Minimax rates of estimation for smooth optimal transport maps

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Abstract. Brenier’s theorem is a cornerstone of optimal transport that guarantees the existence of an optimal transport map $T$ between two probability distributions $P$ and $Q$ over $\mathbb{R}^d$ under certain regularity conditions. The main goal of this work is to establish the minimax rates estimation rates for such a transport map from data sampled from $P$ and $Q$ under additional smoothness assumptions on $T$. To achieve this goal, we develop an estimator based on the minimization of an empirical version of the semi-dual optimal transport problem, restricted to truncated wavelet expansions. This estimator is shown to achieve near minimax optimality using new stability arguments for the semi-dual and a complementary minimax lower bound. These are the first minimax estimation rates for transport maps in general dimension.

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1. INTRODUCTION

Wasserstein distances and the associated optimal transport problem date back to the work of Gaspard Monge [54] and have since then become important tools in pure and applied mathematics [67, 85, 86]. Tools from optimal transport have been successfully employed in machine learning [2, 4, 5, 11, 22, 28, 31, 34, 40, 55, 59, 64, 69, 70, 75] computer graphics [27, 48, 73, 74], statistics [1, 6, 12, 13, 23, 44, 47, 56, 60, 62, 71, 77, 88, 90] and, more recently, computational biology [68, 89].

Monge asked the following question: Given two probability measures $P, Q$ in $\mathbb{R}^d$, how can we transport $P$ to $Q$ while minimizing the total distance traveled by this transport. A classical instantiation of this problem over $\mathbb{R}^d$ is to find a map $T_0: \mathbb{R}^d \to \mathbb{R}^d$ that minimizes the objective

$$\min_T \int_{\mathbb{R}^d} \|T(x) - x\|^2_2 dP(x), \quad \text{s.t. } T_\#P = Q,$$

which is known as the Monge problem, where $T_\#P$ denotes the push-forward of $P$ under $T$, that is,

$$T_\#P(A) = P(T^{-1}(A)), \quad \text{for all Borel sets } A.$$
While cost functions other than \(\|T(x) - x\|_2^2\) could be of interest, this work focuses on the quadratic cost.

The highly non-linear constraint in (1.2) made the mathematical treatment of the Monge problem seem elusive for a long time, until the seminal work of Kantorovich [42, 43], who considered the following relaxation. Instead of looking for a map \(T_0\), look for a transport plan \(\gamma_0\) in the set of all possible probability measures on \(\mathbb{R}^d \times \mathbb{R}^d\) whose marginals coincide with \(P\) and \(Q\), which we denote by \(\Gamma(P, Q)\). This leads to the optimization problem

\[
\min_\gamma \int \|x - y\|_2^2 \, d\gamma(x, y) \quad \text{s.t. } \gamma \in \Gamma(P, Q),
\]

which is known as the *Kantorovich problem*, and whose value is the square of the 2-Wasserstein distance \(W_2^2(P, Q)\) between the two probability measures \(P\) and \(Q\). The two optimization problems are indeed linked: Brenier’s Theorem (Theorem 1), guarantees that under regularity assumptions on \(P\), a solution \(\gamma_0\) to (1.3) is concentrated on the graph of a map \(T_0\), that is, using a suggestive informal notation, \(\gamma_0(x, y) = P(x) \delta_{y=T_0(x)},\) where \(\delta\) denotes a point mass. Moreover, \(T_0\) is the gradient of a convex function \(f_0\).

Statistical optimal transport describes a body of questions that arise when the measures \(P\) and \(Q\) are unknown but samples are available. While the question of estimation of various quantities such as \(W_2^2(P, Q)\), for example, are of central importance, for applications such as domain adaptation and data integration[14–16, 19, 29, 57, 63, 72], the main quantity of interest is the transport map \(T_0\) itself since it can be used to push almost every points in the support of \(P\) to points in the support of \(Q\). The goal of this paper is to study the rates of estimation of a smooth transport map \(T_0\) from samples.

To fix a concrete setup assume that we have at our disposal \(2n\) independent observations \(X_1, \ldots, X_n\) from \(P\) and \(Y_1, \ldots, Y_n\) from \(Q\), based on which we would like to find an estimator \(\hat{T}\) for \(T_0\). This statistical problem poses several challenges:

(i) The most straightforward estimator is obtained by replacing \(P\) and \(Q\) by their empirical counterparts [58]. It leads to a finite-dimensional linear problem that can be approximated very efficiently due to recent algorithmic advances [3, 17, 24, 58]. However, even if the resulting optimizer \(\hat{\gamma}\) is actually a map (matching), which it is not in general, it is not defined outside the sample points. In particular, it does not indicate how to transport a point \(x \notin \{X_1, \ldots, X_n\}\). In contrast, we would like to obtain an estimator \(\hat{T}\) with guarantees in \(L^2(P)\), that is, with convergence of

\[
\|\hat{T} - T_0\|_{L^2(P)}^2 := \int \|\hat{T}(x) - T_0(x)\|_2^2 \, dP(x).
\]

(ii) It is known that the estimator \(W_2^2(\hat{P}, \hat{Q})\) can be a poor proxy for \(W_2^2(P, Q)\) if the underlying dimensionality of the distributions \(P\) and \(Q\) is large, as it suffers from the so-called *curse of dimensionality*. For example, if both \(P\) and \(Q\) are absolutely continuous with respect to the Lebesgue measure in \(\mathbb{R}^d, d \geq 3\), it is known that \(\mathbb{E}[W_2^2(P, \hat{P})] \approx n^{-2/d}\) (see, e.g., [87]). In fact, we show in Theorem 4 that without further assumptions on either \(P, Q\), or \(T_0\), no estimator can have an expected squared loss (1.4) uniformly better than \(n^{-2/d}\).

(iii) While many heuristic approaches have been brought forward to address the previous point, a thorough statistical analysis of the rate of convergence has so far been lacking. This can be partly attributed to the structure (or lack thereof) of problem (1.3). Being a linear optimization problem, it lacks simple stability estimates that are key to establish statistical guarantees.
by relating $\|\hat{T} - T_0\|_{L^2(P)}$ to the sub-optimality gap
\[
\int_{\mathbb{R}^d} \|T(x) - x\|_2^2 \, dP(x) - \int_{\mathbb{R}^d} \|T_0(x) - x\|_2^2 \, dP(x).
\]

In this paper, we aim to address these problems by imposing additional assumptions on the transport map $T_0$ that lead to a rate faster than $n^{-2/d}$. One assumption we impose on the transport map $T_0$ is smoothness, a standard way of alleviating the curse of dimensionality in non-parametric estimation. Another key assumption is based on an observation of Ambrosio published in an article by Gigli [32]. They show that the optimization problem (1.1) has positive curvature, in the sense of a stability estimate
\[
\|T - T_0\|_{L^2(P)}^2 \lesssim \int_{\mathbb{R}^d} \|T(x) - x\|_2^2 \, dP(x) - \int_{\mathbb{R}^d} \|T_0(x) - x\|_2^2 \, dP(x),
\]
provided $T_0 = \nabla f_0$ is Lipschitz continuous on $\mathbb{R}^d$ and $T_\# P = Q$. While this observation does not immediately lend itself to the analysis of an estimator due to the presence of the push-forward constraint, we show in Proposition 8 that under similar assumptions, the so-called semi-dual problem (see (2.6) below) admits a stability estimate.

Due to the rising interest in Optimal Transport as a tool for statistics and machine learning, many empirical regularization techniques have been proposed, ranging from the computationally successful entropic regularization [3, 17, 30], $\ell^2$-regularization [7], smoothness regularization [57], to regularization techniques specifically adapted to the application of domain adaptation [14–16]. Notably, [30] also consider regularization based on the semi-dual objective and reproducing kernel Hilbert spaces. However, the statistical performance of these regularization techniques to estimate transport maps from sampled data has been largely unanswered, with the following exceptions.

The rest of this paper is organized as follows. In Section 2, we review some important concepts of optimal transport, mainly duality and Brenier’s theorem which are instrumental in the definition of our estimator, which is postponed to Section 5. Indeed, since the main goal of this paper is to establish minimax rates of convergence for smooth transport maps, we present these rates in Section 3 and prove lower bounds in the following Section 4, since this proof illustrates well the source of the nonstandard exponent in the rates. We then proceed to Section 5 where we define a minimax optimal estimator constructed as follows. First, we define an estimator for the optimal Kantorovich potential as the solution to the empirical counterpart of the semi-dual problem restricted to a class of wavelet expansions. Then, our estimator is defined as the gradient of this potential. We prove that it achieves the optimal rate in the same section. Finally, some useful facts from convex analysis, approximation theory for wavelets and empirical process theory respectively are gathered in the three appendices.

To the authors’ best knowledge, estimation of transport maps has only been studied in the one-dimensional case under the name uncoupled regression [63] where the sample $Y_1, \ldots, Y_n$ is subject to measurement noise. There, the main statistical difficulty arises from the presence of this additional noise and boils down to obtaining deconvolution guarantees in the Wasserstein distance. Such guarantees were recently obtained under smoothness assumptions on the underlying density [10, 20, 21] but they do not translate directly into rates of estimation for the optimal transport map beyond the 1D case. Note that in the presence of Gaussian measurement noise, the rates of estimation are likely to become logarithmic rather than polynomial as deconvolution is a statistically difficult task.
Notation. For any positive integer $m$, define $[m] := \{1, \ldots, m\}$. We write $|A|$ for the cardinality of a set $A$. The relation $a \lesssim b$ is used to indicate that two quantities are the same up to a constant $C$, $a \leq C b$. The relation $\gtrsim$ is defined analogously, and we write $a \asymp b$ if $a \lesssim b$ and $a \gtrsim b$. We denote by $c$ and $C$ constants that might change from line to line and that may depend on all parameters of the statistical problem except $n$. We abbreviate with $a \lor b$, $a \land b$ the maximum and minimum of $a \in \mathbb{R}$ and $b \in \mathbb{R}$, respectively. For $a \in \mathbb{R}$, the floor and ceiling functions are denoted by $\lfloor a \rfloor$ and $\lceil a \rceil$, indicating rounding $a$ to the next smaller and larger integer, respectively. We use $\text{supp} f$ to denote the support of a function or measure $f$, and $\text{diam} \Omega$ for the diameter of a set $\Omega \subseteq \mathbb{R}^d$. We denote by $B_1$ the unit-ball with respect to the Euclidean distance in $\mathbb{R}^d$, where $d$ should be clear from the context. For a real symmetric matrix $A$ and $\lambda \in \mathbb{R}$, we write $\lambda \preceq A$ if all eigenvalues of $A$ are bounded below $\lambda$, and similarly for $A \succeq \lambda$. Moreover, we denote the smallest and largest eigenvalues of $A$ by $\lambda_{\min}(A)$, $\lambda_{\max}(A)$, respectively.

For $p \in [1, \infty]$, we denote by $\ell^p$ the space $\mathbb{R}^d$ endowed with the usual $\ell^p$ norms $\| \cdot \|_p$ and by $L^p$ the Lebesgue spaces of functions on $\mathbb{R}^d$ or subsets $\Omega \subseteq \mathbb{R}^d$ with respect to the Lebesgue measure $\lambda$ on $\mathbb{R}^d$, whose norms we denote by $\| \cdot \|_{L^p}(\mathbb{R}^d)$ and $\| \cdot \|_{L^p(\Omega)}$, respectively. By abuse of notation, for a different measure $P$, we denote the associated Lebesgue norms by $\| \cdot \|_{L^p(P)}$.

For a function $f : \mathbb{R}^d \ni \Omega \to \mathbb{R}$, we denote by $\partial_i = \partial_i/(\partial x_i)$ its weak derivative in the sense of distributions in direction $x_i$, which coincides with the usual (point-wise) derivative if $f$ is differentiable in $\Omega$. For a multi-index $b \in \mathbb{N}^d$, we set

$$\partial^b f = \frac{\partial}{\partial x_1^{b_1}} \cdots \frac{\partial}{\partial x_d^{b_d}} f,$$

and $|b| = \sum_i b_i$. The symbol $\partial f$ is also used to denote the sub-differential of a convex function $f$, while we use the symbols $\nabla f$ for the gradient of a function $f$ and $Dg$ for the derivative of a vector valued function $g : \mathbb{R}^{d_1} \ni \Omega \to \mathbb{R}^{d_2}$, $\nabla f = (\partial_1 f, \ldots, \partial_d f)^\top$ and $Dg = (\nabla g_1, \ldots, \nabla g_{d_2})^\top$ respectively, and $D^2 f = D\nabla f$ denotes the Hessian of $f$.

If $\Omega \subseteq \mathbb{R}^d$ is a closed set with non-empty interior and $\alpha > 0$, the Hölder spaces on $\Omega$ as defined in Appendix B are denoted by $C^\alpha(\Omega)$ and their associated norms by $\| \cdot \|_{C^\alpha(\Omega)}$. Similarly, the $p$-Sobolev spaces of order $\alpha$ for $p \in [1, \infty]$ are denoted by $W^{\alpha, p}(\Omega)$ with norms $\| \cdot \|_{W^{\alpha, p}(\Omega)}$, as defined in Appendix B.

We say that $\Omega \subseteq \mathbb{R}^d$ is a Lipschitz domain if its boundary can be locally expressed as the sublevel set of a Lipschitz function.

2. BRENIER’S THEOREM AND THE SEMI-DUAL PROBLEM

We begin by recalling the Monge and Kantorovich problems given in Section 1, and that we restrict our attention to the case where the transport cost is given by the squared Euclidean distance. Let $P$, $Q$ be two Borel probability measures on $\mathbb{R}^d$ with finite second moments.

The Monge (primal) problem is defined as

$$\min_T \mathcal{P}_M(T) \quad \text{s.t.} \quad T_\# P = Q,$$

where $\mathcal{P}_M(T) := \frac{1}{2} \int_{\mathbb{R}^d} \| T(x) - x \|_2^2 \, dP(x)$, and the push-forward $T_\# P$ is defined as $T_\# P(A) = P(T^{-1}(A))$ or all Borel sets $A$.

