller than the stochastic fluctuations is quite remarkable and seems to have appeared only in the concurrent work [dBGSLNW22].

**Theorem 3.** The mean squared error and bias are bounded respectively as

$$\mathbb{E}|S_n - S|^2 \lesssim \frac{1}{n}, \quad |\mathbb{E}[S_n] - S| \lesssim \frac{1}{n}.$$  

Moreover, for all $t > 0$, with probability at least $1 - 6e^{-t}$,

$$|S_n - S| \lesssim \frac{t}{n} + \sqrt{\frac{t}{n}}.$$  

This result is achieved by a careful analysis of the empirical dual problem, and is elementary in that it essentially only involves straightforward calculations and standard inequalities arising from strong concavity. In contrast to most of the previous literature on statistical estimation problems in both unregularized and entropic optimal transport, we completely circumvent the control of suprema of empirical processes.

Map. Our second result concerns the problem of estimating the entropic regression function defined in (2.14). To that end, we employ the canonical extension $b_n$ defined in (2.18).

In this work, we consider $b_n$ as an estimator not of the Brenier map but of the entropic regression function $b_*$. In contrast to the unregularized case, the computationally feasible estimator $b_n$ achieves the parametric rate $1/n$ for estimating $b_*$ in arbitrary dimension.

**Theorem 4.** Let $b_*$ and $b_n$ be as in (2.14) and (2.15), respectively. Then

$$\mathbb{E}\|b_n - b_*\|^2_{L^2(\mu)} \lesssim \frac{1}{n}.$$  

Moreover, for all $t > 0$, with probability at least $1 - 8e^{-t}$, it holds

$$\|b_n - b_*\|^2_{L^2(\mu)} \lesssim \frac{t}{n}.$$  

Density. Our third result, proved in almost exactly the same way as our result on entropic map estimation, gives a comparable result for the problem of density estimation.

**Theorem 5.** Let $p_*$ be as in (2.8). Extend the empirical analog $p_n$ from (2.12) as in section 2.3. Then

$$\mathbb{E}\|p_n - p_*\|^2_{L^2(\mu \otimes \nu)} \lesssim \frac{1}{n}.$$  

Moreover, for all $t > 0$, with probability at least $1 - 16e^{-t}$, it holds

$$\|p_n - p_*\|^2_{L^2(\mu \otimes \nu)}, \|p_n - p_*\|^2_{L^2(\mu \otimes \nu)} \lesssim \frac{t}{n}.$$
Note that the high-probability bound above holds in both $L^2(\mu_n \otimes \nu_n)$ as well as $L^2(\mu \otimes \nu)$; while the latter is more natural from a statistical estimation perspective, the former is ultimately more useful for our subsequent applications. In particular, this result readily implies Theorem 4 and is achieved with essentially the same ideas as our estimate on the cost, and so has a simple, easy to understand proof.

In sum, the previous three results show that the statistical picture for entropic optimal transport is fundamentally different than in unregularized optimal transport: fast, parametric, rates hold in arbitrary dimension, and they can be established with simple proofs.

**Coupling.** While these results provide strong evidence that entropic optimal transport is fundamentally tractable, both statistically and computationally, there remains basic questions about the validity of using $\pi_n$ as a plug-in for the coupling $\pi_\star$ in more complex statistical procedures. There, we generally wish to understand the deviations $\pi_\star - \pi_n$. The next result, proved in section 4.3, makes a first step in this direction.

**Theorem 6.** Let $\varphi \in L^\infty(\mu \otimes \nu)$. Then, for all $t > 0$, with probability at least $1 - 18e^{-t^2}$,

$$| (\pi_\star - \pi_n)(\varphi) | \lesssim \frac{\| \varphi \|_{L^\infty(\mu \otimes \nu)} \cdot t}{\sqrt{n}}. \tag{3.1}$$

In particular, the random variable $(\pi_\star - \pi_n)(\varphi)$ is subGaussian with variance proxy of order $1/n$ as in standard empirical process theory even though $\pi_n$ has a dependence in all the observations that is much more complex than a simple average of independent random variables.

In the next section, we refine this result to achieve parametric rates for a broad family of transfer learning tasks based on entropic optimal transport.

**3.2 Application to transfer learning**

Recall that in Theorem 4 we examined the sample complexity of estimating the entropic regression function $b_\star(x) = \mathbb{E}_{\pi_\star}[Y \mid X = x]$. This regression function is the solution to the following least squares problem:

$$b_\star = \arg \min_{h \in L^2(\mu)} \mathbb{E}_{\pi_\star} \| h(X) - Y \|^2. \tag{3.2}$$

Similarly, $b_n$ is its empirical counterpart in the sense that

$$b_n = \arg \min_{h \in L^2(\mu_n)} \mathbb{E}_{\pi_n} \| h(X) - Y \|^2. \tag{3.3}$$

Theorem 4 implies that the solutions of these two problems are close. The goal of this section is to explore how general this phenomenon is. To that end, we consider the more general setup, where in addition to the samples $X = (X_1, \ldots, X_n)$ and $Y = (Y_1, \ldots, Y_n)$, we observe real-valued labels $A_1, \ldots, A_n \in \mathbb{R}$ such that $A_i \sim q(\cdot \mid Y_i)$ for some unknown $q$. As a result, our observations consist of unlabeled observations $X_1, \ldots, X_n$, as well as labeled observations $(Y_1, A_1), \ldots, (Y_n, A_n)$ but the coupling between the labeled and unlabeled observations is not observed. The goal is to predict $A$ from $X$. Without making any assumptions on the coupling between the $X$ and $Y$ variables, this problem is clearly impossible. We thus make the additional assumption that the joint distribution of $(X, Y, A)$, denoted by $\omega$, is given by $(X, Y) \sim \pi_\star$ and $A \sim q(\cdot \mid Y)$.
A relevant benchmark arises when observations consist of $n$ independent triples $(X_i, Y_i, A_i)$, $i = 1, \ldots, n$ where $(X_i, Y_i) \sim \pi^*$ and, conditionally on $Y_i$, $A_i \sim q(\cdot|Y_i)$. In this case, the Schrödinger coupling $\pi^*$ need not be learned from uncoupled data. One of the main statistical messages of this section is that the cost of estimating the Schrödinger coupling is at most the same as the underlying statistical task and thus does not affect the statistical rate $s$. To illustrate this fact, we investigate two statistical questions: regression and classification.

**Regression with a squared loss.** In the transfer learning model above, the regression problem (3.2) generalizes to

$$h^* = \arg\min_{h \in L^2(\mu)} F(h) := \mathbb{E}|h(X) - A|^2,$$

so that

$$h^*_n(x) = \mathbb{E}_\omega[A | X = x] = \mathbb{E}_\omega[Ap^*_n(x, Y)].$$

Analogously, define

$$h_n = \arg\min_{h \in L^2(\mu_n)} \hat{F}(h) := \frac{1}{n^2} \sum_{i,j=1}^n p_n(X_i, Y_j)(h(X_i) - A_j)^2,$$

where $p_n$ is the density defined in (2.12). We extend $h_n$ to an element of $L^2(\mu)$ by using the canonical extension of $p_n$ in the formula for $h_n$: that is, for all $x \in \mathbb{R}^d$, we set

$$h_n(x) := \frac{1}{n} \sum_{j=1}^n A_j p_n(x, Y_j) \quad x \in \mathbb{R}^d.$$

Using this equation and taking successively $A = u_1^T k Y$, where $u_1, \ldots, u_d$ is an orthonormal basis for $\mathbb{R}^d$ and $k \in [d]$, it is easy to see that this model generalizes that of equations (3.2) and (3.3). Incorporating general labels $A$ allows us to model a common practical situation where we are given two datasets, one labeled and the other not, and we wish to transfer the labels from one to the other.

The next theorem is a direct extension of Theorem 4 to the more general setup with labels. Its proof is postponed to subsection 4.4 in the appendix.

**Theorem 7.** Suppose that $\omega$-almost surely, $|A| \leq 1$ and $h^*, h_n$ are defined as in (3.4) and (3.7), respectively. Then

$$\mathbb{E}\|h^* - h_n\|^2_{L^2(\mu)} \lesssim \frac{1}{n}.$$
\( \ell_*(x) = \mathbb{I}(h_*(X) > 1/2) \), where \( \mathbb{I}(\cdot) \) denotes the indicator function and \( h_* \) is the regression function defined in (3.5). This leads us to consider the excess-risk of a classifier \( \ell \), which is defined as [DGL96]

\[
\mathcal{E}(\ell) = \mathbb{P}[\ell(X) \neq Y] - \mathbb{P}[\ell_*(X) \neq Y] \geq 0.
\]

This explicit form of the Bayes classifier together with the availability of a good nonparametric estimator \( h_n \) defined in (3.7) suggest a natural plug-in classifier \( \ell_n \) defined by

\[
\ell_n(x) = \mathbb{I}(h_n(x) > 1/2).
\]

Such estimators were investigated in [AT07] under the classical Mammen-Tsybakov noise condition which controls the steepness of the function \( h_* \) around value 1/2. We recall its definition here for convenience.