Its relaxation, the Kantorovich (primal) problem, is given by

$$\min_\gamma \bar{\mathcal{P}}_K(\gamma) \quad \text{s.t.} \quad \gamma \in \Gamma(P, Q) \quad \text{where} \quad \bar{\mathcal{P}}_K(\gamma) := \frac{1}{2} \int \| x - y \|_2^2 \, d\gamma(x, y), \quad (2.1)$$
and \( \Gamma(P,Q) \) denotes the set of couplings between \( P \) and \( Q \), that is, the set of probability measures \( \gamma \) on \( \mathbb{R}^d \times \mathbb{R}^d \) such that \( \gamma(A \times \mathbb{R}^d) = P(A) \) and \( \gamma(\mathbb{R}^d \times A) = Q(A) \) for all Borel set \( A \subset \mathbb{R}^d \).

The value of problem (2.1) is the square of the 2-Wasserstein distance, denoted by

\[
W_2^2(P,Q) := \min_{\gamma \in \Gamma(P,Q)} \tilde{\mathcal{P}}_K(\gamma).
\]

Note that we can expand the objective in (2.1) as

\[
\tilde{\mathcal{P}}_K(\gamma) = \frac{1}{2} \int \|x - y\|^2 d\gamma(x,y) = \frac{1}{2} \int \|x\|^2 dP(x) + \frac{1}{2} \int \|y\|^2 dQ(y) - \int \langle x,y \rangle d\gamma(x,y),
\]

Since the first two terms above do not depend on \( \gamma \), we obtain the equivalent optimization problem

\[
\max_{\gamma} \mathcal{P}_K(\gamma) \quad \text{s.t.} \; \gamma \in \Gamma(P,Q), \quad \text{where} \quad \mathcal{P}_K(\gamma) := \int \langle x,y \rangle d\gamma(x,y). \tag{2.3}
\]

We focus on this equivalent formulation for the rest of the paper because it is more convenient to work with.

Problem (2.3) is a linear optimization problem, albeit an infinite-dimensional one. Hence, it is natural to consider its dual problem, which is given by

\[
\min_{f,g} \int f(x) dP(x) + \int g(y) dQ(y) \quad \text{s.t.} \quad f(x) + g(y) \geq \langle x,y \rangle, \quad P \otimes Q \text{-a.e},
\]

\[
f \in L^1(P), \; g \in L^1(Q). \tag{2.4}
\]

The dual variables \( f \) and \( g \) are called potentials, and for an optimal pair \((f_0, g_0)\), \( f_0 \) is called a Kantorovich potential.

The dual problem (2.4) can be further simplified: Assume we are given a candidate function \( f \) in (2.4) above. Then, we can formally solve for the corresponding \( g \) to get an optimal \( g \) given by the Legendre-Fenchel conjugate (see Section A) of \( f \):

\[
g_f(y) = \sup_{x \in \mathbb{R}^d} \langle x,y \rangle - f(x) = f^*(y), \tag{2.5}
\]

Plugging solution (2.5) back into the optimization problem leads to the so-called semi-dual problem,

\[
\min \mathcal{S}(f) = \int f(x) dP(x) + \int f^*(y) dQ(y) \quad \text{s.t.} \; f \in L^1(P), \tag{2.6}
\]

where the supremum in (2.5) is interpreted as an essential supremum with respect to \( P \). By transitioning to the semi-dual, we effectively solved for all constraints in (2.4), leaving us with an unconstrained convex problem that is not linear anymore. Under regularity assumptions, a solution to the semi-dual provides a solution to the Monge problem as indicated by the following theorem, which is a cornerstone of modern optimal transport.

**Theorem 1** (Brenier’s theorem, [9,45,65]). Assume \( P \) is absolutely continuous with respect to the Lebesgue measure and that both \( P \) and \( Q \) have finite second moments. Then, a unique optimal solution to (2.2) exists and is of the form \( \gamma_0 = (\text{id}, T_0)_\#P \), where \( T_0 = \nabla f_0 \) is the gradient of a convex function \( f_0 : \mathbb{R}^d \to \mathbb{R} \). In fact, \( f_0 \) can be chosen to be a minimizer of the semi-dual objective in (2.6).

Brenier’s theorem implies that a solution to the semi-dual problem readily gives an optimal transport map. Our strategy is to minimize an approximation of the semi-dual and establish stability results as well as generalization bounds to conclude that the minimizer to the approximation is close to the minimizer of the original problem.
3. MAIN RESULTS

Let \( X_{1:n} = (X_1, \ldots, X_n) \) and \( Y_{1:n} = (Y_1, \ldots, Y_n) \) be \( n \) independent copies of \( X \sim P \) and \( Y \sim Q = (T_0)_\#P \) respectively. Furthermore, assume that \( X_{1:n} \) and \( Y_{1:n} \) are mutually independent. Our goal is to estimate \( T_0 \). To that end, we consider the following set of assumptions on \( P, Q \) and \( T_0 \). Throughout, we fix a constant \( M \geq 2 \).

A1 (Source distribution). Let \( \mathcal{M} = \mathcal{M}(M) \) be the set of all probability measures \( P \) with support \( \Omega = [0, 1]^d \) and that admit a density \( \rho_P \) with respect to the Lebesgue measure such that \( M^{-1} \leq \rho_P(x) \leq M \) for almost all \( x \in \Omega \). Assume that the source distribution \( P \) is in \( \mathcal{M} \).

A2 (Transport map). Let \( \tilde{\Omega} = [-1, 2]^d \) denote the enlargement of \( \Omega \) by 1 in every direction. Let \( \mathcal{T} = \mathcal{T}(M) \) be the set of all differentiable functions \( T: \tilde{\Omega} \to \mathbb{R}^d \) such that \( T = \nabla f \) for some differentiable convex function \( f: \tilde{\Omega} \to \mathbb{R}^d \) and

(i) \( |T(x)| \leq M \) for all \( x \in \tilde{\Omega} \),
(ii) \( M^{-1} \leq DT(x) \leq M \) for all \( x \in \tilde{\Omega} \),
(iii) \( \text{supp} T_\#P = \Omega = [0, 1]^d \).

For \( R > 0 \) and \( \alpha > 1 \), assume that

\[ T_0 \in \mathcal{T}_\alpha = \mathcal{T}_\alpha(M, R) = \{ T \in \mathcal{T}(M) : T \text{ is } \lceil \alpha \rceil \text{-times differentiable and } \| T \|_{C^{\alpha}(\tilde{\Omega})} \leq R \}. \]

Our main result is the following theorem. It characterizes, up to logarithmic factors, the minimax rate of estimation of an \( \alpha \)-smooth transport map \( T_0 \in \mathcal{T}_\alpha \) in the setup described above.

THEOREM 2. Fix \( \alpha \geq 1 \), then

\[
\inf_{T} \sup_{P \in \mathcal{M}, T_0 \in \mathcal{T}_\alpha} \mathbb{E} \left[ \int \| \hat{T}(x) - T_0(x) \|_2^2 \, dP(x) \right] \geq \frac{1}{n} n^{-\frac{2\alpha}{2\alpha + 2}} \vee \frac{1}{n}. \tag{3.1}
\]

where the infimum is taken over all measurable functions \( \hat{T} \) of the data \( X_{1:n} = (X_1, \ldots, X_n) \), \( Y_{1:n} = (Y_1, \ldots, Y_n) \). Moreover, if \( P \in \mathcal{M} \) and \( T_0 \in \mathcal{T}_\alpha \), there exists an estimator \( \hat{T} \), given in Section 5, that is near minimax optimal. More specifically, there exists an integer \( n_0 = n_0(d, \alpha, M, R) \) such that for any \( n \geq n_0 \), it holds,

\[
\sup_{P \in \mathcal{M}, T_0 \in \mathcal{T}_\alpha} \mathbb{E} \left[ \int \| \hat{T}(x) - T_0(x) \|_2^2 \, dP(x) \right] \leq n^{-\frac{2\alpha}{2\alpha + 2}} \log^3(n) \vee \frac{1}{n}. \tag{3.2}
\]

REMARK 3. Assumption A1 can be significantly relaxed with respect to the geometry of \( \Omega \) and the density of \( P \). In fact, the upper bounds are given under more general assumptions in Section 5. Similarly, the assumption A2(iii) that \( \text{supp}(Q) = [0, 1]^d \) can also be relaxed.

However, the constants in the resulting upper bounds exhibit a dependence on the geometry of the supports of both \( P \) and \( Q \) as well as on the enclosing set \( \tilde{\Omega} \) through functional analytical results used in the proofs. While it may be possible to make this dependence explicit in terms of geometric features of the sets \( \text{supp}(P), \text{supp}(Q) \) and \( \tilde{\Omega} \)— see for example [25, 41, 78] for such estimates under restrictive assumptions— providing a uniform control these quantities in terms of easily interpretable properties of the sets is beyond the scope of this article. Instead, we chose to present Theorem 2 under these simplified assumptions to make the results more readable.
We conjecture that the logarithmic terms appearing in the upper bound are superfluous and arise as an artifact of our proof techniques. We briefly make a qualitative comment on the rate \( n^{-\frac{2\alpha}{2\alpha - 2 + d}} \). Note first that it appears from this rate that estimation of transport maps, like the estimation of smooth functions suffers from the curse of dimensionality. However, as \( \alpha \to \infty \), this curse of dimensionality may be mitigated by extra smoothness with the parametric rate \( n^{-1} \) as a limiting case. Note also that we can formally take the limit \( \alpha \to 1 \), which corresponds to the case where no additional smoothness condition holds beyond having a strongly convex Kantorovich potential with Lipschitz gradient. This is essentially the minimal structural condition arising from Brenier’s theorem with additional bounds on the derivative of \( T_0 \). In this case, one formally recovers the rate \( n^{-2/d} \) and we conjecture that this is the minimax rate of estimation in the context where \( T_0 \) is only assumed to be the gradient of a strongly convex function with Lipschitz gradient. If either of these two additional requirements is not fulfilled, our stability results no longer hold. While further investigating this question is of fundamental interest, it is beyond the scope of the present work.

4. LOWER BOUND

In this section we begin by proving the lower bound (3.1) as it sheds light on the source of the non-standard exponent \( \frac{2\alpha}{2\alpha - 2 + d} \) in the minimax rate. We prove the following theorem.

**Theorem 4.** Fix \( \alpha \geq 1 \), and let \( P \) be the uniform distribution on \([0,1]^d\). Then

\[
\inf_{T} \sup_{P \in \mathcal{M}, T_0 \in T_0} \mathbb{E} \left[ \int \| \hat{T}(x) - T_0(x) \|^2 dP(x) \right] \gtrsim n^{-\frac{2\alpha}{2\alpha - 2 + d}} \vee \frac{1}{n},
\]

where the infimum is taken over all measurable functions of the data \( X_1, \ldots, X_n, Y_1, \ldots, Y_n \).

**Proof.** The proof uses standard tools for minimax lower bounds and in particular [80, Theorem 2.5]. It relies on the following construction.

Set \( P = \text{Unif}([0,1]^d) \in \mathcal{M} \), the uniform distribution on the hypercube. For \( \alpha > 1 \), let \( \xi : [0,1] \to \mathbb{R} \) be a non-zero function in \( C^{\alpha+1}(\mathbb{R}^d) \) with support contained in \([0,1]^d\) and define \( g : [0,1]^d \to \mathbb{R} \) by

\[
g(x) = \prod_{i \in [d]} \xi(x_i), \quad x = (x_1, \ldots, x_d).
\]

Let \( m = \lceil \theta n^\frac{1}{2\alpha - 2 + d} \rceil \) be a positive integer where \( \theta \) is a universal constant to be chosen later. We form a regular discretization of the space \([0,1]^d\) by defining the collection of vectors \( \{x^{(j)} : j \in [m]^d\} \subset [0,1]^d \) to have coordinates \( x^{(j)}_i = (j_i - 1)/m, \ i = 1, \ldots, d \) and let

\[
g_j(x) = \frac{\kappa}{m^{\alpha+1}} g(m(x - x^{(j)})),
\]

for a constant \( \kappa > 0 \) to be chosen later.

Next, let \( b \in \mathbb{N}^d \) be a multi-index and observe that the differential operator \( \partial^b \) applied to \( g_j \) yields \( \partial^b g_j(\cdot) = m^{|b| - \alpha - 1} \partial^b g(m(\cdot - x_j)) \). Since \( \xi \in C^{\alpha+1} \), if \( \alpha > 1 \), a second-order Taylor expansion yields that \( g_j \) has uniformly vanishing Hessian: \( \| D^2 g_j \|_\infty \to 0 \) as \( m \to \infty \). In particular, in that case, there exists \( m_0 \) such that \( \| D^2 g_j(x) \|_\infty \leq 1/2 \) for all \( m \geq m_0 \) and \( j \in [m]^d \). If \( \alpha = 1 \), the same can be obtained by choosing \( \kappa \) small enough.

For \( m^d \geq 8 \), the Varshamov-Gilbert lemma [80, Lemma 2.9] guarantees the existence of binary vectors \( \tau^{(1)}, \ldots, \tau^{(K)} \in \{-1,1\}^{[m]^d}, K \geq 2^m^d/8 \) such that \( \| \tau^{(k)} - \tau^{(k')} \|_2^2 \geq m^d/2 \) for \( 1 \leq k \neq k' \leq K \).
With this, we define the following collection of Kantorovich potentials:

$$\phi_k(x) = \frac{1}{2} \|x\|^2 + \sum_{j \in [m]^d} \tau_j^{(k)} g_j(x), \quad k = 1, \ldots, K.$$  

It is easy to see (Lemma 29) that for any $k = 1, \ldots, K$ and $m \geq m_0$, $\nabla \phi_k$ is a bijection from $[0,1]^d$ to $[0,1]^d$. It yields that $T_k := \nabla \phi_k \in T_0(M, R)$ for $M > 2$ and $\kappa$ small enough. We now check the conditions of [80, Theorem 2.5].

First, observe that for $1 \leq k \neq k' \leq K$, it holds that

$$\int_{[0,1]^d} \|\nabla \phi_k(x) - \nabla \phi_{k'}(x)\|^2 \, dx = \frac{\kappa^2}{m^{2\alpha+d}} \sum_{j \in [m]^d} (\tau_j^{(k)} - \tau_j^{(k')})^2 \int_{\mathbb{R}^d} \|\nabla g_j(x)\|^2 \, dx \geq \frac{1}{m^{2\alpha}}.$$  

This yields

$$\int_{[0,1]^d} \|\nabla \phi_k(x) - \nabla \phi_{k'}(x)\|^2 \, dx \gtrsim n^{-\frac{2\alpha}{2\alpha+d}},$$

which completes checking the separation condition (i) of [80, Theorem 2.5].