**Definition 8 (Mammen-Tsybakov noise condition [MT99]).** We say that the distribution \( \omega \) satisfies the Mammen-Tsybakov condition with parameter \( \alpha > 0 \), if there exists a constant \( C_0 > 0 \) such that \( \mu(0 < |h_* - 1/2| \leq \varepsilon) \leq C_0 \varepsilon^\alpha \) for all \( \varepsilon \in (0, 1/2] \).

Note that this condition governs simultaneously how steeply \( h_* \) crosses level 1/2 and how much \( \mu \) puts mass around the noise region \( \{x : h_*(x) = 1/2\} \). For this reason, it is also referred to margin or low noise condition.

In their seminal paper [AT07] establish a key lemma, which relates the excess-risk of a plug-in estimator \( \ell(x) = \mathbb{I}(h(x) > 1/2) \) to that of the pointwise estimation error of \( h_* \) by \( h \); see [AT07], Lemma 3.1. Combining this result with pointwise guarantees for \( h_n \), we establish the following result.

**Theorem 9.** Suppose that \( \omega \) satisfies the Mammen-Tsybakov condition with parameter \( \alpha > 0 \). Then the excess risk of the plug-in classifier \( \ell_n \) defined above has excess risk bounded as

\[
\mathbb{E}[\mathcal{E}(\ell_n)] \lesssim n^{-\frac{1+\alpha}{2}}.
\]

Note that the rate of Theorem 9 is at least as fast as \( 1/\sqrt{n} \) for when \( \alpha = 0 \). As \( \alpha \to \infty \), it can be easily verified that it leads to exponential rates as in [KB05].

### 4. Proofs

In this section we give the proofs for our convergence results in expectation and postpone the proofs of tail bounds to the appendix. Indeed, the proofs in expectation are simpler and already contain the key ingredients to obtain the parametric rates of convergence showcased in section 3.

#### 4.1 Structural results on entropic optimal transport

We begin with some key structural results—chiefly strong concavity for the empirical dual problem—which drive the parametric rates of convergence. The strong concavity result relies on boundedness of the dual potentials which follows from the bounded support assumption 1 and is established by the following proposition, proved in section B.1.
PROPOSITION 10 (Bounded dual potentials and densities). As above, specify the unique dual potentials \((f_n, g_n)\) and \((f, g)\) such that \(\nu_n(g_n) = \nu(g) = 0\), and extend \((f_n, g_n)\) according to \((2.16)\) and \((2.17)\), respectively. Then

\[
\|f_n\|_{L^\infty(\mu)}, \|g_n\|_{L^\infty(\nu)} \leq 2, \quad \|f\|_{L^\infty(\mu)}, \|g\|_{L^\infty(\nu)} \leq 1.
\]

In particular, for \((\mu \otimes \nu)\)-almost every \((x, y)\),

\[
e^{-5\eta} \leq p_n(x, y), \quad p_n(x, y) \leq e^{5\eta}.
\] (4.1)

We remark that, unfortunately, this exponential dependence on \(\eta\) is unavoidable in the worst case. For an example, see [ANWS22, section 3].

Recall that we denote the empirical dual objective by \(\Phi_n\), as in \((2.5)\). The next lemma simply says that \(\Phi_n\) is strongly concave so long as we remove the symmetry \((f, g) \mapsto (f + c, g - c)\) using the condition \(\nu(g) = 0\) and consider only uniformly bounded potentials. More precisely, we work on the convex set of dual potentials

\[
\mathcal{S}_L := \{(f, g) \in L^\infty(\mu_n) \times L^\infty(\nu_n) : \|f\|_{L^\infty(\mu_n)} \vee \|g\|_{L^\infty(\nu_n)} \leq L, \ \nu_n(g) = 0\}.
\]

In this section, we use the shorthand notation \(\langle \cdot, \cdot \rangle_n\) and \(\| \cdot \|_n\) respectively to denote the inner product and norm of \(L^2(\mu_n) \times L^2(\nu_n)\).

We are now in a position to state our first structural result.

**LEMMA 11** (Strong concavity of the empirical dual). For each \(L > 0\), \(\Phi_n\) is \(\delta\)-strongly concave with respect to the norm \(\| \cdot \|_n\) on \(\mathcal{S}_L\) for \(\delta = \eta e^{-\eta(2L+1)}\) in the sense that for any \((f, g), (f', g') \in \mathcal{S}_L\), we have almost surely

\[
\Phi_n(f, g) - \Phi_n(f', g') \geq \langle \nabla \Phi_n(f, g), (f, g) - (f', g') \rangle_n + \frac{\delta}{2} \| (f, g) - (f', g') \|_n^2.
\]

**PROOF.** Fix two pairs \((f, g), (f', g') \in \mathcal{S}_L\). Then it suffices to show that the function

\[
h(t) := \Phi_n((1 - t)f + tf', (1 - t)g + tg'),
\]

satisfies

\[
h''(t) \leq -\delta\| (f, g) - (f', g') \|_n^2, \quad \forall t \in [0, 1].
\]

Fix some \(t \in [0, 1]\). Observe that the linear terms cancel so that

\[
h''(t) = -\frac{\eta}{n^2} \sum_{i,j=1}^n (f(X_i) - f'(X_i) + g(Y_j) - g'(Y_j))^2 \\
\times \exp \left( -\eta \| X_i - Y_j \|^2 + \eta t (f(X_i) + g(Y_j)) + \eta (1 - t)(f'(X_i) + g'(Y_j)) \right).
\]

Using our bounded support Assumption 1, along with the definition of \(\mathcal{S}_L\), yields

\[
h''(t) \leq -\eta e^{-\eta(2L+1)} \cdot \frac{1}{n^2} \sum_{i,j=1}^n (f(X_i) - f'(X_i) + g(Y_j) - g'(Y_j))^2.
\]
Expanding out these squared terms, we use the fact that \( \nu_n(g) = \nu_n(g') = 0 \) to find
\[
\frac{1}{n^2} \sum_{i,j=1}^{n} (f(X_i) - f'(X_i) + g(Y_j) - g'(Y_j))^2 = \| (f, g) - (f', g') \|_n^2 + 2\mu_n (f - f') \cdot \nu_n(g - g')
\]
\[
= \| (f, g) - (f', g') \|_n^2.
\]
Hence the result. 

The following consequence of strong concavity of \( \Phi_n \), known as a Polyak-Łojasiewicz (PL) inequality, is instrumental in our results.

**Proposition 12 (PL inequality for the empirical dual).** Let \( L > 0 \) be such that \( (f_n, g_n) \in \mathcal{S}_L \). Then for any \( (f, g) \in \mathcal{S}_L \),
\[
\Phi_n(f_n, g_n) - \Phi_n(f, g) \leq \frac{e^{\eta(2L+1)}}{2\eta} \| \nabla \Phi_n(f, g) \|_n^2. \tag{4.2}
\]

Proposition 12 is a weaker form of strong concavity that has recently been thoroughly studied in the optimization literature [KNS16], but for the reader’s convenience we include a proof in section B.2.

In light of Proposition 10, we have that \( (\bar{f}_*, \bar{g}_*) := (f_* + \nu_n(g_*), g_* - \nu_n(g_*)) \in \mathcal{S}_2 \) almost surely. On the one hand, together with the PL inequality (4.2) it yields
\[
\Phi_n(f_n, g_n) - \Phi_n(\bar{f}_*, \bar{g}_*) \leq \frac{e^{5\eta}}{2\eta} \| \nabla \Phi_n(f_* + \nu_n(g_*), g_* - \nu_n(g_*)) \|_n^2 = \frac{e^{5\eta}}{2\eta} \| \nabla \Phi_n(f_*, g_*) \|_n^2.
\]

On the other hand, strong concavity in Lemma 11 gives
\[
\Phi_n(f_n, g_n) - \Phi_n(\bar{f}_*, \bar{g}_*) \geq \frac{\eta e^{-5\eta}}{2} \| (f_n - \bar{f}_*, g_n - \bar{g}_*) \|_n^2.
\]

The above two displays imply
\[
\| (f_n - \bar{f}_*, g_n - \bar{g}_*) \|_n \leq \frac{e^{5\eta}}{\eta} \| \nabla \Phi_n(f_*, g_*) \|_n. \tag{4.3}
\]

This inequality has been called “error bound” in the optimization literature and can, in fact, be shown to be equivalent to a PL inequality; see [KNS16, Theorem 2]. As detailed in the next section, inequality (4.3) readily yields dimension-independent rates of estimation for the population dual potentials \((f_*, g_*)\).