To check condition (ii) of [80, Theorem 2.5], recall the Kullback-Leibler (KL) divergence between two measures $Q, P$ such that $Q$ is absolutely continuous with respect to $P$ is defined by

$$D(Q\|P) = \mathbb{E} \log \left( \frac{dQ}{dP}(W) \right), \quad W \sim Q.$$  

In view of Lemma 29, for any $k = 1, \ldots, K$, the measure $Q_k = (\nabla \phi_k)^\# P$ is supported on $[0,1]^d$ and in particular, it is absolutely continuous with respect to $P$. By the change of variables formula, it admits the density

$$\frac{dQ_k}{dP}(y) := \frac{1}{\det D^2 \phi_k((\nabla \phi_k)^{-1}(y))} \mathbb{1}((\nabla \phi_k)^{-1}(y) \in [0,1]^d).$$

Moreover, let $X \sim P$ and $Y \sim Q_k$ be two random variables. It holds

$$D(Q_k\|P) = E \log \left( \frac{dQ_k}{dP}(Y) \right) = \mathbb{E} \log \left( \frac{dQ_k}{dP}(\nabla \phi_k(X)) \right) = - \int_{[0,1]^d} \log \left( \det D^2 \phi_k(x) \right) \, dx. \tag{4.3}$$

Recall that $D^2 \phi_k = I_d + \sum_{j \in [m]^d} \tau_j^{(k)} D^2 g_j$ where $I_d$ denotes the identity matrix in $\mathbb{R}^d$. Therefore, since the functions $g_j$ have disjoint support, we have for all $x \in [0,1]^d$ that

$$\log \left( \det D^2 \phi_k(x) \right) = \sum_{l=1}^d \log \left( 1 + \lambda_l \left( \sum_{j \in [m]^d} \tau_j^{(k)} D^2 g_j(x) \right) \right) = \sum_{l=1}^d \sum_{j \in [m]^d} \log \left( 1 + \tau_j^{(k)} \lambda_l \left( D^2 g_j(x) \right) \right),$$

where $\lambda_l(A)$ denotes the $l$th eigenvalue of a matrix $A$. Since $\log(1 + z) \geq z - z^2/2$ for all $z > 0$,

$$\log \left( \det D^2 \phi_k(x) \right) \geq \sum_{j \in [m]^d} \tau_j^{(k)} \mathrm{Tr} (D^2 g_j(x)) - \frac{1}{2} \sum_{j \in [m]^d} \|D^2 g_j(x)\|_F^2,$$  

where $\| \cdot \|_F$ denotes the Frobenius norm. Thus,

$$D(Q_k\|P) \leq - \sum_{j \in [m]^d} \tau_j^{(k)} \int_{[0,1]^d} \mathrm{Tr} (D^2 g_j(x)) \, dx + \frac{1}{2} \sum_{j \in [m]^d} \int_{[0,1]^d} \|D^2 g_j(x)\|_F^2 \, dx.$$  

On the one hand, by the divergence theorem and the fact that $g_j$ has bounded support,
\[
\int_{[0,1]^d} \text{Tr}(D^2 g_j(x)) \, dx = \int_{\partial[0,1]^d} \nabla \cdot \nabla g_j(x) \, dx = 0,
\]
where $\partial[0,1]^d$ denotes the boundary of the unit hypercube. On the other hand
\[
\sum_{j \in [m]^d} \int_{[0,1]^d} \|D^2 g_j(x)\|_F^2 \, dx = \frac{\kappa^2}{m^{2\alpha-2+d}} \sum_{j \in [m]^d} \int_{\mathbb{R}^d} \|D^2 g(x)\|_F^2 \, dx \lesssim \frac{1}{m^{2\alpha-2}}.
\]

The above three displays yield
\[
D(P \otimes P_k \otimes P \otimes P) = nD(Q_k \| P) \lesssim \frac{n}{m^{2\alpha-2}} \leq (m/\theta)^d \leq \frac{\log K}{9}
\]
for $\theta$ large enough. This completes checking (ii) in \cite[Theorem 2.5]{02} and hence the proof of the first part of the minimax lower bound.

To show the remaining lower bound of $1/n$, repeat the same argument as above with the two potentials $\phi_0(x) = \|x\|^2/2$ and $\phi_1(x) = \phi_0(x) + (\tilde{\theta}/\sqrt{n})g(x)$ for $\tilde{\theta}$ chosen to ensure $\phi_0, \phi_1 \in \mathcal{T}_\alpha$. The separation condition is given by
\[
\int_{[0,1]^d} \|\nabla \phi_0(x) - \nabla \phi_1(x)\|^2 \, dx = \frac{\tilde{\theta}^2}{n} \int_{[0,1]^d} \|\nabla g(x)\|^2 \, dx \gtrsim \frac{1}{n},
\]
and the KL divergence between the associated probability distributions can be estimated by
\[
D(P \otimes P_1 \otimes P \otimes P) = nD(Q_1 \| P) \lesssim \frac{\tilde{\theta}^2 n}{n} \int_{[0,1]^d} \|D^2 g(x)\|_F^2 \, dx \lesssim \frac{1}{9},
\]
for $\tilde{\theta}$ large enough.

Looking back at this proof, we get a better understanding of the exponent in the minimax rate $n^{-\frac{2\alpha}{2\alpha+d}}$. Indeed, the numerator $2\alpha$ in the exponent comes from the fact that we estimate an $\alpha$ smooth transport map in squared $L^2$-distance. However, rather than seeing the usual $2\alpha + d$ denominator that one would expect in the traditional Gaussian white noise model \cite{14} for example, we get a denominator of $2(\alpha-1)+d$. This is due to the fact the information structure, measured in terms of Kullback-Leibler divergence, is governed by the derivative of the signal, i.e., the Hessian of the $\alpha + 1$ smooth Kantorovich potential; see (4.3). This, in turn, follows directly from the Monge-Ampère equation (4.2).

Given that the rate $n^{-\frac{2\alpha}{2(\alpha+k)-d}}$ is the minimax rate of estimation of the $k$ derivative of a signal observed in the Gaussian white noise model, the rate that we obtain is formally that of an “anti-derivative” in this model. Of course, in the absence of a multivariate version of the fundamental theorem of calculus, it is unclear how to define this notion. Nevertheless, similar rates arise in the estimation of the invariant measure of a diffusion process when smoothness is imposed on the drift \cite{18, 76}. This is not surprising as the drift is the gradient of the logarithm of the density of the invariant density in an overdamped Langevin process.

Finally, note that the multivariate case is singularly different from the traditional univariate case where the rate of estimation of linear functionals such as anti-derivatives is known to be parametric regardless of the smoothness of the signal \cite{14}. 

5. UPPER BOUNDS

In this section, we give an estimator \( \hat{T} \) that achieves the near optimal rate (3.2). We present this estimator under the following more general assumptions on the distribution and the geometry of the support of both \( P \) and \( Q = (T_0)_# P \). We also need slightly weaker conditions on the regularity of the transport map (Sobolev instead of Hölder regularity). After stating these weaker assumptions, we present our estimator and restate the main upper bound. Its proof relies on a separate control of approximation error and stochastic error, similar to a standard bias-variance tradeoff.

5.1 Assumptions

Throughout, we fix two constants \( M \geq 2, \beta > 1 \).

**B1** (Source distribution). Let \( \mathcal{M} = \mathcal{M}(M) \) be the set of all probability measures \( P \) whose support \( \Omega_P \) is a bounded and connected Lipschitz domain, and that admit a density \( \rho_P \) with respect to the Lebesgue measure such that \( M^{-1} \leq \rho_P(x) \leq M \) for almost all \( x \in \Omega_P \). Assume that the measure \( P \in \mathcal{M} \).

**B2** (Transport map). For any \( P \in \mathcal{M} \) with support \( \Omega_P \), let \( \tilde{\Omega}_P \) denote a convex set with Lipschitz boundary such that \( \text{diam}(\tilde{\Omega}_P) \leq M \), and \( \Omega_P + M^{-1}B_1 \subseteq \tilde{\Omega}_P \). Let \( \mathcal{T} = \tilde{T}(M) \) be the set of all differentiable functions \( T : \tilde{\Omega}_P \to \mathbb{R}^d \) such that \( T = \nabla f \) for some differentiable convex function \( f : \tilde{\Omega}_P \to \mathbb{R} \) and

\[
\begin{aligned}
(i) \quad & |T(x)| \leq M \text{ for all } x \in \tilde{\Omega}_P, \\
(ii) \quad & M^{-1} \leq DT(x) \leq M \text{ for all } x \in \tilde{\Omega}_P.
\end{aligned}
\]

For \( R > 0 \) and \( \alpha > 1 \), assume that

\[
T_0 \in \mathcal{T}_\alpha = \mathcal{T}_\alpha(M,R) = \{ T \in \mathcal{T}(M) : \|T\|_{C^\beta(\tilde{\Omega}_P)} \vee \|T\|_{W^{\alpha,2}(\tilde{\Omega}_P)} \leq R \}.
\]

These new conditions have two implications. First, they imply regularity of the Kantorovich potential \( f_0 \), where \( T_0 = \nabla f_0 \), and second, they imply some conditions on the pushforward measure \( Q = (T_0)_# P \) that subsume the generalization of Assumption A2(iii). These results are gathered in the following proposition (see Section D.1 for a proof).

**Proposition-Definition 5.** Assume that \( P \) satisfies B1, \( T_0 \) satisfies B2 and let \( \mathcal{X} = \mathcal{X}(M) \) be the set of all twice continuously differentiable functions \( f : \tilde{\Omega}_P \to \mathbb{R} \) such that

\[
\begin{aligned}
(i) \quad & |f(x)| \leq M^2 \text{ and } |\nabla f(x)| \leq M \text{ for all } x \in \tilde{\Omega}_P, \\
(ii) \quad & M^{-1} \leq D^2 f(x) \leq M \text{ for all } x \in \tilde{\Omega}_P, \\
(iii) \quad & Q = \nabla f_0 \# P \text{ has a connected and bounded Lipschitz support } \Omega_Q \text{ and admits a density } \rho_Q \text{ with respect to the Lebesgue measure that satisfies } M^{-(d+1)} \leq \rho_Q(y) \leq M^{d+1} \text{ for all } y \in \Omega_Q.
\end{aligned}
\]

Then there exists a Kantorovich potential \( f_0 \in \mathcal{X}(M) \) such that \( T_0 = \nabla f_0 \) and

\[
\|f_0\|_{C^{\beta+1}(\tilde{\Omega}_P)} \vee \|f_0\|_{W^{\alpha+1,2}(\tilde{\Omega}_P)} \leq R + M^3. \tag{5.1}
\]

Note that the simplified Assumptions A1 and A2 from Section 3 follow from B1 and B2 in the case \( \Omega_P = \Omega = [0,1]^d \) and \( \tilde{\Omega}_P = \Omega = [-1,2]^d \). Additionally, the simplified assumptions restrict the class of transport maps to those such that \( \Omega_Q = [0,1]^d \) and for which \( \beta = \alpha \). Indeed, noting that \( \|T_0\|_{W^{\alpha,2}(\tilde{\Omega})} \lesssim \|T_0\|_{C^{\alpha}(\tilde{\Omega})} \), we can fold the two smoothness conditions into one.
5.2 Estimator

To construct an estimator for $T_0$, we observe that if we had access to a Kantorovich potential $f_0$, then $T_0 = \nabla f_0$ by Brenier’s Theorem, Theorem 1. In turn, $f_0$ is the minimum of the semi-dual objective (2.6). Hence, we replace population quantities with sample ones in its definition to obtain an empirical loss function. Moreover, to account for the assumed smoothness of the transport map and to ensure stability of the objective, we constrain our minimization problem to smooth and strongly convex Kantorovich potentials, restricted to a compact superset of the support of $P$. Then, our estimator is the gradient of the solution to this stochastic optimization problem.

More precisely, for a measurable function $f$, let us write

$$Pf = \int f(x) \, dP(x), \quad Qf = \int f(y) \, dQ(y), \quad \hat{P}f = \frac{1}{n} \sum_{i=1}^{n} f(X_i), \quad \hat{Q}f = \frac{1}{n} \sum_{j=1}^{n} f(Y_j),$$

where, as in Section 3, $X_1:n = (X_1, \ldots, X_n)$ and $Y_1:n = (Y_1, \ldots, Y_n)$ are $n$ i.i.d. samples from $P$ and $Q$, respectively, that are mutually independent as well. Recall from Section 2 that the semi-dual objective is defined as $S(f) = Pf + Qf^*$ for $f \in L^1(P)$, where $f^*$ denotes the convex conjugate of $f$. Replacing both $P$ and $Q$ by their empirical counterparts, we obtain the empirical semi-dual,

$$\hat{S}(f) = \hat{P}f + \hat{Q}f^*. \quad (5.2)$$

In order to incorporate smoothness regularization into the minimization of (5.2), we consider the restriction of potentials $f$ to a wavelet expansion of finite degree, a strategy which is frequently used in non-parametric estimation [33, 35]. For the purpose of this section, it is enough to think about wavelets as a graded orthogonal basis of $L^2(\mathbb{R}^d)$, leading to nested subspaces

$$V_0 \subseteq V_1 \subseteq \cdots \subseteq V_J \subseteq \cdots \subseteq L^2(\mathbb{R}^d),$$

that roughly correspond to increasing frequency ranges of the continuous Fourier transform of a function $f \in L^2(\mathbb{R}^d)$. Truncated wavelet decompositions yield good approximations for smooth functions and we control their approximation error in Lemma 11. We only consider the span $V_J(\tilde{\Omega}_P)$ of those basis functions of the wavelet expansion whose support has non-trivial intersection with $\tilde{\Omega}_P$. This is a finite dimensional vector space as long as the elements of the wavelet basis have compact support. The cut-off parameter $J$ is chosen according to the regularity of $f_0$ in assumption B2, see Section 5.6, or alternatively can be chosen adaptively by a straightforward but technical extension using a penalization scheme [53] that we omit for readability. Alternatively, other selection methods such as Lepski’s method [50–52] could be used. In order to ensure the necessary regularity and the compact support of the elements of the wavelet basis, we assume throughout that the wavelet basis is given by Daubechies wavelets of sufficient order. For a more detailed treatment of wavelets, we refer the reader to Section B.

To ensure stability of the minimizer of the semi-dual with respect to perturbations of the input distributions $P$ and $Q$, we further restrict the potentials $f$ to mimic the assumptions in Proposition-Definition 5, in particular, we enforce upper and lower bounds on the Hessian $D^2f$ on $\tilde{\Omega}_P$ by demanding $f \in \mathcal{X}(2M)$.

Combined, both wavelet regularization and strong convexity lead to the set

$$\mathcal{F}_J = \mathcal{X}(2M) \cap V_J(\tilde{\Omega}_P) \quad (5.3)$$
of candidate potentials, based on which we define the estimators

$$\hat{f}_J \in \arg\min_{f \in F_J} S(f), \quad \hat{T}_J = \nabla \hat{f}_J,$$

for the Kantorovich potential and transport map, respectively.

Note that since we consider candidate potentials only on the compact set $\tilde{\Omega}_P$, $f^*$ above is defined as

$$f^*(y) = \sup_{x \in \tilde{\Omega}_P} \langle x, y \rangle - f(x) = f^*(x) - (f + \iota_{\tilde{\Omega}_P})(x), \quad y \in \mathbb{R}^d,$$

where $\iota_{\tilde{\Omega}_P}$ is the usual indicator function in convex analysis (see Section A).

With this, we can restate the upper bound of Theorem 2.

**Theorem 6.** Under assumptions $B1$ and $B2$, there exists $n_0 \in \mathbb{N}$ and $J$ such that for $n \geq n_0$,

$$\mathbb{E}_{(X_1, n, Y_1)} \left[ \int \| \hat{T}_J(x) - T_0(x) \|^2_2 \, dP(x) \right] \leq C \left[ n^{- \frac{2\alpha}{2\alpha + 2} \log(n)^3} \lor \frac{1}{n} \right],$$

where $n_0$, $C$, and $J$ may depend on $d, M, R, \Omega_P, \Omega_Q, \tilde{\Omega}_P, n_0$ may additionally depend on $\beta$, and $C$ may additionally depend on $\alpha$.

The cutoff $J$ depends on $\alpha$ if $d \geq 3$, but in the cases $d = 1$ and $d = 2$, $J$ can be chosen independently from $\alpha$.

**Remark 7.** A few remarks are in order.

(i) Similar upper bounds hold with high probability and can be inferred from the proof.

(ii) As written, the estimator $\hat{f}_J$ is not directly implementable since the calculation of $f^*$ involves computing a maximum over a continuous subset of $\mathbb{R}^d$. While this limitation can be overcome by a discretization of the space, it is not practical even in moderate dimensions and we leave the search for an estimator that yields comparable rates to $\hat{f}$ while being amenable to fast computation as a topic of future research.

(iii) The estimator employed in Theorem 6 can be made adaptive to the unknown smoothness parameter $\alpha$ using a standard penalization scheme [53]. We omit this straightforward extension and instead focus on establishing minimax rates of estimation. For more a more detailed account, we refer the reader to [38].

In the rest of this section, we present the proof of Theorem 6. We begin by stating our key result, which relates the semi-dual objective to the square of our measure of performance. This result also allows us to employ a fixed-point argument when controlling the risk of our estimator using empirical process theory. Combined with approximation results for truncated wavelet expansions, these lead to a bias-variance tradeoff that achieves the minimax lower bound of Theorem 4 up to log factors.

### 5.3 Stability of optimal transport maps

In this section, we leverage the assumed regularity of the optimal transport map to relate the suboptimality gap in the semi-dual objective function $S$ and the $L^2$-distance of interest.

**Proposition 8.** Under assumptions $B1 – B2$, for all $f \in X(2M)$ as defined in Proposition-Definition 5, we have

$$\frac{1}{8M} \| \nabla f(x) - \nabla f_0(x) \|^2_{L^2(P)} \leq S(f) - S(f_0) \leq 2M \| \nabla f(x) - \nabla f_0(x) \|^2_{L^2(P)} \quad (5.5)$$
and
\[ \frac{1}{4M} \| \nabla f^*(y) - \nabla f^*_0(y) \|^2_{L^2(Q)} \leq S(f) - S(f_0). \] (5.6)

**Proof.** It follows from Proposition-Definition 5(ii) and a second-order Taylor expansion that \( f \) is of quadratic type [46] around every \( x \in \Omega_P \):
\[ \frac{1}{2L} \| z - x \|^2_2 \leq f(z) - f(x) - \langle \nabla f(x), z - x \rangle \leq \frac{L}{2} \| z - x \|^2_2, \quad \text{for } x \in \Omega_P, z \in \tilde{\Omega}_P, \] (5.7)
for all \( L \geq 2M \). It turns out that these conditions are sufficient to obtain the desired result.

The upper bound in (5.7) is of the form
\[ f(z) \leq q_x(z) = f(x) + \langle \nabla f(x), z - x \rangle + \frac{L}{2} \| z - x \|^2_2 + t_{\Omega_P}(z). \]

Since the convex conjugate is order reversing and because the convex conjugate \( q^*_x \) of the quadratic function \( q_x \) can be computed explicitly (Lemma 19), we have
\[ f^*(\nabla f_0(x)) \geq q^*_x(\nabla f_0(x)) = \frac{1}{2L} \| \nabla f_0(x) - \nabla f(x) \|^2_2 + \langle x, \nabla f_0(x) \rangle - f(x) - \frac{L}{2} d^2 \left( \frac{\nabla f_0(x) - \nabla f(x)}{L} - x, \tilde{\Omega}_P \right). \]

The squared distance term vanishes for \( L = 4M \): by the triangle inequality \( \| \nabla f_0(x) - \nabla f(x) \|_2 \leq 4M \) and since \( x \in \Omega_P \), it holds that
\[ \frac{\nabla f_0(x) - \nabla f(x)}{L} - x \in \tilde{\Omega}_P. \]

Together with the fact that \( Q = (\nabla f_0)_\# P \), this yields
\[ S(f) = Pf + Qf^* = \int [f(x) + f^*(\nabla f_0(x))]dP(x) \geq \frac{1}{8M} \| \nabla f - \nabla f_0 \|^2_{L^2(P)} + \int \langle x, \nabla f_0(x) \rangle dP(x). \]

Moreover, by strong duality, we have
\[ S(f_0) = Pf_0 + Qf^*_0 = \int \langle x, \nabla f_0(x) \rangle dP(x). \]

The above two displays yield \( S(f) - S(f_0) \geq (8M)^{-1} \| \nabla f - \nabla f_0 \|^2_{L^2(P)} \). In the same way, using the lower bound in (5.7), we get that \( S(f) - S(f_0) \leq 2M \| \nabla f - \nabla f_0 \|^2_{L^2(P)} \), which concludes the proof of (5.5).

It turns out that (5.6) is even easier to prove. Indeed, by Proposition-Definition 5(ii) and Lemma 15, we get that the upper bound in (5.7) is also true for \( f^* \) on all of \( \mathbb{R}^d \). In this case, we can simply take \( L = 2M \) and get similar results. \( \square \)

There are many ways to leverage strong convexity in order to obtain faster rates of convergence, often known as fixed-point arguments [33,46,53]. In this work, we employ van de Geer’s “one-shot” localization technique originally introduced in [81] and stated in a form close to our needs in [82].
5.4 Control of the stochastic error via empirical processes

In light of Proposition 8, the performance of our estimator \( \hat{T}_J = \nabla f_J \) defined in (5.4) requires the control of \( S(\hat{f}_J) - S(f_0) \), which can be achieved using tools from empirical process theory. To that end, for any \( f \), define

\[ S_0(f) = S(f) - S(f_0) \quad \text{and} \quad \hat{S}_0(f) = \hat{S}(f) - \hat{S}(f_0), \]

and let \( \bar{f}_J \in F_J \). We observe that by optimality of \( \hat{f}_J \) for \( \hat{S} \),

\[ S_0(\hat{f}_J) - S_0(\bar{f}_J) \leq [S_0(\hat{f}_J) - \hat{S}_0(\hat{f}_J)] + [\hat{S}_0(\bar{f}_J) - S_0(\bar{f}_J)]. \]

To proceed, we control the localized empirical process

\[ \sup_{f \in F_J : S_0(f) \leq \tau^2} |S_0(f) - \hat{S}_0(f)|. \]

for some fixed \( \tau^2 > 0 \). More precisely, we prove the following result in Appendix D.2.

**Proposition 9.** Let assumptions B1 – B2 be fulfilled and define \( F_J \) as in (5.3). For any \( \tau > 0 \), define

\[ F_J(\tau^2) := \{ f \in F_J : S_0(f) \leq \tau^2 \}, \]

and for any integer \( J \) and dimension \( d \geq 1 \), define \( \kappa_J \) by

\[ \kappa_J = \begin{cases} 1 & \text{if } d = 1, \\ \sqrt{J} & \text{if } d = 2, \\ 0 & \text{if } d \geq 3. \end{cases} \]

Then, there exists \( C_1 = C_1(d, M, \Omega_P, \Omega_{\hat{P}}, \Omega_Q) > 0 \) such that with probability at least \( 1 - \exp(-t) \),

\[ \sup_{f \in F_J(\tau^2)} |S_0(f) - \hat{S}_0(f)| \leq C_1 \left( \phi_J(\tau^2) + \tau \sqrt{\frac{t}{n} + \frac{t}{n}} \right), \]

where

\[ \phi_J(\tau^2) = \frac{2^J(d-2)/2}{\sqrt{n}} \sqrt{\log \left( 1 + \frac{C_1}{\tau} \right) + \frac{2^J(d-2)J^2}{n} \log \left( 1 + \frac{C_1}{\tau} \right) + \frac{\tau}{\sqrt{n}} \kappa_J.} \]

Equipped with this result, we can apply van de Geer’s localization technique. To simplify the presentation, assume that \( \hat{f} = \hat{f}_J \in \text{argmin}_{f \in F_J} S(f) \) exists. If not, we may repeat the proof with an \( \varepsilon \)-approximate minimizer and let \( \varepsilon \to 0 \). Throughout the proof, we write \( \hat{f} = \hat{f}_J \) and \( \| \cdot \| \rightarrow \| \cdot \|_{L^2(P)} \)

Fix \( \sigma > 0 \) to be defined later and set

\[ \hat{f}_s = s \hat{f} + (1 - s) \bar{f}, \quad s = \frac{\sigma}{\sigma + \| \nabla \hat{f} - \nabla \bar{f} \|}. \]

Note that since \( s \in [0,1] \) and \( F_J \) is convex, we have \( \hat{f}_s \in F_J \).

On the one hand, \( \hat{f}_s \) is localized in the sense that

\[ \| \nabla \hat{f}_s - \nabla \bar{f} \| = s \| \nabla \hat{f} - \nabla \bar{f} \| = \frac{\sigma \| \nabla \hat{f} - \nabla \bar{f} \|}{\sigma + \| \nabla \hat{f} - \nabla \bar{f} \|} \leq \sigma. \]
By Proposition 8 and the triangle inequality respectively, this yields
\[ S_0(\hat{f}_s) \leq 2M \|\nabla \hat{f}_s - \nabla f_0\|^2 \leq 4M (\sigma^2 + \|\nabla \bar{f} - \nabla f_0\|^2) =: \tau^2. \]

Therefore, \( \hat{f}_s \in \mathcal{F}_J(\tau^2) \). For the same reason, we also have that \( \bar{f} \in \mathcal{F}_J(\tau^2) \).

On the other hand, \( f_s \), akin to \( \bar{f} \), has empirical risk smaller than \( f \). Indeed, by convexity of \( \hat{S} \) and the fact that \( \bar{f} \) minimizes \( \hat{S} \) over \( \mathcal{G} \), we obtain
\[ \hat{S}(\hat{f}_s) \leq s\hat{S}(\bar{f}) + (1-s)\hat{S}(\bar{f}) \leq \hat{S}(\bar{f}), \]
which yields
\[ S_0(\hat{f}_s) \leq S_0(\bar{f}) + \sup_{f \in \mathcal{F}_J(\tau^2)} |S_0(f) - \hat{S}_0(f)|. \]
Together with Jensen’s inequality and Proposition 8 respectively, the above display yields
\[ \|\nabla \hat{f}_s - \nabla \bar{f}\|^2 \leq 2\|\nabla \hat{f}_s - \nabla f_0\|^2 + 2\|\nabla f_0 - \nabla \bar{f}\|^2 \leq 4MS_0(\hat{f}_s) + 4MS_0(f) \]
\[ \leq 8MS_0(\bar{f}) + 8M \sup_{f \in \mathcal{F}_J(\tau^2)} |S_0(f) - \hat{S}_0(f)|. \]

Next, note for \( s \) as in (5.10), we have that \( \|\nabla \hat{f}_s - \nabla \bar{f}\| \geq \sigma/2 \) iff \( \|\nabla \bar{f} - \nabla \bar{f}\| \geq \sigma. \) Hence
\[ \mathbb{P}(\|\nabla \bar{f} - \nabla f_0\| \geq \sigma + \|\nabla \bar{f} - \nabla f_0\|) \leq \mathbb{P}(\|\nabla \hat{f}_s - \nabla \bar{f}\|^2 \geq \sigma^2/4) \]
\[ \leq \mathbb{P}(\sup_{f \in \mathcal{F}_J(\tau^2)} |S_0(f) - \hat{S}_0(f)| \geq \frac{\sigma^2}{32M} - \hat{S}_0(\bar{f})) \]
\[ = \mathbb{P}(\sup_{f \in \mathcal{F}_J(\tau^2)} |S_0(f) - \hat{S}_0(f)| \geq \frac{\tau^2}{128M^2} - \frac{1}{32M}\|\nabla \bar{f} - \nabla f_0\|^2 - \hat{S}_0(\bar{f})). \]

Recalling Proposition 9, we take \( \sigma \) such that
\[ \frac{\tau^2}{128M^2} \geq S_0(\bar{f}) + \frac{1}{32M}\|\nabla \bar{f} - \nabla f_0\|^2 + C_1 \left( \frac{\sigma^2}{\sqrt{n}} + \tau \sqrt{\frac{t}{n} + \frac{t}{n}} \right), \tag{5.11} \]
so that we get
\[ \mathbb{P}(\|\nabla \bar{f} - \nabla f_0\| \geq \sigma + \|\nabla \bar{f} - \nabla f_0\|) \leq e^{-t}. \]

In particular, recalling Proposition 8, we can check that (5.11) is fulfilled if we choose \( \sigma \) such that
\[ \sigma^2 \geq S_0(\bar{f}) + \frac{2J(d-2)J^2}{n} \log \left( 1 + \frac{C_2\sqrt{n}}{2J(d-2)/2J} \right) + \frac{\sigma^2}{n} + \frac{t}{n}, \]
for a suitable choice of \( C_2 > 0 \).