We conclude with a tool that becomes useful when assessing the quality of the canonical extensions employed in this paper. It is essentially a consequence of the Lipschitzness of the exponential and logarithm on bounded intervals. Its proof is postponed to Appendix B.

**Proposition 13 (Comparison inequalities for dual potentials and densities).** For \( \mu \)-almost every \( x, \)
\[
| f_*(x) - f_n(x) | \leq \left| \frac{1}{n} \sum_{j=1}^{n} e^{-\eta \| x - Y_j \|^2 + \eta g_*(Y_j)} - \nu (e^{-\eta \| x - \cdot \|^2 + \eta g_*(\cdot)} \right| + \| g_\nu - g_n \|_{L^1(\nu_\mu)}.
\]
Similarly, for \( \nu \)-almost every \( y \),

\[
|\bar{g}(y) - g_n(y)| \lesssim \frac{1}{n} \sum_{i=1}^{n} e^{-\eta \|X_i - y\|^2 + \eta f_i(X_i)} - \mu(e^{-\eta \|y\|^2 + \eta f_i()} + \|\bar{f}_* - f_n\|_{L^1(\mu_n)},
\]

And for \((\mu \otimes \nu)\)-almost every \((x, y)\),

\[
|p_*(x, y) - p_n(x, y)| \lesssim |\bar{f}_*(x) - f_n(x)| + |\bar{g}_*(y) - g_n(y)|.
\]

### 4.2 Rates of convergence in expectation

We begin with an important, albeit simple, argument to establish our convergence results. Central to our proof is the fact that we only need to measure empirical deviations at \((f_*, g_*)\), the optimal dual potentials.

**Lemma 14.** Let \( \Phi \) and \( \Phi_n \) be the dual objectives defined in (2.4) and (2.5) respectively. Moreover, let \((f_*, g_*)\) be the pair of potentials that maximizes \( \Phi \) and such that \( \nu(g_*) = 0 \). Then

\[
\mathbb{E}\|\nabla \Phi_n(f_*, g_*)\|^2 \leq \frac{2e^{10\eta}}{n},
\]

where \( \|\cdot\|_n \) denotes the norm of \( L^2(\mu_n) \times L^2(\nu_n) \).

**Proof.** Recall that \( p_* \) is defined in (2.8) so by (2.7) we get

\[
\mathbb{E}\|\nabla \Phi_n(f_*, g_*)\|^2 = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[ 1 - \frac{1}{n} \sum_{j=1}^{n} p_*(X_i, Y_j) \right]^2 + \frac{1}{n} \sum_{j=1}^{n} \mathbb{E} \left[ 1 - \frac{1}{n} \sum_{i=1}^{n} p_*(X_i, Y_j) \right]^2
\]

\[
= \frac{1}{n^2} \left( \sum_{j,l=1}^{n} \text{Cov} \left[ 1 - p_*(X_1, Y_j), 1 - p_*(X_1, Y_l) \right] + \sum_{i,k=1}^{n} \text{Cov} \left[ 1 - p_*(X_i, Y_1), 1 - p_*(X_k, Y_1) \right] \right),
\]

where \( X_i \sim \mu, Y_j \sim \nu \) with \( X_1, \ldots, X_n \) mutually independent, and \( Y_1, \ldots, Y_n \) mutually independent. In particular, in light of the marginal constraints listed in (2.9), it holds that

\[
\text{Cov} \left[ 1 - p_*(X_i, Y_j), 1 - p_*(X_k, Y_l) \right] = 0, \quad \forall (i, j) \neq (k, l).
\]

As a result,

\[
\mathbb{E}\|\nabla \Phi_n(f_*, g_*)\|^2 \leq \frac{2}{n} \text{Var} \left[ 1 - p_*(X_1, Y_1) \right] = \frac{2}{n} \text{Var} \left( p_*(X_1, Y_1) \right) \leq \frac{2e^{10\eta}}{n},
\]

where in the inequality, we used (4.1).

**Bias of cost.** We here give the proof of the bias inequality part of Theorem 3. Recall that the population and empirical cost are denoted, respectively,

\[
S := \pi_*(\|x - y\|^2) + \frac{1}{\eta} \text{KL}(\pi_*|\mu \otimes \nu), \quad S_n := \pi_n(\|x - y\|^2) + \frac{1}{\eta} \text{KL}(\pi_n|\mu_n \otimes \nu_n).
\]
Our goal is to establish the bias bound of Theorem 3: $|\mathbb{E}[S_n] - S| \lesssim 1/n$. To that end, observe that
\[
S_n - S = \Phi_n(f_n, g_n) - \Phi(f_*, g_*) = \{\Phi_n(f_n, g_n) - \Phi_n(f_*, g_*)\} + \{\Phi_n(f_*, g_*) - \Phi(f_*, g_*)\}.
\]
Since $\mathbb{E}[\Phi_n] = \Phi$, we get
\[
\mathbb{E}[S_n] - S = \mathbb{E}[\Phi_n(f_n, g_n) - \Phi_n(f_*, g_*)]. \tag{4.5}
\]
Using this equation and optimality of $(f_n, g_n)$, we can conclude $\mathbb{E}[S_n] \geq S$; $S_n$ has a non-negative bias. Thus, it suffices to focus on upper-bounding the right-hand side of (4.5). To do this, recall first that in light of Proposition 10, we have that $(f_* + \nu_n(g_*), g_* - \nu_n(g_*)) \in S_2$ almost surely. Therefore, the PL inequality in Proposition 12 yields
\[
\Phi_n(f_n, g_n) - \Phi_n(f_*, g_*) = \Phi_n(f_n, g_n) - \Phi_n(f_* + \nu_n(g_*), g_* - \nu_n(g_*)) \tag{4.6}
\leq e^{5\eta}/2\eta \|\nabla \Phi_n(f_* + \nu_n(g_*), g_* - \nu_n(g_*))\|^2_{L^2(\mu_n \otimes \nu_n)} = e^{5\eta}/2\eta \|\nabla \Phi_n(f_*, g_*)\|^2_{L^2(\mu_n \otimes \nu_n)}. \tag{4.7}
\]
Applying Lemma 14, we get
\[
\mathbb{E}[\Phi_n(f_n, g_n) - \Phi_n(f_*, g_*)] \leq e^{15\eta}/\eta \cdot 1/n.
\]

**Squared error of cost.** We now show how to augment the above proof technique to yield the squared error bound in Theorem 3. Note that from here on, we suppress constants depending only on $\eta$ as explained in the notation section. Begin by applying Young’s inequality to see
\[
\mathbb{E}|S_n - S|^2 \leq 2\mathbb{E}|\Phi_n(f_n, g_n) - \Phi_n(f_*, g_*)|^2 + 2\mathbb{E}|\Phi_n(f_*, g_*) - \Phi(f_*, g_*)|^2. \tag{4.8}
\]
For the first term, observe that $\Phi_n(f_n, g_n) \geq \Phi_n(f_*, g_*)$. Since the square function is monotonic on the positive real line, we can apply Proposition 12 to yield
\[
\mathbb{E}|\Phi_n(f_n, g_n) - \Phi_n(f_*, g_*)|^2 \lesssim \mathbb{E}\|\nabla \Phi_n(f_*, g_*)\|^4_n.
\]
We observe that by Proposition 10 and (2.7), $\|\nabla \Phi_n(f_*, g_*)\|_n \lesssim 1$ almost surely. Thus, we can apply Lemma 14 to conclude
\[
\mathbb{E}|\Phi_n(f_n, g_n) - \Phi_n(f_*, g_*)|^2 \lesssim \mathbb{E}\|\nabla \Phi_n(f_*, g_*)\|^4_n \lesssim \mathbb{E}\|\nabla \Phi_n(f_*, g_*)\|^2_n \lesssim 1/n.
\]
For the second term in (4.8), we observe that
\[
\mathbb{E}|\Phi_n(f_*, g_*) - \Phi(f_*, g_*)|^2 \leq 4\mathbb{E}|(\mu_n - \mu)(f_*)|^2 + 4\mathbb{E}|(\nu_n - \nu)(g_*)|^2
\]
\[
+ \frac{4}{\eta^2}\mathbb{E}|(\mu_n \otimes \nu_n - \mu \otimes \nu)(p_* - 1)|^2
\]
\[
\lesssim \frac{1}{n} + \mathbb{E}|(\mu_n \otimes \nu_n - \mu \otimes \nu)(p_* - 1)|^2,
\]
where we use the uniform boundedness from Proposition 10. We observe that by the marginal constraints (2.9), Jensen’s inequality, and (2.7),

\[
|\langle \mu \otimes \nu_n - \mu \otimes \nu \rangle (p^*_n - 1) \rangle |^2 = |\langle \mu \otimes \nu_n \rangle (p^*_n - 1) \rangle |^2 \leq \frac{1}{n} \sum_{i=1}^{n} \left( \frac{1}{n} \sum_{j=1}^{n} p^*_n(X_i, Y_j) - 1 \right)^2 \leq \| \nabla \Phi_n (f^*_n, g^*_n) \|^2 .
\]

Applying Lemma 14 once more, we conclude that

\[
\mathbb{E}|\langle \mu \otimes \nu_n - \mu \otimes \nu \rangle (p^*_n - 1) \rangle |^2 \lesssim \frac{1}{n} .
\]

This yields the result.