With this and applying again Proposition 8, we get that with probability at least \( 1 - e^{-t} \), it holds
\[ \|\nabla \hat{f} - \nabla f_0\|^2 \lesssim \|\nabla \bar{f} - \nabla f_0\|^2 + \frac{2J(d-2)J^2}{n} \log \left( 1 + \frac{C_2\sqrt{n}}{2J(d-2)/2J} \right) + \frac{\sigma^2}{n} + \frac{t}{n}. \]
Moreover, integrating the tail with respect to \( t \) readily yields by Fubini’s theorem that
\[ \mathbb{E}\|\nabla \hat{f} - \nabla f_0\|^2 \lesssim \|\nabla \bar{f} - \nabla f_0\|^2 + \frac{2J(d-2)J^2}{n} \log \left( 1 + \frac{C_2\sqrt{n}}{2J(d-2)/2J} \right) + \frac{\sigma^2}{n}. \]

We have proved the following result.
PROPOSITION 10. Let $B1 - B2$ hold and define $F_J$ as in (5.3). Then, the estimator $\hat{T}_J$ defined in (5.4) satisfies

$$
\mathbb{E}\|\hat{T}_J - T_0\|_{L^2(P)}^2 \lesssim \inf_{f \in F_J} \|\nabla f - T_0\|_{L^2(P)}^2 + \frac{2^{(d-2)J^2}}{n} \log \left(1 + \frac{C_2 \sqrt{n}}{2^{(d-2)/2}J} \right) + \frac{x_J^2}{n}. \quad (5.12)
$$

Moreover, with probability at least $1 - \exp(-t)$,

$$
\|\hat{T}_J - T_0\|_{L^2(P)}^2 \lesssim \inf_{f \in F_J} \|\nabla f - T_0\|_{L^2(P)}^2 + \frac{2^{(d-2)J^2}}{n} \log \left(1 + \frac{C_2 \sqrt{n}}{2^{(d-2)/2}J} \right) + \frac{x_J^2 + t}{n}.
$$

5.5 Control of the approximation error

Next, we control the approximation error $\inf_{f \in F_J} \|\nabla f - \nabla f_0\|_{L^2(P)}$ that appears in Proposition 10. In fact, it is sufficient to control $\|\nabla f - \nabla f_0\|_{L^2(P)}$ where $\hat{f} = P_J$ ext $f_0$ is the truncation of $f_0$ to its first $J$ wavelet scales after extending $f_0$ to all $\mathbb{R}^d$. In light of Lemma 21, we may assume that $\hat{f}$ has the same $C^\alpha$- and $W^{\alpha, 2}$-norm as $f$ up to a constant depending on $\hat{\Omega}_p$.

To control the approximation associated with truncating a wavelet decomposition, we rely on the following lemma for Besov functions.

LEMMA 11. Let $f \in B_{p, q}^s(\mathbb{R}^d)$ and denote by $P_J$ its projection onto the first scale $J$ wavelet coefficients. That is, if

$$
f = \sum_{j=0}^{\infty} \sum_{g \in G^j} \sum_{k \in \mathbb{Z}^d} \gamma_{k}^{j, g} \psi_{k}^{j, g}, \quad \text{we set} \quad P_J f = \sum_{j=0}^{J} \sum_{g \in G^j} \sum_{k \in \mathbb{Z}^d} \gamma_{k}^{j, g} \psi_{k}^{j, g},
$$

where $\psi_{k}^{j, g}$ are multi-dimensional Daubechies wavelets and $G^j$ the associated index sets as in Section B. Then, for all $1 \leq p, q \leq \infty$, $s \geq 0$,

$$
\|P_J f\|_{B_{p, q}^s(\mathbb{R}^d)} \leq \|f\|_{B_{p, q}^s}, \quad (5.13)
$$

$$
\|P_J f - f\|_{B_{p, q}^s(\mathbb{R}^d)} \leq \|f\|_{B_{p, q}^s}. \quad (5.14)
$$

Moreover, for every $q' \in [1, \infty]$, $s' > 0$, and $1 \leq p \leq p' \leq \infty$ such that $s - d/p > s' - d/p'$,

$$
\|P_J f - f\|_{B_{p', q'}^s(\mathbb{R}^d)} \lesssim 2^{-J(s-d/p-(s'-d/p'))}\|f\|_{B_{p', q'}^s}.
$$

In particular: If $f \in C^{\alpha+1}$ for $\alpha > 1$, then $\|f - P_J f\|_{C^2} \lesssim 2^{-J(\alpha-1)}\|f\|_{C^{\alpha+1}}$ and if $f \in W^{\alpha+1, 2}$, for $\alpha > 0$, then $\|f - P_J f\|_{W^{1, 2}} \lesssim 2^{-J\alpha}\|f\|_{W^{\alpha+1, 2}}$.

PROOF. Write $\gamma$ for the wavelet coefficients of $f$. The statements (5.13) and (5.14) follow immediately from the wavelet characterization of the Besov norms, (B.2).

To prove the remaining statements, note that for every $j$, because $\|\cdot\|_{H^s} \leq \|\cdot\|_{H^0}$ and $\|\cdot\|_q$ and $\|\cdot\|_{q'}$ are comparable up to a constant due to $|G^j| \leq 2^d$ being finite,

$$
2^j(s' + \frac{d}{p'} - \frac{d}{p}) \left[ \sum_{g \in G^j} \left( \sum_{k \in \mathbb{Z}^d} |\gamma_{k}^{j, g}|^p \right)^{q'/p'} \right]^{1/q'} \lesssim 2^j(s' - \frac{d}{p'} - (s - d/p)) 2^{j(s + \frac{d}{p} - \frac{d}{p'})} \left[ \sum_{g \in G^j} \left( \sum_{k \in \mathbb{Z}^d} |\gamma_{k}^{j, g}|^p \right)^{q/p} \right]^{1/q} \lesssim 2^{j(s' - \frac{d}{p'} - (s - d/p))} 2^{j(s + \frac{d}{p} - \frac{d}{p'})} \left[ \sum_{g \in G^j} \left( \sum_{k \in \mathbb{Z}^d} |\gamma_{k}^{j, g}|^p \right)^{q/p} \right]^{1/q} \lesssim 2^{j(s' - \frac{d}{p'} - (s - d/p))} 2^{j(s + \frac{d}{p} - \frac{d}{p'})} \|f\|_{B_{p, q}^s}.
$$
Then, plugging this into the wavelet expansion of $\Pi_J f - f$, we obtain

$$
\|\Pi_J f - f\|_{B^{q'}_{p',q'}}^q = \sum_{j=J+1}^{\infty} 2^j q'(s' + \frac{d}{p'} - \frac{d}{2}) \sum_{g \in G} \left( \sum_{k \in \mathbb{Z}^d} |\hat{f}_j(k)|^p \right)^{q'/p'}
\lesssim \sum_{j=J+1}^{\infty} 2^j q'(s' - \frac{d}{p'} - (s' - \frac{d}{2})) \|f\|_{B^{q'}_{p',q'}}^q \lesssim 2^j q'(s' - \frac{d}{p'} - (s' - \frac{d}{2})) \|f\|_{B^{q'}_{p',q'}}^q,
$$

Finally, to obtain the special cases, note that $\|\cdot\|_{B^{q}_{p,\infty}} \lesssim \|\cdot\|_{C^*} \lesssim \|\cdot\|_{B^{q}_{1,\infty}}$ and $\|\cdot\|_{W^{1,2}} = \|\cdot\|_{B^{2}_{2,2}}$ by Theorem 20.

The above lemma together with Proposition-Definition 5 allows us to check that $\tilde{f} \in \mathcal{F}_J$. Indeed, by Weyl's inequality, we have for any $x \in \tilde{\Omega}_P$ that

$$
\lambda_{\min}(D^2 \Pi_J \text{ext } f_0(x)) \geq D^2 f_0(x) - \|D^2 \Pi_J \text{ext } f_0(x)\|_{\text{op}} \geq M - C \|\Pi_J \text{ext } f_0 - f_0\|_{C^2(\tilde{\Omega}_P)}.
$$

It follows from Lemma 11 that $\|\Pi_J \text{ext } f_0 - f_0\|_{C^2(\tilde{\Omega}_P)} \lesssim 2^{-(\beta - 1)J}(M^3 + R) \leq M/2$, if

$$
J \geq J_0 := C_3 \frac{1}{\beta - 1} \log \left( \frac{2M^3 + 2R}{M} \right),
$$

and $C_3 = C_3(d, \beta, \tilde{\Omega}_P)$ is large enough. This yields $\lambda_{\min}(D^2 \Pi_J \text{ext } f_0(x)) \geq M/2$ and $\tilde{f}$ is strongly convex. Similarly, we get that $\lambda_{\max}(D^2 \Pi_J \text{ext } f_0(x)) \leq 2M$ and hence that $\tilde{f} \in \mathcal{F}_J$. Thus,

$$
\inf_{f \in \mathcal{F}_J} \|\nabla f - \nabla f_0\|_{L^2(\mathcal{P})}^2 \leq \|\nabla \tilde{f} - \nabla f_0\|_{L^2(\mathcal{P})} \lesssim \int_{\tilde{\Omega}_P} \|\nabla f - \nabla f_0\|_{L^2(\mathcal{P})}^2 \, d\mu(x) \leq \|f - f_0\|^2_{L^2(\mathcal{P})} \lesssim R^2 2^{-2J\alpha},
$$

where we used Assumption B2 and Lemma 11.

We have thus proved that

$$
\inf_{f \in \mathcal{F}_J} \|\nabla f - \nabla f_0\|_{L^2(\mathcal{P})} \lesssim R^2 2^{-2J\alpha} \quad \text{for } J \geq J_0. \tag{5.15}
$$

### 5.6 Bias-variance tradeoff

We are now in a position to complete the proof of Theorem 6. Combining the bounds (5.12) and (5.15), we get

$$
\mathbb{E}\|\hat{T}_J - T_0\|^2_{L^2(\mathcal{P})} \lesssim R^2 2^{-2J\alpha} + 2^{J(d-2)} J^2 \frac{\log(n)}{n} + \frac{1 + \kappa_J^2}{n},
$$

where $\kappa_J$ is defined in (5.8). We conclude the proof by optimizing with respect to $J$. It yields

$$
\mathbb{E}\|\hat{T}_J - T_0\|^2_{L^2(\mathcal{P})} \lesssim \begin{cases} 
\frac{n^{-1}}{n} & \text{if } d = 1, \\
\frac{n^{-1}(\log n)^3}{n} & \text{if } d = 2, \\
\frac{n^{2d-2+\frac{\alpha}{d-2}}}{n} \log^3(n) & \text{if } d \geq 3.
\end{cases}
$$

We note that since $\alpha > 1$, in the first two cases, $d \in \{1, 2\}$, the cut-off $J$ can be picked independently from $\alpha$. Finally, high-probability bounds can be obtained in a similar manner.

**Acknowledgments.** The authors would like to thank Richard Nickl pointing out to relevant references on the estimation of invariant measures in the multivariate Gaussian white noise model.
APPENDIX A: CONVEX ANALYSIS

In this section, we recall some useful facts from convex analysis. We refer the reader to [36] for a comprehensive treatment.

Recall that a set $U \subseteq \mathbb{R}^d$ is convex if for all $x, y \in U, t \in [0, 1], tx + (1 - t)y \in U$. A function $f: U \to \mathbb{R} \cup \{+\infty\}$ is convex if for all $x, y \in U, t \in [0, 1]$, it holds that

$$f(tx + (1 - t)y) \leq tf(x) + (1 - t)f(y).$$

Moreover, we call a function $\mu$-strongly convex if for all $x, y \in U, t \in [0, 1]$, we have

$$f(tx + (1 - t)y) \leq tf(x) + (1 - t)f(y) - \frac{\mu}{2}t(1 - t)\|x - y\|^2.$$

For twice differentiable functions, it is often more convenient to employ the following analytic criterion for strong convexity.

**Lemma 12 ([36, Theorem B.4.3.1])**. Let $U \subseteq \mathbb{R}^d$ be an open convex set and $f: U \to \mathbb{R}$ twice differentiable. Then, $f$ is $\mu$-strongly convex if and only if $\lambda_{\min}(D^2 f(x)) \geq \mu$ for all $x \in U$.

Note that even if $U \subseteq \mathbb{R}^d$ is a proper convex subset of $\mathbb{R}^d$, we can always consider a function $f: U \to \mathbb{R} \cup \{+\infty\}$ to be defined on all of $\mathbb{R}^d$ by setting it to $+\infty$ outside of $U$. To that end, let $\iota_U$ be the indicator function defined by

$$\iota_U(x) = \begin{cases} 0, & x \in U \\ +\infty, & \text{otherwise.} \end{cases}$$

We define the extension of $f$ outside $U$ by $f + \iota_U$, which by abuse of notation we also denote by $f$.

Note that if $f$ is (strongly) convex on $U$ then its extension outside $U$ is also (strongly) convex. We call $\text{dom}(f) = \{ x \in \mathbb{R}^d : f(x) < +\infty \}$ the domain of a convex function.

We now recall two important notions associated with convex functions $f$.

The subdifferential of $f$ at $x \in \text{dom}(f)$ is defined as

$$\partial f(x) = \{ a \in \mathbb{R}^d : f(y) \geq \langle a, y - x \rangle + f(x) \text{ for all } y \in \mathbb{R}^d \}.$$ 

As indicated by the following lemma, the subdifferential reduces to the gradient for differentiable functions.

**Lemma 13 ([36, Corollary D.2.1.4])**. Let $f: \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$ be a convex function. If $f$ is differentiable at $x \in \mathbb{R}^d$ with gradient $\nabla f(x)$, then $\partial f(x) = \{\nabla f(x)\}$.

Conversely, if $\partial f(x) = \{a\}$ consists of only a single element, then $f$ is differentiable at $x$ with gradient $\nabla f(x) = a$.

The convex conjugate, or Legendre-Fenchel conjugate, is defined for any function $f: \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$ as

$$f^*(y) = \sup_{x \in \mathbb{R}^d} \langle x, y \rangle - f(x), \quad y \in \mathbb{R}^d.$$ 

By considering $f + \iota_U$, this definition extends to functions $f: U \to \mathbb{R} \cup \{+\infty\}$.

We recall the following standard facts about the convex conjugate, stated here without proof (see [36, Part E] for details).
Lemma 14. If $f: \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$ is convex and lower semi-continuous, then $f^{**} = f$.