**Map.** We explain here how to prove Theorem 4. Recall that we use the notation

\[
b^*_n(x) = \mathbb{E}_{\pi^*_n}[Y | X = x] = \int y p^*_n(x, y) \, d\nu(y),
\]

\[
b_n(x) = \mathbb{E}_{\pi_n}[Y | X = x] = \frac{1}{n} \sum_{j=1}^{n} Y_j p_n(x, Y_j) .
\]

It holds

\[
\| b^*_n - b_n \|_{L^2(\mu)}^2 \leq 2 \left\| b^*_n - \frac{1}{n} \sum_{j=1}^{n} Y_j p^*_n(\cdot, Y_j) \right\|_{L^2(\mu)}^2 + 2 \left\| \frac{1}{n} \sum_{j=1}^{n} Y_j p^*_n(\cdot, Y_j) - b_n \right\|_{L^2(\mu)}^2 
\]

\[
\leq 2 \left\| b^*_n - \frac{1}{n} \sum_{j=1}^{n} Y_j p^*_n(\cdot, Y_j) \right\|_{L^2(\mu)}^2 + 2 \frac{1}{2n} \sum_{j=1}^{n} \| p_n(\cdot, Y_j) - p^*_n(\cdot, Y_j) \|_{L^2(\mu)}^2 ,
\]

where in the second inequality, we used Jensen’s inequality together with the bound \( \| Y_j \| \leq 1/2 \). The first term is straightforward to control in expectation:

\[
\mathbb{E} \left\| b^*_n - \frac{1}{n} \sum_{j=1}^{n} Y_j p^*_n(\cdot, Y_j) \right\|_{L^2(\mu)}^2 = \frac{1}{n} \int \| y p^*_n(x, y) - b^*_n(x) \|^2 \, d\mu(x) \, d\nu(y) \lesssim \frac{1}{n} ,
\]

where the last inequality follows by once again applying Proposition 10. For the second term in (4.9), observe that Proposition 13 and Young’s inequality implies

\[
\frac{1}{2n} \sum_{j=1}^{n} \| p_n(\cdot, Y_j) - p^*_n(\cdot, Y_j) \|_{L^2(\mu)}^2 \lesssim \| \tilde{f}^*_n - f_n \|^2_{L^2(\mu)} + \| \tilde{g}^*_n - g_n \|^2_{L^2(\nu_n)} .
\]

The next Lemma is useful in this proof and the subsequent proof for the density. It is immediate from Propositions 10 and 13.

**Lemma 15.** We have

\[
\mathbb{E} \| f_n - \tilde{f}^*_n \|^2_{L^2(\mu)} \lesssim \mathbb{E} \| g_n - \tilde{g}^*_n \|^2_{L^2(\nu_n)} + \frac{1}{n} ,
\]

and

\[
\mathbb{E} \| g_n - \tilde{g}^*_n \|^2_{L^2(\nu)} \lesssim \mathbb{E} \| f_n - \tilde{f}^*_n \|^2_{L^2(\mu_n)} + \frac{1}{n} .
\]
Applying Lemma 15 yields
\[ \mathbb{E}\|b_\ast - b_n\|_{L^2(\mu)}^2 \lesssim \mathbb{E}\|\bar{g}_\ast - g_n\|_{L^2(\nu_n)}^2 + \frac{1}{n}. \]
To conclude, we combine (4.3) together with Lemma 14 to get the desired bound on \( \mathbb{E}\|\bar{g}_\ast - g_n\|_{L^2(\nu_n)}^2 \).

**Density.** Proposition 13 and Young’s inequality implies
\[ \|p_n - p_\ast\|_{L^2(\mu \otimes \nu)}^2 \lesssim \|f_n - \bar{f}_\ast\|_{L^2(\mu)}^2 + \|g_n - \bar{g}_\ast\|_{L^2(\nu)}^2. \]
Hence by Lemma 15,
\[ \mathbb{E}\|p_n - p_\ast\|_{L^2(\mu \otimes \nu)}^2 \lesssim \mathbb{E}[\|f_n - \bar{f}_\ast\|_{L^2(\mu_n)}^2 + \|g_n - \bar{g}_\ast\|_{L^2(\nu_n)}^2] + \frac{1}{n}. \]
To conclude, we combine again (4.3) together with Lemma 14.

**Extending to the full results.** To give the results in probability, we replace each use of expectations with appropriate concentration inequalities in the above proofs. Because the main ideas are all present in the proofs in expectation, we leave these extensions to Appendix A.

### 4.3 Fluctuations of bounded test functions

We now give the proof of our main result on the difference \( (\pi_n - \pi_\ast)(\varphi) \) where \( \varphi \) is a bounded test function. Recall that Theorem 6 says that, for all \( t > 0 \), with probability at least \( 1 - 8e^{-t^2} \),
\[ |(\pi_\ast - \pi_n)(\varphi)| \lesssim \frac{\|\varphi\|_{L^\infty(\mu \otimes \nu)} \cdot t}{\sqrt{n}}. \]
To begin, we assume without loss of generality that \( \|\varphi\|_{L^\infty(\mu \otimes \nu)} = 1 \). We break up the bound into two terms, and use the uniform boundedness of \( \varphi \) to yield
\[ |(\pi_n - \pi_\ast)(\varphi)| \leq \frac{1}{n^2} \sum_{i,j=1}^n |p_n(X_i, Y_j) - p_\ast(X_i, Y_j)| + \frac{1}{n^2} \sum_{i,j=1}^n (p_\ast(X_i, Y_j)\varphi(X_i, Y_j) - \pi_\ast(\varphi)). \]
The first term can be controlled using the results from the previous section. Specifically, Theorem 5 implies that with probability at least \( 1 - 16e^{-t^2} \),
\[ \frac{1}{n^2} \sum_{i,j=1}^n |p_n(X_i, Y_j) - p_\ast(X_i, Y_j)| \lesssim \frac{t}{\sqrt{n}}. \]
For the second term above, we can rewrite it as
\[ \frac{1}{n^2} \sum_{i,j=1}^n (p_\ast(X_i, Y_j)\varphi(X_i, Y_j) - \pi_\ast(\varphi)) = (\mu_n \otimes \nu_n - \mu \otimes \nu)(p_\ast \varphi). \]
Thus, this second term resembles an empirical sample from \( \mu \otimes \nu \), except that we have joined together samples from \( \mu \) and \( \nu \). This difference is, however, benign. Using a trick from U-statistics [Hoe63], we can, in fact, control the size of the above process by that of a *bona fide* sample from \( \mu \otimes \nu \) of size \( n \). This technique is encapsulated in the following Lemma.
Lemma 16. Suppose $a \in L^{\infty}(\mu \otimes \nu)$ is such that $(\mu \otimes \nu)(a) = 0$. Then, for all $t > 0$, with probability at least $1 - 2e^{-t}$ over $X$ and $Y$,

$$|((\mu_n \otimes \nu_n)(a)| \leq \sqrt{\frac{2t}{n}} \|a\|_{L^{\infty}(\mu \otimes \nu)}.$$

Proof. Apply Chernoff’s bound to see that for any $\lambda > 0$,

$$\mathbb{P}_{X,Y}[((\mu_n \otimes \nu_n)(a) > t] \leq e^{-\lambda t} \mathbb{E}_{X,Y}[\exp\{\lambda (\mu_n \otimes \nu_n)(a)\}].$$

We can now apply the key idea from Hoeffding’s paper [Hoe63]. By counting terms, we observe that we can rewrite $(\mu_n \otimes \nu_n)(a)$ as

$$(\mu_n \otimes \nu_n)(a) = \frac{1}{n!} \sum_{\sigma \in \Sigma_n} \frac{1}{n} \sum_{k=1}^{n} a(X_k, Y_{\sigma(k)}),$$

where $\Sigma_n$ is the set of permutations on $n$ elements. Combining this observation with Jensen’s inequality yields the bound

$$\mathbb{P}_{X,Y}[((\mu_n \otimes \nu_n)(a) > t] \leq e^{-\lambda t} \mathbb{E}_{X,Y}\left[\frac{1}{n!} \sum_{\sigma \in \Sigma_n} \exp\left\{\frac{\lambda}{n} \sum_{k=1}^{n} a(X_k, Y_{\sigma(k)})\right\}\right]$$

$$\leq e^{-\lambda t} \mathbb{E}_{X,Y}\left[\frac{1}{n!} \sum_{\sigma \in \Sigma_n} \exp\left\{\frac{\lambda}{n} \sum_{k=1}^{n} a(X_k, Y_{\sigma(k)})\right\}\right].$$