Lemma 15. Let $U$ be a closed, convex set. If $f: U \rightarrow \mathbb{R}$ is $\mu$-strongly convex, then $\text{dom}(f^*) = \mathbb{R}^d$, and $\nabla f^*$ is $\mu^{-1}$-Lipschitz:
\[
\|\nabla f^*(x) - \nabla f^*(y)\|_2 \leq \frac{1}{\mu} \|x - y\|_2, \quad \forall x, y \in \mathbb{R}^d.
\]

Lemma 16. Denote by $f: \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$ a lower semi-continuous and convex function. Then, for $x, y \in \mathbb{R}^d$,
\[
f^*(y) = \langle x, y \rangle - f(x) \iff y \in \partial f(x) \iff x \in \partial f^*(y).
\]

Lemma 17. If $f, g: U \rightarrow \mathbb{R}$, $f(x) \leq g(x)$ for all $x \in U$, then $f^*(y) \geq g^*(y)$ for all $y \in \mathbb{R}$.

Lemma 18. Given two functions $f, g: U \rightarrow \mathbb{R}$ for a compact set $U$. Abusing notation, denote the convex conjugate of the function $f + \mu_U$ by $f^*$. Then, $\|f^* - g^*\|_{L^\infty(U)} \leq \|f - g\|_{L^\infty(U)}$.

The next lemma provides an explicit form for the convex conjugate of a quadratic function. It is instrumental in the stability proof for the semi-dual objective function (see Proposition 8).

Lemma 19. Let $a > 0$, $b, t \in \mathbb{R}^d$, $c \in \mathbb{R}$ and let $U \subseteq \mathbb{R}^d$ be a closed, convex set. Define
\[
q_t(x) = \frac{a}{2} \|x - t\|_2^2 + \langle b, x - t \rangle + c + \mu_U(x), \quad x \in \mathbb{R}^d.
\]
Then,
\[
q_t^*(y) = \frac{\|y - b\|^2}{2a} + \langle t, y \rangle - c - \frac{a}{2} d^2 \left( \frac{y - b}{a} - t, U \right),
\]
where $d^2$ denotes the squared distance $d^2(x, U) = \inf_{y \in U} \|x - y\|_2^2$.

Proof. Note first that for any $y \in \mathbb{R}^d$,
\[
q_t^*(y) = \sup_{x \in \mathbb{R}^d} \langle x, y \rangle - q(x - t) = \sup_{x \in \mathbb{R}^d} \langle x + t, y \rangle - q(x) = q^*(y) + \langle t, y \rangle,
\]
where
\[
q(x) = \frac{a}{2} \|x\|_2^2 + b^\top x + c + \mu_{U+t}(x)
\]
Moreover,
\[
q^*(y) = \sup_{x \in \mathbb{R}^d} \langle x, y \rangle - q(x) = -\inf_{x \in \mathbb{R}^d} \{q(x) - \langle x, y \rangle\}.
\]
Writing
\[
q(x) - \langle x, y \rangle = \frac{a}{2} \|x - y - \frac{b}{a}\|_2^2 - \frac{\|y - b\|^2}{2a} + c + \mu_{U+t}(x)
\]
we see that the infimum in (A.2) is achieved by the projection $\bar{x}$ of $(y - b)/a$ onto the closed convex set $U + t$. Moreover, the value of the objective at $\bar{x}$ is given by
\[
q(\bar{x}) - \langle \bar{x}, y \rangle = \frac{a}{2} d^2 \left( \frac{y - b}{a}, U + t \right) - \frac{\|y - b\|^2}{2a} + c = \frac{a}{2} d^2 \left( \frac{y - b}{a} - t, U \right) - \frac{\|y - b\|^2}{2a} + c
\]
Together with (A.1) and (A.2), this completes the proof of the lemma. \qed
APPENDIX B: WAVELETS AND FUNCTION SPACES

In this section, we give a brief overview of the different function spaces used in the paper and how their norms can be related to their wavelet coefficients.

First, we recall the definition of Hölder and Sobolev spaces. Let $\Omega \subseteq \mathbb{R}^d$ be a closed set with non-empty interior and denote by $C_u(\Omega)$ the set of uniformly continuous functions on $\Omega$. The Hölder norms for any $f \in C_u(\Omega)$ are defined as follows. For any integer $k \geq 0$ and $f$ that admits continuous derivatives up to order $k$, define

$$\|f\|_{C^k(\Omega)} := \sum_{|\beta| \leq k} \|\partial^\beta f\|_{L^\infty(\Omega)},$$

and for any real number $\alpha > 0$, define

$$\|f\|_{C^\alpha(\Omega)} := \|f\|_{C^{\lfloor \alpha \rfloor}(\Omega)} + \sum_{|\beta| = \lfloor \alpha \rfloor} \sup_{x \neq y, x, y \in \Omega} \frac{|\partial^\beta f(x) - \partial^\beta f(y)|}{\|x - y\|_2^{\alpha - \lfloor \alpha \rfloor}}.$$

The space $C^\alpha(\Omega)$ is then defined as the set of functions for which this norm is finite. For a vector valued function $T: \Omega \to \mathbb{R}^d$, $T = (T_1, \ldots, T_d)^\top$, we similarly define the norms as the sum over the individual norms,

$$\|T\|_{C^\alpha(\Omega)} := \sum_{i=1}^d \|T_i\|_{C^\alpha(\Omega)}.$$

Similarly, for an integer $k \geq 0$ and $p \in [1, \infty]$, the Sobolev norms are defined as

$$\|f\|_{W^{k,2}(\Omega)} := \sum_{|\beta| \leq k} \|\partial^\beta f\|_{L^p(\Omega)},$$

where the derivative $\partial^\beta$ is to be understood in the sense of distributions and the Sobolev space $W^{m,2}(\Omega)$ is the space of all functions for which this norm is finite. This definition can be extended to $\alpha > 0$, for example by defining $W^{\alpha,2}(\Omega)$ as the Besov space $B^{\alpha,2}_{2,2}(\Omega)$, which we define shortly.

Next, we define wavelet bases and Besov spaces, following the definitions given in [79, Section 3], and we refer the reader to this reference for further details on wavelets. Denote by $\psi_M \in C^r(\mathbb{R})$ and $\psi_F \in C^r(\mathbb{R})$ a compactly supported wavelet and scaling function, respectively, for example Daubechies wavelets. This implies that

$$\psi^j_k = \begin{cases} \psi_F(x - k), & j = 0, k \in \mathbb{Z}, \\ 2^{j-1/2} \psi_M(2^{j-1}x - k), & j \in \mathbb{N}, k \in \mathbb{Z}, \end{cases}$$

is an orthonormal basis of $L^2(\mathbb{R})$. To obtain a basis of $L^2(\mathbb{R}^d)$, for $j \in \mathbb{N}$, set

$$G^j = \{\mathfrak{F}, \mathfrak{M}\}^d \setminus \{(\mathfrak{F}, \ldots, \mathfrak{F})\}, \quad G^0 = \{(\mathfrak{F}, \ldots, \mathfrak{F})\},$$

and for $g \in G^j \cup G^0$,

$$\Psi^g_k(x) = \prod_{i=1}^n \psi_g(x_i - k_i), \quad k \in \mathbb{Z}^d.$$  

This gives the orthonormal basis

$$\Psi^j_k = \begin{cases} \psi^j_k(x), & j = 0, g \in G^0, k \in \mathbb{Z}^d \\ 2^{(j-1)d/2} \psi^j_k(2^{j-1}x), & j \in \mathbb{N}, g \in G^j, k \in \mathbb{Z}^d. \end{cases}$$
Wavelet coefficients, defined as the expansion coefficients with respect to the above basis for $L^2(\mathbb{R}^d)$ functions, can be used to characterize the so-called Besov spaces: Let $1 \leq p, q \leq \infty$, $s \geq 0$, and let the regularity of the above wavelets satisfy

$$r > s \vee \left(\frac{2d}{p} + \frac{d}{2} - s\right).$$

With this, if $f$ admits the wavelet representation

$$f = \sum_{j=0}^{\infty} \sum_{g \in G^j} \sum_{k \in \mathbb{Z}^d} \gamma_{j,g} \Psi_{j,g}^k,$$

we define the family of norms $\|f\|_{B^s_{p,q}}$ by

$$\|f\|_{B^s_{p,q}} := \|\gamma\|_{B^s_{p,q}} := \left[ \sum_{j=0}^{\infty} 2^{jq(s + \frac{d}{2} - \frac{d}{p})} \sum_{g \in G^j} \left( \sum_{k \in \mathbb{Z}^d} |\gamma_{j,g}^k|^p \right)^{q/p} \right]^{1/q}. \quad (B.1)$$

In particular, by the orthonormality of the wavelets $\{\Psi_{j,g}^k\}_{j,g,k}$,

$$\|f\|_{B^0_{2,2}} = \|\gamma\|_{\ell^2} = \|f\|_{L^2(\mathbb{R}^d)}.$$ 

For a bounded Lipschitz domain $\Omega \subseteq \mathbb{R}^d$, we can define the Besov spaces $B^s_{p,q}(\Omega)$ by restrictions of functions on $\mathbb{R}^d$ with norm

$$\|f\|_{B^s_{p,q}(\Omega)} := \inf\{\|g\|_{B^s_{p,q}(\mathbb{R}^d)} : g|_{\Omega} = f\}.$$ 

Note that since we work with compactly supported wavelets, for a function $f$ with compact support, only a finite number of wavelet coefficients are non-vanishing in (B.1). In particular, for non-zero wavelet coefficients are contained in a set $\Lambda(j)$ with $|\Lambda(j)| \lesssim 2^{jd}$.

The following theorem collects some basic properties of Besov spaces and their relationship to Hölder and Sobolev spaces.

**Theorem 20.** Let $\Omega \subseteq \mathbb{R}^d$ be a bounded Lipschitz domain.

(i) [33, Proposition 4.3.6] Let $s, s' > 0$, $1 \leq p, p', q, q' \leq \infty$. Then, the following inclusions hold in the sense of continuous embeddings:

(a) $B^s_{p,q} \subseteq B^{s'}_{p',q'}$, if $q \leq q'$,

(b) $B^s_{p,q} \subseteq B^{s'}_{p',q'}$, if $s > s'$,

(ii) [79, Theorem 1.122] Let $k \in \mathbb{N}$. Then, $W^{k,2}(\Omega) = B^k_{2,2}(\Omega)$ and we define $W^{\alpha,2}(\Omega) := B^\alpha_{2,2}(\Omega)$ for $\alpha > 0$ not an integer.

(iii) [79, Theorem 1.122], [33, Proposition 4.3.20] Let $\alpha > 0$. If $\alpha$ is not integer, then

$$C^{\alpha}(\Omega) = B^{\alpha}_{\infty,\infty}(\Omega),$$

If $\alpha$ is integer, then

$$B^{\alpha}_{1,\infty}(\Omega) \subseteq C^{\alpha}(\Omega) \subseteq B^{\alpha}_{\infty,\infty}(\Omega). \quad (B.3)$$
Note that the proof in [33] of (B.3) is given in 1D, but extends naturally to arbitrary dimensions by summability of the wavelet coefficients.

A very useful tool in order to handle function spaces on domains is the availability of extension operators that preserve the norms. The following theorem guarantees the existence of such an extension operator that is the same among all Besov spaces. This allows us to characterize Besov functions on domains via the wavelet coefficients of their extensions.

**THEOREM 21** (Extension operator, [79, Theorem 1.105], [66]). Let \( \Omega \subseteq \mathbb{R}^d \) be a bounded Lipschitz domain. Then, there exists a linear extension operator \( \text{ext} \) that preserves \( L^2, C^\beta, \) and \( W^{\alpha,2} \) norms. That is, there exists an extension operator \( \text{ext} = \text{ext}(\Omega) \) such that for \( A \in \{ L^2, C^\beta, W^{\alpha,2} : \beta > 0, \alpha > 0 \} \), there exist constants \( C = C(\Omega, A) \) with

\[
\| \text{ext} f \|_{A(\mathbb{R}^d)} \leq C \| f \|_{A(\Omega)}, \quad \text{and} \quad \text{ext} f |_{\Omega} = f, \quad \text{for } f \in A.
\]

We conclude this section by a lemma that provides uniform control of a function by its wavelet coefficients. It is useful to control bracketing entropy numbers.

**LEMMA 22.** Let \( f \in V_j(\mathbb{R}^d) \) with wavelet coefficients \( \gamma_{j,k} \) for compactly supported mother and father wavelets. Then, \( \| f \|_\infty \lesssim 2^{jd/2} \| \gamma \|_\infty \lesssim 2^{jd/2} \| \gamma \|_2 \).

**PROOF.** Let \( x \in \mathbb{R}^d \) and write

\[
|f(x)| = \left| \sum_{j=0}^J \sum_{g \in G^j, k \in \mathbb{Z}^d} \gamma_{j,k}^g \psi_{j,k}^g(x) \right| \leq \| \gamma \|_\infty \sum_{j=0}^J \sum_{g \in G^j, k \in \mathbb{Z}^d} |\psi_{j,k}^g(x)| \lesssim \| \gamma \|_\infty \sum_{j=0}^J 2^{jd/2} \lesssim 2^{jd/2} \| \gamma \|_\infty,
\]

where we used Hölder’s inequality and the fact that only a finite number of \( k \) enters the summation for each fixed \( x \in \mathbb{R}^d \). The last inequality is trivial. \( \square \)

**APPENDIX C: METRIC ENTROPY AND SUPREMA OF STOCHASTIC PROCESSES**

Here, we collect some basic results about empirical processes that are needed in the proofs. Note that because all suprema we deal with are over subsets of finite dimensional vector spaces, we do not consider issues of measurability in the remainder.