Now, we observe that for any fixed permutation $\sigma$, the joint law of $(X_1, Y_{\sigma(1)}), \ldots, (X_n, Y_{\sigma(n)})$, is identical to that of $z_1, \ldots, z_n$ where $z_k \sim \mu \otimes \nu$ are independent and identically distributed. Let $Z$ denote such an iid sample $(z_1, \ldots, z_n)$. Thus we can change the order of summation to yield

$$\mathbb{E}_{X,Y}\left[\frac{1}{n!} \sum_{\sigma \in \Sigma_n} \exp\left\{\frac{\lambda}{n} \sum_{k=1}^{n} a(X_k, Y_{\sigma(k)})\right\}\right] = \frac{1}{n!} \sum_{\sigma \in \Sigma_n} \mathbb{E}_{X,Y}\left[\exp\left\{\frac{\lambda}{n} \sum_{k=1}^{n} a(X_k, Y_{\sigma(k)})\right\}\right]$$

$$= \mathbb{E}_{Z} \left[\exp\left\{\frac{\lambda}{n} \sum_{k=1}^{n} a(z_k)\right\}\right].$$

Applying Hoeffding’s Lemma and optimizing over $\lambda$ we find

$$\mathbb{P}_{X,Y}[((\mu_n \otimes \nu_n)(a) > t] \leq \exp\left\{-\frac{nt^2}{2\|a\|_{L^{\infty}(\mu \otimes \nu)}^2}\right\}.$$

The analogous argument works for the other tails. Combining these bounds yields the result. □

With thisLemma 16 in hand, we can conclude the proof of Theorem 6 using the uniform boundedness of $p_*$ from Proposition 10.
4.4 Proofs for transfer learning

Proof of Theorem 7 for transfer regression. Observe

\[ \|h^* - h_n\|_{L^2(\mu)}^2 \leq 2\|h^* - \frac{1}{n} \sum_{j=1}^n A_j p^*(\cdot, Y_j)\|_{L^2(\mu)}^2 + 2\|\frac{1}{n} \sum_{j=1}^n A_j (p^*(\cdot, Y_j) - p_n(\cdot, Y_j))\|_{L^2(\mu)}^2 \]

\[ \leq 2\|h^* - \frac{1}{n} \sum_{j=1}^n A_j p^*(\cdot, Y_j)\|_{L^2(\mu)}^2 + 2\|\frac{1}{n} \sum_{j=1}^n p^*(\cdot, Y_j) - p_n(\cdot, Y_j)\|_{L^2(\mu)}^2. \]

The result in expectation then follows as in the proof of Theorem 4 once we observe that

\[ \mathbb{E}\|h^* - \frac{1}{n} \sum_{j=1}^n A_j p^*(\cdot, Y_j)\|_{L^2(\mu)}^2 = \frac{1}{n} \mathbb{E}\|A_1 p^*(\cdot, Y_1) - h^*\|_{L^2(\mu)}^2 \lesssim \frac{1}{n}. \]

Proof of Theorem 9 for transfer classification. We start essentially as in the proof of Theorem 7 without integration. Applying the triangle inequality and Jensen’s inequality, we get that for any \( x \), it holds

\[ |h_n(x) - h^*(x)| \leq \left| \frac{1}{n} \sum_{j=1}^n A_j p^*(x, Y_j) - \mathbb{E}_\omega [A p^*(x, Y)] \right| + \frac{1}{n} \sum_{j=1}^n |p^*(x, Y_j) - p_n(x, Y_j)|. \quad (4.10) \]

To control the first term, we use the boundedness from Proposition 10 to apply Hoeffding’s inequality to get that with probability \( 1 - 2e^{-t} \) it holds for any \( x \) that

\[ \left| \frac{1}{n} \sum_{j=1}^n A_j p^*(x, Y_j) - \mathbb{E}_\omega [A p^*(x, Y)] \right| \lesssim \sqrt{\frac{t}{n}}. \]

For the second term, recall that (4.4) yields

\[ \frac{1}{n} \sum_{j=1}^n |p^*(x, Y_j) - p_n(x, Y_j)| \lesssim |\hat{f}^*(x) - \hat{f}_n(x)| + \|\bar{g}^* - g_n\|_{L^1(\nu_n)}. \]

Moreover, controlling first term using Proposition 13 yields

\[ \frac{1}{n} \sum_{j=1}^n |p^*(x, Y_j) - p_n(x, Y_j)| \lesssim \left| \frac{1}{n} \sum_{j=1}^n e^{-\eta \|x - Y_j\|_2^2 + \eta g_n(Y_j)} - \nu(e^{-\eta \|x - \cdot\|_2^2 + \eta g_n(\cdot)}) \right| + \|\bar{g}^* - g_n\|_{L^1(\nu_n)}. \]

Using Hoeffding’s inequality, we get that with probability at least \( 1 - 2e^{-t} \),

\[ \left| \frac{1}{n} \sum_{j=1}^n e^{-\eta \|x - Y_j\|_2^2 + \eta g_n(Y_j)} - \nu(e^{-\eta \|x - \cdot\|_2^2 + \eta g_n(\cdot)}) \right| \lesssim \sqrt{\frac{t}{n}}. \]

Moreover, Equation (4.3) together with Lemma 18 imply that with probability at least \( 1 - 4e^{-t} \),

\[ \|\bar{g}^* - g_n\|_{L^1(\mu_n)} \leq \|\bar{g}^* - g_n\|_{L^2(\mu_n)} \lesssim \sqrt{\frac{t}{n}}. \]
Collecting terms, we get that for any $x$, with probability at least $1 - 8e^{-t}$,

$$|h_n(x) - h_\star(x)| \lesssim \sqrt{\frac{t}{n}}.$$  \hspace{1cm} (4.11)

We are now in a position to apply Lemma 3.1 in [AT07] which implies that under the Mammen-Tsybakov noise condition above, the pointwise deviation inequality (4.11) readily yields the desired bound on the excess-risk of the plug-in classifier.

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**Appendix A: Omitted proofs for sample complexity**

In this section we give the proofs of the high probability statements in Theorems 3, 4, and 5. In section A.1, we state and prove our main tail bound. In section A.2 we state and prove the lemma comparing the extended dual potentials to their non-extended versions. The theorems are then proved in sections A.3, A.4, and A.5, respectively.

**A.1 The tail bound**

To provide results with control on the tails, we frequently use the following direct consequence of the bounded differences inequality.

**Lemma 17.** Suppose $Z_1, \ldots, Z_m$ are independent mean-zero random variables taking values in a Hilbert space $(H, \| \cdot \|_H)$. Suppose there is some $C > 0$ such that for each $k = 1, \ldots, m$, $\|Z_k\|_H \leq C$. Then, for all $t > 0$, with probability at least $1 - 2e^{-t}$,

$$\left\| \frac{1}{m} \sum_{k=1}^m Z_k \right\|_H^2 \leq \frac{8C^2t}{m}.$$

Using this concentration inequality, we can prove the following Lemma which is at the heart of our results.

**Lemma 18.** Define $\nabla \Phi_n$ as in (2.6) and $\langle \cdot, \cdot \rangle_n$ and $\| \cdot \|_n$ as the inner product and norm of $L^2(\mu_n) \times L^2(\nu_n)$, as in section 2. Then for all $t > 0$, with probability at least $1 - 4e^{-t}$ over both $\mathcal{X}$ and $\mathcal{Y}$,

$$\|\nabla \Phi_n(f_\star, g_\star)\|_n^2 \lesssim \frac{t}{n}.$$
Proof. Recall from (2.7) that
\[
\|\nabla \Phi_n(f_\star, g_\star)\|_n^2 = \frac{1}{n} \sum_{i=1}^{n} \left( 1 - \frac{1}{n} \sum_{j=1}^{n} p_\star(X_i, Y_j) \right)^2 + \frac{1}{n} \sum_{j=1}^{n} \left( 1 - \frac{1}{n} \sum_{i=1}^{n} p_\star(X_i, Y_j) \right)^2, \tag{A.1}
\]
We show the bound for the first term, the proof for the second term is analogous.
Let \(A_j := (1 - p_\star(X_i, Y_j)) n \in \mathbb{R}^n \) for \(j = 1, \ldots, n\), and put
\[
\bar{A}_n := \frac{1}{n} \sum_{j=1}^{n} A_j.
\]
Conditionally on \(X\), the vectors \(A_j\) are independent and have zero mean by the marginal equation (2.9). Moreover, using the uniform boundedness of \(p_\star\) from Proposition 10, we find \(\|A_j\| \lesssim \sqrt{n}\). Applying Lemma 17 we find with probability at least \(1 - 2e^{-t}\) over \(Y\) with \(X\) fixed,
\[
\frac{1}{n} \sum_{i=1}^{n} \left( 1 - \frac{1}{n} \sum_{j=1}^{n} p_\star(X_i, Y_j) \right)^2 \lesssim \frac{t}{n}.
\]
Using the analogous statement for the second term in (A.1) yields the result. \(\square\)

A.2 Controlling the extended dual potentials

We need the next Lemma, which is the high probability analog to Lemma 15.

Lemma 19. Fix any \(t > 0\), and let \((f_n, g_n)\) be extended as in section 2.3. Then with probability at least \(1 - 2e^{-t}\) over \(Y\),
\[
\|\tilde{f}_\star - f_n\|_{L^2(\mu)}^2 \lesssim \|\tilde{g}_\star - g_n\|_{L^2(\nu_n)}^2 + \frac{t}{n}.
\]
Similarly, with probability at least \(1 - 2e^{-t}\) over \(X\),
\[
\|\tilde{g}_\star - g_n\|_{L^2(\nu)}^2 \lesssim \|\tilde{f}_\star - f_n\|_{L^2(\mu_n)}^2 + \frac{t}{n}.
\]

Proof. We prove the first statement, the second is analogous. Note that it follows readily from Lemma 17 that with probability at least \(1 - 2e^{-t}\) over \(Y\), it holds
\[
\left\| \frac{1}{n} \sum_{j=1}^{n} e^{-\eta\|\cdot - Y_j\|^2 + \nu g_\star(Y_j)} - \nu e^{-\eta\|\cdot - y\|^2 + \nu g_\star(y)} \right\|_{L^2(\mu)}^2 \lesssim \frac{t}{n}.
\]
Together with Proposition 13, this completes the proof. \(\square\)

A.3 Proof of tail control for costs

To yield the result, we can use the same proof as in the expectation case but with tail control replacing the expectation of \(\Phi_n(f_\star, g_\star) - \Phi(f_\star, g_\star)\), and \(\|\nabla \Phi_n(f_\star, g_\star)\|_n\). To begin, we write
\[
|S_n - S| \leq |\Phi_n(f_n, g_n) - \Phi_n(f_\star, g_\star)| + |\Phi_n(f_\star, g_\star) - \Phi(f_\star, g_\star)|. \tag{A.2}
\]
For the first term on the right-hand side above, Proposition 12 implies
\[ |\Phi_n(f_n, g_n) - \Phi_n(f_\ast, g_\ast)| = \Phi_n(f_n, g_n) - \Phi_n(f_\ast, g_\ast) \lesssim \|\nabla \Phi_n(f_\ast, g_\ast)\|_n^2. \]
So using Lemma 18 we find that with probability at least 1 \( - 4e^{-t} \) over both \( \mathcal{X} \) and \( \mathcal{Y} \),
\[ |\Phi_n(f_n, g_n) - \Phi_n(f_\ast, g_\ast)| \lesssim \frac{t}{n}. \]
For latter term in (A.2), we can write
\[ \Phi_n(f_\ast, g_\ast) - \Phi(f_\ast, g_\ast) = (\mu_n \otimes \nu_n - \mu \otimes \nu)(f_\ast + g_\ast - \frac{1}{\eta}p_\ast). \]
Using the uniform boundedness from Proposition 10, we can apply Lemma 16 to find that with probability at least 1 \( - 2e^{-t} \) over \( \mathcal{X}, \mathcal{Y} \)
\[ |(\mu_n \otimes \nu_n - \mu \otimes \nu)(f_\ast + g_\ast - \frac{1}{\eta}p_\ast)| \lesssim \sqrt{\frac{t}{n}}. \]
Applying both of these tails bounds to (A.2) yields the result.

**A.4 Proof of tail control for maps**

We start by bounding
\[ \|b_\ast - b_n\|_{L^2(\mu)}^2 \lesssim \left\| \frac{1}{n} \sum_{j=1}^n Y_j p_\ast(\cdot, Y_j) - b_\ast(\cdot) \right\|_{L^2(\mu)}^2 + \left\| \frac{1}{n} \sum_{j=1}^n Y_j (p_\ast(\cdot, Y_j) - p_n(\cdot, Y_j)) \right\|_{L^2(\mu)}^2. \]
For the first term, we apply the bounded differences inequality, Lemma 17. In this way, we see that for all \( t > 0 \), with probability at least 1 \( - 2e^{-t} \) over \( \mathcal{Y} \),
\[ \left\| \frac{1}{n} \sum_{j=1}^n Y_j p_\ast(\cdot, Y_j) - b_\ast(\cdot) \right\|_{L^2(\mu)}^2 \lesssim \frac{t}{n}. \]
Hence, we can focus on the second term.

Using Jensen’s and Proposition 13 yields
\[ \left\| \frac{1}{n} \sum_{j=1}^n Y_j (p_\ast(\cdot, Y_j) - p_n(\cdot, Y_j)) \right\|_{L^2(\mu)}^2 \lesssim \frac{1}{n} \sum_{j=1}^n \left\| p_\ast(\cdot, Y_j) - p_n(\cdot, Y_j) \right\|_{L^2(\mu)}^2 \lesssim \|\bar{f}_\ast - f_n\|_{L^2(\mu)}^2 + \|\bar{g}_\ast - g_n\|_{L^2(\nu_n)}^2. \]
Applying Lemma 19 we obtain that with probability at least 1 \( - 4e^{-t} \) over \( \mathcal{Y} \),
\[ \|b_\ast - b_n\|_{L^2(\mu)}^2 \lesssim \frac{t}{n} + \|\bar{g}_\ast - g_n\|_{L^2(\nu_n)}^2. \]
Hence, we may use Equation (4.3) to find that
\[ \|b_\ast - b_n\|_{L^2(\mu)}^2 \lesssim \frac{t}{n} + \|\nabla \Phi_n(f_\ast, g_\ast)\|_n^2, \]
and now we can use Lemma 18 to conclude.
A.5 Proof of tail control for densities

For the bound in $L^2(\mu_n \otimes \nu_n)$, Proposition 13 implies
\[
\|p_n - p_*\|_{L^2(\mu_n \otimes \nu_n)}^2 \lesssim \|\tilde{f}_n - f_n\|_{L^2(\mu_n)}^2 + \|\tilde{g}_n - g_n\|_{L^2(\nu_n)}^2.
\]
Applying (4.3) and Lemma 18, we can conclude.

For the bound in $L^2(\mu \otimes \nu)$, put $\tilde{f}_* := f_* + \nu_n(g_*)$ and $\tilde{g}_* := g_* - \nu_n(g_*)$ are as in Proposition 13. Then Proposition 13 implies
\[
\|p_n - p_*\|_{L^2(\mu \otimes \nu)}^2 \lesssim \|\tilde{f}_* - f_n\|_{L^2(\mu)}^2 + \|\tilde{g}_* - g_n\|_{L^2(\nu)}^2,
\]
Applying Lemma 19 we find that with probability at least $1 - 4e^{-t}$ over $\mathcal{X}, \mathcal{Y}$
\[
\|p_n - p_*\|_{L^2(\mu \otimes \nu)}^2 \lesssim \|\tilde{f}_* - f_n\|_{L^2(\mu_n)}^2 + \|\tilde{g}_* - g_n\|_{L^2(\nu_n)}^2 + \frac{t}{n}.
\]
Applying (4.3) and Lemma 18, we can conclude.

Appendix B: Further proofs

B.1 Proof of Proposition 10

The proof is essentially that of [MNW19, Prop. 1], just with different notation and slightly different assumptions. We include it in this appendix for the reader’s convenience. We begin by showing the result for $(f_*, g_*)$.

The $\mu$-marginal constraint for $\pi_*$, namely (2.9), implies that for $\mu$-almost every $x$,
\[
1 = \int e^{-\eta\|x-y\|^2 - f_*(x) - g_*(y)}d\nu(y) \geq e^{-\eta(1-f_*(x))} \int e^{\eta g_*(y)}d\nu(y) \geq e^{-\eta(1-f_*(x))},
\]
where the first inequality follows by Assumption 1, the second inequality by Jensen’s together with the convention that $\nu(g_*) = 0$. This implies $f_*(x) \leq 1 \mu$-almost everywhere. Hence, we can use the marginal constraint (2.9) for $\nu$-almost every $y$ to yield
\[
1 = \int e^{-\eta\|x-y\|^2 - f_*(x) - g_*(y)}d\mu(x) \leq e^{\eta(1+g_*(y))}.
\]

Whence $g_*(y) \geq -1$ for $\nu$-almost every $y$.