Denote the bracketing number of a set \( \mathcal{F} \) with respect to a norm \( \| \cdot \| \) by \( N_{[-]}(\delta, \mathcal{F}, \| \cdot \|) \) and define the Dudley integral as

\[
D_{[-]}(\sigma, \mathcal{F}, \| \cdot \|) = \int_0^\sigma \sqrt{1 + \log N_{[-]}(\delta, \mathcal{F}, \| \cdot \|)} \, d\delta.
\] (C.1)

**THEOREM 23** (Bernstein chaining, [83, Lemma 3.4.2]). Let \( \mathcal{F} \) be a class of measurable functions such that \( \mathbb{E}[f^2] < \sigma^2 \) and \( \| f \|_\infty \leq M \) for all \( f \in \mathcal{F} \). Then,

\[
\mathbb{E}\left[ \sup_{f \in \mathcal{F}} |\sqrt{n}(\hat{P} - P)f| \right] \lesssim D_{[-]}(\sigma, \mathcal{F}, L_2(P)) \left( 1 + \frac{D_{[-]}(\sigma, \mathcal{F}, L_2(P))}{\sigma^2 \sqrt{n}} M \right).
\]

**THEOREM 24** (Concentration, see [53, Equation (5.50)], going back to [8]). Under the same assumptions as Theorem 23,

\[
\mathbb{P}\left( \sup_{f \in \mathcal{F}} \sqrt{n}|(\hat{P} - P)f| \geq 2\mathbb{E}[\sup_{f \in \mathcal{F}} \sqrt{n}|(\hat{P} - P)f|] + \sigma \sqrt{2x} + \frac{M}{\sqrt{n}} x \right) \leq \exp(-x).
\]
LEMMA 25 (Bracketing numbers from \(L^\infty\) covering numbers). Let \(P\) be a probability measure and \(A \subseteq \mathcal{F}\) be a set of functions with \(N(\mathcal{F}, L^\infty(P), \delta/2) \leq \phi(\delta)\) then \(N(\mathcal{F}, L^2(P), \delta) \leq \phi(\delta)\). Moreover, if for every function in the original class \(f \in \mathcal{F}\), \(E[f^2] < \sigma^2\) and \(\|f\|_{L^\infty(P)} < M\), then every bracket \([f_1, f_2]\) above (note that \(f_1\) and \(f_2\) need not be members of \(\mathcal{F}\)) satisfies

\[
E[f_j^2] < 2\sigma^2 + \frac{1}{2}\delta^2, \quad \|f_j\|_{L^\infty(\nu)} < M + \delta/2, \quad j \in \{1, 2\}.
\]

Proof. Denote by \(\{f_1, \ldots, f_N\}\) the centers of a minimal \(\delta/2\)-covering of \(\mathcal{F}\) in \(L^\infty(P)\). Let \(i \in \{1, \ldots, N\}\). Then, each \(\delta/2\) ball around \(f_i\) is contained in the bracket \([f_i - \delta/2, f_i + \delta/2]\). Moreover, the \(L^2(P)\) diameter of the above bracket is bounded by its \(L^\infty(P)\) diameter, which is \(\delta\), so the collection of those brackets yields the desired covering with brackets.

The rest of the lemma follows from

\[
E[(f \pm \delta/2)^2] \leq 2E[f^2] + \frac{1}{2}\delta^2, \quad \|f \pm \nu\delta/2\|_{L^\infty(\nu)} \leq \|f\|_{L^\infty(\nu)} + \frac{\delta}{2}.
\]

The following lemma can be shown by directly specifying a grid or by a volume argument such as [84, Proposition 4.2.12].

LEMMA 26 (Covering numbers for norm balls). Fix \(p \in \mathbb{N}\) and denote by \(B_\infty(A)\) the \(\ell^\infty\) ball of \(\mathbb{R}^d\) with radius \(A\). Then, \(N(B_\infty(A), \| \cdot \|_\infty, \delta) \leq (3A/\delta)^d\).

LEMMA 27 ([61, Lemma 10.3]). For \(\alpha > 0\),

\[
\int_0^\alpha \sqrt{\log(1 + t^{-1})} \, dt \leq \alpha \sqrt{1 + \log(1 + \alpha^{-1})}.
\]

APPENDIX D: OMITTED PROOFS

D.1 Proof of Proposition-Definition 5

We proceed in order of statement of the results.

(i) It follows from B2 that there exists \(f_0\) such that \(\nabla f_0 = T_0\) and by B2(ii) that \(|\nabla f_0(x)| \leq M\) for all \(x \in \tilde{\Omega}_P\). Moreover, since \(f_0\) is defined up an additive constant, assume that \(f_0(x_0) = 0\) for some \(x_0 \in \Omega_P\). A first order Taylor expansion yields that for any \(x \in \tilde{\Omega}_P\),

\[
|f_0(x)| = |f_0(x) - f_0(x_0)| \leq \sup_{z \in \tilde{\Omega}_P} \|\nabla f_0(z)\|_2\|x - x_0\|_2 \leq M \text{diam}(\tilde{\Omega}_P) \leq M^2,
\]

where in the second inequality, we used B2(i) and in the second one, we used that \(\text{diam}(\tilde{\Omega}_P) \leq M\) according to B2.

(ii) follows immediately from B2(ii).

(iii) By Lemma 12 and (ii) above, \(f_0\) is strongly convex on \(\text{int}(\tilde{\Omega}_P)\) and can be extended to \(+\infty\) outside of \(\tilde{\Omega}_P\) and thus be also be considered a strongly convex function on \(\mathbb{R}^d\). By Lemmas 15 and 16, we conclude that \(T_0 = \nabla f_0\) is a bijection from \(\Omega_P\) onto its image \(\Omega = \text{supp}(\nabla f_0)_\#\mathbb{P}\), with both \(\nabla f_0\) and \((\nabla f_0)^{-1}\) being continuously differentiable; in other words, \(\nabla f_0\) is a \(C^1\)-diffeomorphism.
between $\Omega_P$ and $\Omega_Q$. Since $C^1$-diffeomorphisms preserve Lipschitz domains [37, Theorem 4.1] and connectedness, we can conclude that $\Omega_Q$ is a connected and bounded Lipschitz domain.

We now turn to check the condition on the density $\rho_Q$ that appears in (iii). To that end, note that by the change of variables formula, $Q$ has the density

$$\rho_Q(y) = \frac{1}{|\det D^2f_0((\nabla f_0)^{-1}(y))|} \rho_P((\nabla f_0)^{-1}(y)) 1(y \in \Omega_Q).$$

This readily yields the desired bound in light of B1 which assumes boundedness of $\rho_P$ and (ii) which gives boundedness of the Hessian $D^2f_0$.

Finally, as in (i), (5.1) follows from a first order expansion: For any $x \in \tilde{\Omega}_P$, note that on the one hand

$$|f_0(x)| = |f_0(x) - f_0(x_0)| \leq \|T_0\|_2 M \leq M^2$$

so that $\|f_0\|_{L^\infty} \leq M^2$ and $\|f_0\|_{L^2} \leq M^3$. Together with the fact that $T_0 = \nabla f_0$, this allows us to shift the smoothness index by one speaking about potentials.

**D.2 Proof of Proposition 9**

We first bound the expectation of the supremum of interest and then obtain the high-probability bound via concentration. To begin, note that

$$\hat{S}_0(f) - S_0(f) = (\hat{P} - P)(f - f_0) + (\hat{Q} - Q)(f^* - f_0^*),$$

which yields

$$\mathbb{E}[\sup_{f \in \mathcal{F}_J(\tau^2)} |\hat{S}_0(f) - S_0(f)|] \leq \mathbb{E}[\sup_{f \in \mathcal{F}_J(\tau^2)} |(\hat{P} - P)(f - f_0)| + \mathbb{E}[\sup_{f \in \mathcal{F}_J(\tau^2)} |(\hat{Q} - Q)(f^* - f_0^*)|] =: T_1 + T_2.$$

We first focus on the $T_2$-term. Once understood, the $T_1$-term can be bounded similarly.

**Bound on $T_2$-term.**

We estimate $T_2$ from above by two suprema, corresponding to low and high frequencies. To this end, we center all functions and consider the extension of a restriction of the functions to $\Omega_Q$, which allows us to use wavelet expansions for harmonic analysis.

First, because $(\hat{Q} - Q)(g + c) = (\hat{Q} - Q)g$ for every function $g$ and constant $c \in \mathbb{R}$, we may assume without loss of generality that

$$\int_{\Omega_Q} (f^*(z) - f_0^*(z)) \, d\lambda(z) = 0 \quad \forall f \in \mathcal{F}_J.$$

Note that $f^*$ and $f_0^*$ are defined over all of $\mathbb{R}^d$ but we do not control their norms over the whole space. To overcome this limitation, with a slight abuse of notation, we denote by $\text{ext } f^*$ (resp. $\text{ext } f_0^*$) the Lipschitz extension of the restriction of $f^*$ (resp. $f_0^*$) to $\Omega_Q$. The existence of a linear extension operator is guaranteed by Theorem 21. In particular, we control the norms of $\text{ext } f^*$ and $\text{ext } f_0^*$.

For a function $g$ with wavelet expansion

$$g = \sum_{j=0}^{\infty} \sum_{g \in G^j} \sum_{k \in \mathbb{Z}^d} \gamma_k g^j_k \psi_k^j,$$
as defined in Section B, we define the two $L^2$-projections

$$\Pi_J g = \sum_{j=0}^{J} \sum_{g \in G^j} \sum_{k \in \mathbb{Z}^d} \gamma_k^j \Psi_k^j,$$

$$\Pi_{>J} g = \sum_{j=J+1}^{\infty} \sum_{g \in G^j} \sum_{k \in \mathbb{Z}^d} \gamma_k^j \Psi_k^j.$$

With this, we write $T_2 = T_{2,1} + T_{2,2}$, where

$$T_{2,1} = \mathbb{E}[\sup_{f \in F_j(\tau^2)} |(\hat{Q} - Q)\Pi_J \text{ext}(f^* - f_0^*)|], \quad T_{2,2} = \mathbb{E}[\sup_{f \in F_j(\tau^2)} |(\hat{Q} - Q)\Pi_{>J} \text{ext}(f^* - f_0^*)|].$$

Note that the projected functions are again well-defined continuous functions: By assumption, all $f$ and $f_0$ are strongly convex, hence their conjugates have Lipschitz-continuous gradients and therefore bounded $B_{2,\infty}^{2,\infty}(\Omega_Q)$-norm. In turn, their projections also have bounded $B_{2,\infty}^{2,\infty}(\Omega_Q)$-norm, and by Theorem 21, this implies that both $\Pi_J \text{ext}(f^* - f_0^*)$ and $\Pi_{>J} \text{ext}(f^* - f_0^*)$ are in $C^s(\mathbb{R}^d)$, for $s < 2$, and hence they are continuous.

**Bound on $T_{2,1}$-term.**

Recall that it follows from Proposition-Definition 5 that $\Omega_Q$ is a connected Lipschitz domain, so we can apply the Poincaré-Wirtinger inequality, Lemma 30, together with (5.6) from Proposition 8, to get

$$\int_{\Omega_Q} (f^* - f_0^*)^2 \, d\lambda \lesssim \int_{\Omega_Q} \|\nabla f^* - \nabla f_0^*\|^2 \, d\lambda \lesssim \tau^2,$$

where we used that we assumed $f^* - f_0^*$ to be centered.

Hence, $f \in F_j(\tau^2)$ implies $\|f^* - f_0^*\|_{W^{1,2}(\Omega_Q)} \lesssim \tau$, and therefore due to the properties of the extension operator $\text{ext}$,

$$\|\text{ext}(f^* - f_0^*)\|_{W^{1,2}(\mathbb{R}^d)} \leq C_4 \tau, \quad (D.2)$$

for some constant $C_4 = C_4(M, \Omega_Q)$. Since $\Pi_J$ is a non-expansive operator on Besov spaces, it follows from the above display that

$$T_{2,1} \leq \sup\{|(\hat{Q} - Q)h| : h \in V_J(\mathbb{R}^d), \|h\|_{W^{1,2}(\mathbb{R}^d)} \leq C_4 \tau\}.$$

Bounding the empirical process over this standard function class can now be performed as follows. Observe first that for any function $h \in V_J(\mathbb{R}^d)$ with wavelet decomposition

$$h = \sum_{j=0}^{J} \sum_{g \in G^j} \sum_{k \in \mathbb{Z}^d} \gamma_k^j \Psi_k^j,$$

the condition $\|h\|_{W^{1,2}(\mathbb{R}^d)} \leq C_4 \tau$ is equivalent to

$$\sum_{j=0}^{J} \sum_{g \in G^j} \sum_{k \in \mathbb{Z}^d} 2^{2j} |\gamma_k^j|^2 \leq C_4^2 \tau^2.$$

Next, by symmetrization, for independent copies of Rademacher random variables $\varepsilon_i, i = 1, \ldots, n$,

$$\mathbb{E} \sup\{|(\hat{Q} - Q)h| : h \in V_J(\mathbb{R}^d), \|h\|_{W^{1,2}(\mathbb{R}^d)} \leq C_4 \tau\} \leq \mathbb{E} \sup\frac{1}{n} \sum_{i=1}^{n} \varepsilon_i h(Y_i),$$

where $Y_i$ are independent Rademacher random variables.
where both suprema are taken over the set \( \mathfrak{G}_J = \{ h \in V_J(\mathbb{R}^d), \| h \|_{W_1^2(\mathbb{R}^d)} \leq C_4 \tau \} \). To control the Rademacher process, fix \( h \in \mathfrak{G}_J \) with wavelet decomposition (D.3). By the Cauchy-Schwarz inequality,

\[
\sum_{i=1}^n \varepsilon_i h(Y_i) \leq \left( \sum_{i=1}^n 2^{2j_i} |\gamma_k^{j_i} g|^2 \right)^{1/2} \left( \sum_{i=1}^n \left( \sum_{j=1}^n \varepsilon_i \Psi_k^{j_i g}(Y_i) \right)^2 \right)^{1/2} \leq C_4 \tau \left( \sum_{i=1}^n \left( \sum_{j=1}^n \varepsilon_i \Psi_k^{j_i g}(Y_i) \right)^2 \right)^{1/2},
\]

where here and below, all sums without indices are over \( \{ 0 \leq j \leq J, g \in G^j, k \in \mathbb{Z}^d \} \). Since the right-hand side in the display above does not depend on \( h \), we get by Jensen’s inequality that

\[
\mathbb{E} \sup \frac{1}{n} \sum_{i=1}^n \varepsilon_i h(Y_i) \leq \frac{C_4 \tau}{n} \left( \mathbb{E} \sum_{i=1}^n \left( \sum_{j=1}^n \varepsilon_i \Psi_k^{j_i g}(Y_i) \right)^2 \right)^{1/2}.
\]