We now claim that $\mu(f_*) \geq 0$. To see this, start by observing that the primal Sinkhorn problem (2.1), has a non-negative optimal value, and so by Theorem 1, the dual objective evaluated at $(f_*, g_*)$ is non-negative. Hence
\[
0 \leq \mu(f_*) + \nu(g_*) - \frac{1}{\eta}(\mu \otimes \nu)(e^{-\eta\|x-y\|^2 - f_*(x) - g_*(y)}) + \frac{1}{\eta} = \mu(f_*) ,
\]
where we used the marginal constraint (2.9) and the convention $\nu(g_*) = 0$. Using this fact, we can mimic the proof that $f_*(x) \leq 1$ above to show that $g_*(y) \leq 1$ for $\nu$ almost all $y$. We similarly find $f_*(x) \geq -1$ for $\mu$ almost all $x$, finishing the proof for $(f_*, g_*)$. 


The exact same argument shows $\|f_n\|_{\infty(\mu_n)}, \|g_n\|_{\infty(\nu_n)} \leqslant 1$. In fact, this readily yields a stronger result for canonical extensions. Indeed, recall that for every $x \in \mathbb{R}^d$, the canonical extension of $f_n$ defined in (2.16) satisfies, for any $x \in \mathbb{R}^d$,

$$f_n(x) = -\frac{1}{\eta} \ln \left( \frac{1}{n} \sum_{j=1}^{n} e^{-\eta \|x-Y_j\|^2 + n g_n(Y_j)} \right) \geq -1.$$

For $\mu$-almost every $x$, we also find

$$f_n(x) = -\frac{1}{\eta} \ln \left( \frac{1}{n} \sum_{j=1}^{n} e^{-\eta \|x-Y_j\|^2 + n g_n(Y_j)} \right) \leq -1.$$

Hence $\|f_n\|_{\infty(\mu)} \leq 2$. Applying the same argument for $g_n$ completes the bounds on dual potentials.

Bounds on densities readily follow from the above bounds on dual potentials together with the definitions (2.8) and (2.12).

**B.2 Proof of Proposition 12**

Proposition 12 follows from the following proposition.

**Proposition 20 (Polyak-Łojasiewicz inequality).** Let $C \subset \mathcal{H}$ be a convex subset of a Hilbert space $\mathcal{H}$. Let $\rho: \mathcal{H} \to \mathbb{R}$ be an $\alpha$-strongly convex on $C$. Then, it holds

$$\rho(v) - \inf_{\mathcal{H}} \rho \leq \frac{1}{2\alpha} \|\nabla \rho(v)\|^2 \quad \forall v \in C.$$

**Proof.** By definition of strong convexity, for all $v, w \in C$,

$$\rho(w) \geq \rho(v) + \langle \nabla \rho(v), w - v \rangle + \frac{\alpha}{2} \|w - v\|^2.$$

The minimum over $w \in \mathcal{H}$ of the right-hand side is achieved at $w = v - \nabla \rho(v)/\alpha$ and is given by

$$\rho(v) - \frac{1}{2\alpha} \|\nabla \rho(v)\|^2.$$

Since $\rho(w)$ exceeds this quantity for all $w \in C$, we also have

$$\inf_{\mathcal{H}} \rho \geq \rho(v) - \frac{1}{2\alpha} \|\nabla \rho(v)\|^2.$$

Re-arranging yields the result.

**B.3 Proof of Proposition 13**

Define

$$\tilde{f}_n(x) := -\frac{1}{\eta} \ln \left( \frac{1}{n} \sum_{j=1}^{n} e^{-\eta \|x-Y_j\|^2 + \eta g_n(Y_j)} \right).$$
We have, as in the proof of Proposition 10, the bound, $|\tilde{f}_*(x)| \leq 3$. Moreover, we get

$$ |\tilde{f}_*(x) - f_n(x)| \leq |\tilde{f}_*(x) - \tilde{f}_*(x)| + |\tilde{f}_*(x) - f_n(x)|. $$

To bound the first term, we use (2.10) together with the Lipschitzness of the logarithm and exponential maps that follows from the uniform bounds on each term. We obtain the following estimate

$$ |\tilde{f}_*(x) - \tilde{f}_*(x)| = \left| \frac{1}{\eta} \ln \left( \frac{1}{n} \sum_{j=1}^{n} e^{-\eta \|x-Y_j\|^2 + \eta \tilde{g}_*(Y_j)} \right) - \frac{1}{\eta} \ln \left( \int e^{-\eta \|x-y\|^2 + \eta \tilde{g}_*(y)} d\nu(y) \right) \right| $$

$$ = \left| \frac{1}{\eta} \ln \left( \frac{1}{n} \sum_{j=1}^{n} e^{-\eta \|x-Y_j\|^2 + \eta \tilde{g}_*(Y_j)} \right) - \frac{1}{\eta} \ln \left( \frac{1}{n} \sum_{j=1}^{n} e^{-\eta \|x-Y_j\|^2 + \eta \tilde{g}_*(Y_j)} \right) \right| $$

$$ \lesssim \left| \frac{1}{n} \sum_{j=1}^{n} e^{-\eta \|x-Y_j\|^2 + \eta \tilde{g}_*(Y_j)} - \nu(e^{-\eta \|x-\|^2 + \eta \tilde{g}_*(\cdot)}) \right|. $$

Using the same technique we get the following bound for the second term:

$$ |\tilde{f}_*(x) - f_n(x)| = \left| \frac{1}{\eta} \ln \left( \frac{1}{n} \sum_{j=1}^{n} e^{-\eta \|x-Y_j\|^2 + \eta g_n(Y_j)} \right) - \frac{1}{\eta} \ln \left( \frac{1}{n} \sum_{j=1}^{n} e^{-\eta \|x-Y_j\|^2 + \eta \tilde{g}_*(Y_j)} \right) \right| $$

$$ \lesssim \| \tilde{g}_* - g_n \|_{L^1(\nu_n)}. $$

This yields the bound on $|\tilde{f}_*(x) - f_n(x)|$ and the bound of $|\tilde{g}_*(y) - g_n(y)|$ follows using the same argument.

To prove the bound on $|p_*(x, y) - p_n(x, y)|$, we again apply the boundedness from Proposition 10 and the Lipschitzness of the exponential on bounded intervals to yield

$$ |p_n(x, y) - p_*(x, y)| = |e^{-\eta \|x-y\|^2 + \eta f_*(x) + \eta g_n(y)} - e^{-\eta \|x-y\|^2 + \eta f_*(x) + \eta \tilde{g}_*(y)}| $$

$$ = |e^{-\eta \|x-y\|^2 + \eta f_*(x) + \eta g_n(y)} - e^{-\eta \|x-y\|^2 + \eta f_*(x) + \eta \tilde{g}_*(y)}| $$

$$ \lesssim |f_n(x) + g_n(y) - \tilde{f}_*(x) - \tilde{g}_*(y)| $$

$$ \leq |f_n(x) - \tilde{f}_*(x)| + |g_n(y) - \tilde{g}_*(y)|. $$

References

[ANWS22] Jason M Altschuler, Jonathan Niles-Weed, and Austin J Stromme. Asymptotics for semidiscrete entropic optimal transport. SIAM Journal on Mathematical Analysis, 54(2):1718–1741, 2022.

[AT07] Jean-Yves Audibert and Alexandre B. Tsybakov. Fast learning rates for plug-in classifiers. Ann. Statist., 35(2):608–633, 2007.

[AWR17] Jason Altschuler, Jonathan Weed, and Philippe Rigollet. Near-linear time approximation algorithms for optimal transport via Sinkhorn iteration. In Advances in Neural Information Processing Systems, pages 1964–1974, 2017.

[Ber20] Robert J Berman. The Sinkhorn algorithm, parabolic optimal transport and geometric Monge–Ampère equations. Numerische Mathematik, 145(4):771–836, 2020.
[BGN21] Espen Bernton, Promit Ghosal, and Marcel Nutz. Entropic optimal transport: geometry and large deviations. \textit{arXiv preprint arXiv:2102.04397}, 2021.

[CFTR17] Nicolas Courty, Rémi Flamary, Devis Tuia, and Alain Rakotomamonjy. Optimal transport for domain adaptation. \textit{IEEE Transactions on Pattern Analysis and Machine Intelligence}, 39(9):1853–1865, 2017.

[Cut13] Marco Cuturi. Sinkhorn distances: Lightspeed computation of optimal transport. In C.J. Burges, L. Bottou, M. Welling, Z. Ghahramani, and K.Q. Weinberger, editors, \textit{Advances in Neural Information Processing Systems}, volume 26. Curran Associates, Inc., 2013.

[dBGSLNW22] Eustasio del Barrio, Alberto Gonzalez-Sanz, Jean-Michel Loubes, and Jonathan Niles-Weed. An improved central limit theorem and fast convergence rates for entropic transportation costs, 2022.