Since \( Y_i \in \Omega_Q \), a compact set by assumption, for given \( j \) and \( g \), \( \Psi_k^{j_i g}(Y_i) \) is non-zero only for \( k \in \Lambda(j) \) where \( \Lambda(j) \) depends on the diameter of \( \Omega_Q \), and \( |\Lambda(j)| \lesssim 2^{jd} \). Together with the independence of the \( \varepsilon_i \), this yields

\[
\mathbb{E} \sum_{i=1}^n \left( \sum_{j=1}^n \varepsilon_i \Psi_k^{j_i g}(Y_i) \right)^2 = \sum_{0 \leq j \leq J} \sum_{g \in G^j, k \in \Lambda(j)} \frac{1}{2^{2j}} \mathbb{E} [\Psi_k^{j_i g}(Y_i)^2].
\]

By Proposition-Definition 5(iii) and the fact that the \( \Psi_k^{j_i g} \) form an orthonormal basis in \( L^2(\mathbb{R}^d) \),

\[
\mathbb{E} [\Psi_k^{j_i g}(Y_i)^2] \lesssim \int_{\Omega_Q} \Psi_k^{j_i g}(y)^2 \, d\lambda(y) \leq \int_{\mathbb{R}^d} \Psi_k^{j_i g}(y)^2 \, d\lambda(y) = 1.
\]

Thus,

\[
\sum_{0 \leq j \leq J} \sum_{g \in G^j, k \in \Lambda(j)} \frac{1}{2^{2j}} \mathbb{E} [\Psi_k^{j_i g}(Y_i)^2] \lesssim n \sum_{0 \leq j \leq J} \frac{2^{jd}}{2^{2j}} \lesssim \begin{cases} n, & d = 1, \\ nJ, & d = 2, \\ n2^{J(d-2)}, & d \geq 3. \end{cases}
\]

We have proved that

\[
T_{2,1} \lesssim \frac{\tau}{\sqrt{n}} \tau_J, \quad \tau_J := \begin{cases} 1, & d = 1, \\ \sqrt{J}, & d = 2, \\ 2^{d-2}, & d \geq 3. \end{cases}
\]

**Bound on \( T_{2,2} \)-term.**

To control the term \( T_{2,2} \), we use a chaining bound for bracketing entropy (Theorem 23). To that end, we exhibit bounds on the \( L^\infty \)-covering numbers of the corresponding function space, which in turn implies control of \( L^2 \)-bracketing numbers. The idea is to bound the covering numbers in the original space \( \mathcal{F}_J(\tau^2) \) and exploit continuity properties of the transformations that lead to the function class in the definition of \( T_{2,2} \), in particular the operation of taking the convex conjugate.

Define the function space

\[
\tilde{\mathcal{F}}_J(\tau^2) = \{ \Pi_{\geq J} \text{ext}(f^\ast - f_0^\ast) : f \in \mathcal{F}_J(\tau^2) \},
\]

where \( \Pi_{\geq J} \) is the projection onto the functions \( f \in \mathcal{F}_J(\tau^2) \) with wavelet decomposition \( f^\ast \). We use a chaining bound for bracketing entropy (Theorem 23).
and let \( f_1, f_2 \in \mathcal{F}_J(\tau^2) \) have wavelet coefficients given by the sequences \( \gamma_1 \) and \( \gamma_2 \). Observe that by linearity of the projection and extension operators, we have for any cutoff \( J' \geq 0 \),

\[
\| \Pi_{> J} \text{ext}(f_1^* - f_0^*) - \Pi_{> J} \text{ext}(f_2^* - f_0^*) \|_{L^\infty(\Omega_Q)} = \| \Pi_{> J} \text{ext}(f_1^* - f_2^*) \|_{L^\infty(\Omega_Q)} \\
\leq \| \Pi_{> J'} \Pi_{> J} \text{ext}(f_1^* - f_2^*) \|_{L^\infty(\Omega_Q)} + \| \Pi_{> J'} \Pi_{> J} \text{ext}(f_1^* - f_2^*) \|_{L^\infty(\Omega_Q)}.
\]

To control the first term in the right-hand side above, in the following lemma, we establish bounds on the potentials in \( \tilde{F}_J(\tau^2) \). Its proof is deferred to the next section.

**Lemma 28.** There exists a constant \( C_5 = C_5(M, \Omega_P, \tilde{\Omega}_P, \Omega_Q) \geq M \) such that for all \( f \in \mathcal{X}(2M) \),

\[
\| \text{ext} f^* \|_{B_{\infty, \infty}^2(\mathbb{R}^d)} \leq \frac{C_5}{2}.
\]

Moreover, under assumptions \( B1 - B2 \), \( \| \text{ext} f_0^* \|_{B_{\infty, \infty}^2(\mathbb{R}^d)} \leq C_5/2 \) as well.

It follows from Lemma 28 that there exists \( C_5 \geq M \) such that for any \( f \in \mathcal{F}(\tau^2) \), we have

\[
\| \Pi_{> J} \text{ext}(f_1^* - f_2^*) \|_{B_{\infty, \infty}^2} \leq C_5.
\]

Therefore, by Lemma 11, we get

\[
\| \Pi_{> J'} \Pi_{> J} \text{ext}(f_1^* - f_2^*) \|_{L^\infty(\Omega_Q)} \leq 2^{-2J'} \| \Pi_{> J'} \text{ext}(f_1^* - f_2^*) \|_{B_{\infty, \infty}^2} \leq \varepsilon
\]

if we choose \( J' = \lceil \log (C_5/\varepsilon)/2 \rceil \) so that \( C_5 2^{-2J'} \leq \varepsilon \).

To control the second term, we get from Lemma 22 that

\[
\| \Pi_{> J'} \Pi_{> J} \text{ext}(f_1^* - f_2^*) \|_{L^\infty(\Omega_Q)} \leq 2^{J'/2} \| \Pi_{> J'} \gamma \|_2 \leq 2^{J'/2} \| \gamma \|_2 = 2^{J'/2} \| \text{ext}(f_1^* - f_2^*) \|_{L^2(\mathbb{R}^d)}.
\]

Moreover, using respectively the fact that \( \text{ext} \) is a Lipschitz operator on Besov spaces, \( \Omega_Q \) is bounded and the convex conjugate is non-expansive in \( L^\infty \) by Lemma 18, we have

\[
\| \text{ext}(f_1^* - f_2^*) \|_{L^2(\mathbb{R}^d)} \lesssim \| f_1^* - f_2^* \|_{L^2(\Omega_Q)} \lesssim \| f_1^* - f_2^* \|_{L^\infty(\Omega_Q)} \leq \| f_1 - f_2 \|_{L^\infty(\tilde{\Omega}_P)} \lesssim 2^{J/2} \| \gamma_1 - \gamma_2 \|_\infty,
\]

where in the last inequality, we used Lemma 22. We have proved that

\[
\| \Pi_{> J} \text{ext}(f_1^* - f_0^*) - \Pi_{> J} \text{ext}(f_2^* - f_0^*) \|_{L^\infty(\Omega_Q)} \leq C_6 2^{(J+J')d/2} \| \gamma_1 - \gamma_2 \|_\infty + \varepsilon,
\]

for some constant \( C_6 = C_6(M, \tilde{\Omega}_P, \Omega_Q) \). This inequality allows us to control the \( L^\infty \)-bracketing numbers of \( \tilde{F}_J(\tau^2) \) using \( \ell^\infty \)-covering numbers for the wavelet coefficients. To control the latter, note that for all \( f \in \mathcal{F}_J(\tau^2) \subset \mathcal{X}(2M) \), it holds \( \| f \|_{B_{\infty, \infty}^2(\mathbb{R}^d)} \lesssim M \) so that \( \| \gamma \|_\infty \lesssim M \leq C_5 \).

Moreover, these wavelet coefficients are in a space of dimension at most \( C 2^{Jd} \), \( C > 0 \) because \( \mathcal{F}_J(\tau^2) \subseteq V_J(\tilde{\Omega}_P) \). Hence, choosing \( \varepsilon = c\delta \) with a suitably small constant \( c = c(M, \Omega_Q) \), Lemmas 25, 26, and the previous display yield

\[
\log N_{[\| \cdot \|_{L^2(\Omega_Q)}, \delta]}(\tilde{F}_J(\tau^2), \delta) \leq \log N(\tilde{F}_J(\tau^2), \| \cdot \|_{L^\infty(\Omega_Q)}, \delta) \lesssim 2^{Jd} J \log \left( \frac{C_5}{\delta} \right).
\]
To apply the chaining bound of Theorem 23, note that by (D.2) and Lemma 28, respectively, combined with Lemma 11, we have
\[ \| g \|_{L^2(\mathbb{R}^d)} \leq C_4 2^{-J \tau}, \quad \| g \|_{L^\infty(\mathbb{R}^d)} \leq C_5 2^{-2J}, \quad \text{for } g \in \tilde{F}_J(\tau^2). \]
Thus,
\[ T_{2,2} \lesssim \frac{1}{\sqrt{n}} \mathcal{D}_{\|}(1 + \frac{\mathcal{D}_{\|}}{C_4 2^{-2J} \tau^2 \sqrt{n}} 2^{-2J}) = \frac{1}{\sqrt{n}} \mathcal{D}_{\|} \left( 1 + \frac{\tau}{\tau^2 \sqrt{n}} \right), \]
where \( \mathcal{D}_{\|} = \mathcal{D}_{\|}(C_4 2^{-J \tau}, \tilde{F}_J(\tau^2), L^2(Q)) \) is the Dudley integral defined in (C.1). Moreover, by (D.5) and Lemma 27, we have
\[ \mathcal{D}_{\|} \lesssim \int_0^{C d^{-J \tau}} \sqrt{1 + 2^{J d} \log(C_5/\delta)} \, d\delta \lesssim \tau 2^{d-2} J \log(1 + C_5/\tau), \]
and therefore,
\[ T_{2,2} \lesssim \frac{2^{J - 2}}{\sqrt{n}} J \sqrt{\log(1 + C_5/\tau)} + \frac{2^{J(d-2)} J^2}{n} \log(1 + C_5/\tau). \]
Together with (D.4), we have \( T_2 \lesssim \phi_J(\tau^2) \) with \( \phi_J \) defined as in (5.9) and we absorbed \( \tau_J \) for \( d \geq 3 \) into the first term on the right-hand side.

**Bounding \( T_1 \).** \( T_1 \) can be bounded completely analogously to how we bounded \( T_2 \), with the exception that Lemma 18 is not needed. Thus, we obtain \( T_1 \lesssim \phi_J(\tau^2) \).

**Final bound and concentration.** Collecting the above bounds on \( T_1 \) and \( T_2 \), we get
\[ \mathbb{E} \left[ \sup_{f \in \mathcal{F}_J(\tau^2)} | \hat{S}_0(f) - \mathcal{S}_0(f) | \right] \lesssim \phi_J(\tau^2). \]
To obtain a bound that holds with high probability, we apply the concentration result of Theorem 24. For this, note that (D.1) can be written as
\[ \hat{S}_0(f) - \mathcal{S}_0(f) = ((\hat{P} \otimes \hat{Q}) - (P \otimes Q))((f - f_0) \otimes (f^* - f_0^*)), \]
where \( P \otimes Q \) denotes the product measure and \( (f \otimes g)(x, y) = f(x) + g(y) \). Following the same argument as in the proof of Lemma 28, we get
\[ \|(f - f_0) \otimes (f^* - f_0^*)\|_{L^\infty(\Omega_P \times \Omega_Q)} \leq C_5. \]
Moreover, similarly to Proposition 8, we have for any \( f \in \mathcal{F}_J(\tau^2) \) that
\[ \|(f - f_0) \otimes (f^* - f_0^*)\|_{L^2(P \otimes Q)} \leq C_4 \tau. \]
We can therefore apply Theorem 24 and conclude that with probability at least \( 1 - e^{-t} \), it holds that
\[ \sup_{f \in \mathcal{F}_J(\tau^2)} \left| S_0(f) - \hat{S}_0(f) \right| \lesssim \phi_J(\tau^2) + \tau \sqrt{\frac{t}{n} + \frac{t}{n}}, \]
which concludes our proof.
D.3 Proof of Lemma 28

By the boundedness conditions in the definition of $\mathcal{X}(2M)$ in Proposition-Definition 5, we have for $y \in \Omega_Q$ that

$$|f^*(y)| = \left| \sup_{x \in \Omega_P} \langle x, y \rangle - f(x) \right| \leq C_5(M).$$

Moreover, by Lemma 15, $\nabla f^*$ is $(2M)^{-1}$-Lipschitz. Therefore, since $\Omega_Q$ is bounded,

$$\|\text{ext } f^*\|_{B_{2,\infty}(\Omega_Q)} \lesssim_{\Omega_Q} \|f^*\|_{C^2(\Omega_Q)} \lesssim C_5.$$

We can similarly deduce the second claim by Proposition-Definition 5 since $f_0 \in \mathcal{X}(M)$, possibly choosing a larger $C_5$.

APPENDIX E: ADDITIONAL LEMMAS

**Lemma 29.** In the notation of the proof of Theorem 4, for any $k = 1, \ldots, K$ and $m \geq m_0$, $\nabla \phi_k$ is a bijection from $[0, 1]^d$ to $[0, 1]^d$.

**Proof of Lemma 29.** By construction, $\phi_k$ is strongly convex and has Lipschitz continuous derivatives, hence so does its convex conjugate $\phi_k^*$. In particular, $\phi_k^*$ is defined on all of $\mathbb{R}^d$ and for each $y$,

$$\phi_k^*(y) = \sup_x \langle x, y \rangle - \phi_k(x).$$

Hence, the equation $\nabla \phi_k(x) = y$ has a unique solution $x(y)$ for every $y \in \mathbb{R}^d$ which implies that $\nabla \phi_k$ is injective and that for any $y \in [0, 1]^d$, there exists $x = x(y) \in \mathbb{R}^d$ such that $\nabla \phi_k(x) = y$. It remains to check that $x(y) \in [0, 1]^d$ for all $y \in [0, 1]^d$. To that end, note that $\phi_k(x) = \|x\|^2/2$ for $x \notin [0, 1]^d$. Hence $x(y) = y$ whenever $y \notin [0, 1]^d$. In particular, if $y \in [0, 1]^d$, we must have $x(y) \in [0, 1]^d$. This completes the proof.

**Lemma 30 (Poincaré inequality, [26, Section 5.8.1], [49, Theorem 13.27]).** Let $\Omega \subseteq \mathbb{R}^d$ be a bounded and connected Lipschitz domain. Then, there exists a constant $C = C(d, \Omega)$ such that for any function $f \in W^{1,2}(\Omega)$,

$$\|f - \int \Omega f(x) \, d\lambda(x)\|_{L^2(\Omega)} \leq C \|\nabla u\|_{L^2(\Omega)}.$$

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