[DDBD21] George Deligiannidis, Valentin De Bortoli, and Arnaud Doucet. Quantitative uniform stability of the iterative proportional fitting procedure. \textit{arXiv preprint arXiv:2108.08129}, 2021.

[Del22] Alex Delalande. Nearly tight convergence bounds for semi-discrete entropic optimal transport. In \textit{International Conference on Artificial Intelligence and Statistics}, pages 1619–1642. PMLR, 2022.

[DGL96] L. Devroye, L. Györfi, and G. Lugosi. \textit{A probabilistic theory of pattern recognition}, volume 31 of \textit{Applications of Mathematics (New York)}. Springer-Verlag, New York, 1996.

[DGS21] Nabarun Deb, Promit Ghosal, and Bodhisattva Sen. Rates of estimation of optimal transport maps using plug-in estimators via barycentric projections. \textit{Advances in Neural Information Processing Systems}, 34:29736–29753, 2021.

[DMG20] Simone Di Marino and Augusto Gerolin. An optimal transport approach for the Schrödinger bridge problem and convergence of Sinkhorn algorithm. \textit{Journal of Scientific Computing}, 85(2):1–28, 2020.

[EMR15] Matthias Erbar, Jan Maas, and Michiel Renger. From large deviations to Wasserstein gradient flows in multiple dimensions. \textit{Electronic Communications in Probability}, 20:1–12, 2015.

[EN21] Stephan Eckstein and Marcel Nutz. Quantitative stability of regularized optimal transport. \textit{arXiv preprint arXiv:2110.06798}, 2021.

[FHN+19] Aden Forrow, Jan-Christian Hütter, Mor Nitzan, Philippe Rigollet, Geoffrey Schiebinger, and Jonathan Weed. Statistical optimal transport via factored couplings. In \textit{The 22nd International Conference on Artificial Intelligence and Statistics}, pages 2454–2465. PMLR, 2019.

[GCB+19] Aude Genevay, Lénaic Chizat, Francis Bach, Marco Cuturi, and Gabriel Peyré. Sample complexity of Sinkhorn divergences. In \textit{The 22nd International Conference on Artificial Intelligence and Statistics}, pages 1574–1583. PMLR, 2019.

[GNB21] Promit Ghosal, Marcel Nutz, and Espen Bernton. Stability of entropic optimal transport and Schrödinger bridges. \textit{arXiv preprint arXiv:2106.03670}, 2021.

[GX21] Florian Gunsilius and Yuliang Xu. Matching for causal effects via multimarginal optimal transport. \textit{arXiv preprint arXiv:2112.04398}, 2021.

[Hoe63] Wassily Hoeffding. Probability inequalities for sums of bounded random variables. \textit{J. Amer. Statist. Assoc.}, 58:13–30, 1963.
[HR21] Jan-Christian Hütter and Philippe Rigollet. Minimax estimation of smooth optimal transport maps. *Ann. Statist.*, 49(2):1166–1194, 2021.

[KB05] Vladimir Koltchinskii and Olexandra Beznosova. Exponential convergence rates in classification. In Peter Auer and Ron Meir, editors, *Learning Theory*, pages 295–307, Berlin, Heidelberg, 2005. Springer Berlin Heidelberg.

[KNS16] Hamed Karimi, Julie Nutini, and Mark Schmidt. Linear convergence of gradient and proximal-gradient methods under the Polyak-Lojasiewicz condition. In *Joint European Conference on Machine Learning and Knowledge Discovery in Databases*, pages 795–811. Springer, 2016.

[KTM20] Marcel Klatt, Carla Tameling, and Axel Munk. Empirical regularized optimal transport: statistical theory and applications. *SIAM Journal on Mathematics of Data Science*, 2(2):419–443, 2020.

[Léo13] Christian Léonard. A survey of the Schrödinger problem and some of its connections with optimal transport. *arXiv preprint arXiv:1308.0215*, 2013.

[LSPC19] Giulia Luise, Saverio Salzo, Massimiliano Pontil, and Carlo Ciliberto. Sinkhorn barycenters with free support via Frank-Wolfe algorithm. *Advances in Neural Information Processing Systems*, 32:9322–9333, 2019.

[LZKS21] Hugo Lavenant, Stephen Zhang, Young-Heon Kim, and Geoffrey Schiebinger. Towards a mathematical theory of trajectory inference. *arXiv preprint arXiv:2102.09204*, 2021.

[MBNWW21] Tudor Manole, Sivaraman Balakrishnan, Jonathan Niles-Weed, and Larry Wasserman. Plugin estimation of smooth optimal transport maps. *arXiv preprint arXiv:2107.12364*, 2021.

[MNW19] Gonzalo Mena and Jonathan Niles-Weed. Statistical bounds for entropic optimal transport: sample complexity and the central limit theorem. *Advances in Neural Information Processing Systems*, 32, 2019.

[MNW21] Tudor Manole and Jonathan Niles-Weed. Sharp convergence rates for empirical optimal transport with smooth costs. *arXiv preprint arXiv:2106.13181*, 2021.

[MT99] E. Mammen and A. B. Tsybakov. Smooth discrimination analysis. *Ann. Statist.*, 27(6):1808–1829, 1999.

[MVB+21] Boris Muzellec, Adrien Vacher, Francis Bach, François-Xavier Vialard, and Alessandro Rudi. Near-optimal estimation of smooth transport maps with kernel sums-of-squares. *arXiv preprint arXiv:2112.01907*, 2021.

[NW21] Marcel Nutz and Johannes Wiesel. Entropic optimal transport: Convergence of potentials. *Probability Theory and Related Fields*, pages 1–24, 2021.

[NWR19] Jonathan Niles-Weed and Philippe Rigollet. Estimation of Wasserstein distances in the spiked transport model. *arXiv preprint arXiv:1909.07513*, 2019.

[Pal19] Soumik Pal. On the difference between entropic cost and the optimal transport cost. *arXiv preprint arXiv:1905.12206*, 2019.

[PC19] Gabriel Peyré and Marco Cuturi. Computational optimal transport. *Foundations and Trends in Machine Learning*, 11(5-6):355–607, 2019.

[PNW21] Aram-Alexandre Pooladian and Jonathan Niles-Weed. Entropic estimation of optimal transport maps. *arXiv preprint arXiv:2109.12004*, 2021.

[RW18] Philippe Rigollet and Jonathan Weed. Entropic optimal transport is maximum-likelihood deconvolution. *Comptes Rendus Mathematique*, 356(11):1228–1235, 2018.
Philippe Rigollet and Jonathan Weed. Uncoupled isotonic regression via minimum wasserstein deconvolution. *Information and Inference: A Journal of the IMA*, 8(4):691–717, 2019.

Filippo Santambrogio. *Optimal transport for applied mathematicians*, volume 87 of *Progress in Nonlinear Differential Equations and their Applications*. Birkhäuser/Springer, Cham, 2015. Calculus of variations, PDEs, and modeling.

Erwin Schrödinger. Über die umkehrung der naturgesetze. *Sitzungsberichte der Preussischen Akademie der Wissenschaften: Physikalisch-Mathematische Klasse*, pages 144–153, 1931.

Erwin Schrödinger. Sur la théorie relativiste de l’électron et l’interprétation de la mécanique quantique. *Annales de l’institut Henri Poincaré*, 2(4):269–310, 1932.

Justin Solomon, Fernando de Goes, Gabriel Peyré, Marco Cuturi, Adrian Butscher, Andy Nguyen, Tao Du, and Leonidas Guibas. Convolutional Wasserstein distances: efficient optimal transportation on geometric domains. *ACM Trans. Graph.*, 34(4):66:1–66:11, July 2015.

Richard Sinkhorn. A relationship between arbitrary positive matrices and doubly stochastic matrices. *The Annals of Mathematical Statistics*, 35(2):876–879, 1964.

Geoffrey Schiebinger, Jian Shu, Marcin Tabaka, Brian Cleary, Vidya Subramanian, Aryeh Solomon, Joshua Gould, Siyan Liu, Stacie Lin, Peter Berube, et al. Optimal-transport analysis of single-cell gene expression identifies developmental trajectories in reprogramming. *Cell*, 176(4):928–943, 2019.

William Torous, Florian Gunsilius, and Philippe Rigollet. An optimal transport approach to causal inference. *arXiv preprint arXiv:2108.05858*, 2021.

Cédric Villani. *Topics in optimal transportation*, volume 58 of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, RI, 2003.

Cédric Villani. *Optimal transport*, volume 338 of *Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences]*. Springer-Verlag, Berlin, 2009. Old and new.

Adrien Vacher, Boris Muzellec, Alessandro Rudi, Francis Bach, and François-Xavier Vialard. A dimension-free computational upper-bound for smooth optimal transport estimation. In *Proceedings of Thirty Fourth Conference on Learning Theory*, pages 4143–4173. PMLR, 2021.