Minimax Estimation of Quadratic Fourier Functionals

SHASHANK SINGH$^1$ BHARATH K. SRIPERUMBUDUR$^2$ and BARNABÁS PÓCZOS$^1$

$^1$Carnegie Mellon University, Pittsburgh, PA 15213, USA
E-mail: sss1@cs.cmu.edu; bapoczos@cs.cmu.edu

$^2$Pennsylvania State University, University Park, PA 16802, USA E-mail: bks18@psu.edu

We study estimation of (semi-)inner products between two nonparametric probability distributions, given IID samples from each distribution. These products include relatively well-studied classical $L^2$ and Sobolev inner products, as well as those induced by translation-invariant reproducing kernels, for which we believe our results are the first. We first propose estimators for these quantities, and the induced (semi)norms and (pseudo)metrics. We then prove non-asymptotic upper bounds on their mean squared error, in terms of weights both of the inner product and of the two distributions, in the Fourier basis. Finally, we prove minimax lower bounds that imply rate-optimality of the proposed estimators over Fourier ellipsoids.

1. Introduction

Let $X$ be a compact subset of $\mathbb{R}^D$ endowed with the Borel $\sigma$-algebra and let $\mathcal{P}$ denote the family of all Borel probability measures on $X$. For each $P \in \mathcal{P}$, let $\phi_P : \mathbb{R}^D \to \mathbb{C}$ denote the characteristic function of $P$ given by

$$
\phi_P(z) = \mathbb{E}_{X \sim P} \left[ \psi_z(X) \right] \quad \text{for all } z \in \mathbb{R}^D, \quad \text{where } \psi_z(x) = \exp(i \langle z, x \rangle)
$$

(1)

denotes the $i^{th}$ Fourier basis element, in which $\langle \cdot, \cdot \rangle$ denotes the Euclidean inner product on $\mathbb{R}^D$.

For any family $a = \{a_z\}_{z \in Z} \subseteq \mathbb{R}$ of real-valued coefficients indexed by a countable set $Z$, define a set of probability measures

$$
\mathcal{H}_a := \left\{ P \in \mathcal{P} : \sum_{z \in Z} \frac{\left| \phi_P(z) \right|^2}{a_z^2} < \infty \right\}.
$$

Now fix two unknown probability measures $P, Q \in \mathcal{H}_a$. We study estimation of the semi-inner product$^1$

$$
\langle P, Q \rangle_a = \sum_{z \in Z} \frac{\phi_P(z) \overline{\phi_Q(z)}}{a_z^2},
$$

(2)

$^1$For a complex number $\xi = a + bi \in \mathbb{C}$, $\overline{\xi} = a - bi \in \mathbb{C}$ denotes the complex conjugate of $\xi$. A semi-inner product has all properties of an inner product, except that $\langle P, P \rangle = 0$ does not imply $P = 0$. 


as well as the squared seminorm $\|P\|_a^2 := \langle P, P \rangle_a$ and squared pseudometric $\|P - Q\|_a^2$, using $n$ i.i.d. samples $X_1, ..., X_n \sim P$ and $Y_1, ..., Y_n \sim Q$ from each distribution. Specifically, we assume that $P$ and $Q$ lie in a smaller subspace $\mathcal{H}_b \subseteq \mathcal{H}_a$ parameterized by a $\mathcal{Z}$-indexed real family $b = \{b_z\}_z \in \mathcal{Z}$. In this setting, we study the minimax $\mathcal{L}^2$ error $M(a, b)$ of estimating $\langle P, Q \rangle_a$, over $P$ and $Q$ lying in a (unit) ellipsoid with respect to $\| \cdot \|_b$; that is, the quantity

$$M(a, b) := \inf_{\hat{S}} \sup_{\|P\|_b, \|Q\|_b \leq 1} \frac{1}{n} \int_{X_1, ..., X_n \sim P} \left( \frac{\hat{S}(X_1, ..., X_n, Y_1, ..., Y_n) - \langle P, Q \rangle_a}{\langle P, Q \rangle_a} \right)^2 \, dP, \quad (3)$$

where the infimum is taken over all estimators $\hat{S}$ (i.e., all complex-valued functions $\hat{S} : \mathcal{X}^{2n} \to \mathbb{C}$ of the data).

We study how the rate of the minimax error $M(a, b)$ is primarily governed by the rates at which $a_z$ and $b_z$ decay to 0 as $\|z\| \to \infty$.\(^2\) This has been studied extensively in the Sobolev (or polynomial-decay) case, where, for some $t > s \geq 0$, $a_z = \|z\|^{-s}$ and $b_z = \|z\|^{-t}$, corresponding to estimation of $s$-order Sobolev inner products under $t$-order Sobolev smoothness assumptions on the Lebesgue density functions $p$ and $q$ of $P$ and $Q$ (as described in Example 3 below) [Bickel and Ritov, 1988, Donoho and Nussbaum, 1990, Laurent and Massart, 2000, Singh et al., 2016]. In this case, the rate of $M(a, b)$ has been identified (by Bickel and Ritov [1988], Donoho and Nussbaum [1990], and Singh et al. [2016], in increasing generality) as \(^3\)

$$M(a, b) \asymp \max \left\{ n^{-1}, n^{-\frac{2(s-t)}{4s+4t}} \right\}, \quad (4)$$

so that the “parametric” rate $n^{-1}$ dominates when $t \geq 2s + D/4$, and the slower rate $n^{-\frac{2(s-t)}{4s+4t}}$ dominates otherwise. Laurent and Massart [2000] additionally showed that, for $t < 2s + D/4$, $M(a, b)$ increases by a factor of $(\log n)^{\frac{4(s-t)}{t+4s}}$ in the “adaptive” case, when the tail index $t$ is not assumed to be known to the estimator.

However, the behavior of $M(a, b)$ for other (non-polynomial) decay rates of $a$ and $b$ has not been studied, despite the fact that, as discussed in Section 1.1, other rates of decay of $a$ and $b$, such as Gaussian or exponential decay, correspond to inner products and assumptions commonly considered in nonparametric statistics. The goal of this paper is therefore to understand the behavior of $M(a, b)$ for general sequences $a$ and $b$.

Although our results apply more generally, to simply summarize our results, consider the case where $a$ and $b$ are “radial”; i.e. $a_z$ and $b_z$ are both functions of some norm $\|z\|$. Under mild assumptions, we show that the minimax convergence rate is then a function of the quantities

$$A_{\zeta_n} = \sum_{\|z\| \leq \zeta_n} a_z^{-2} \quad \text{and} \quad B_{\zeta_n} = \sum_{\|z\| \leq \zeta_n} b_z^{-2},$$

\(^2\)By equivalence of finite-dimensional norms, the choice of norm here affects only constant factors.

\(^3\)Here and elsewhere, $\asymp$ denotes equality up to constant factors.
which can be thought of as measures of the “strengths” of $\| \cdot \|_a$ and $\| \cdot \|_b$, for a particular choice of a “smoothing” (or “truncation”) parameter $\zeta_n \in (0, \infty)$. Specifically, we show

$$M(a, b) \asymp \max \left\{ \left( \frac{A_{\zeta_n}}{B_{\zeta_n}} \right)^2, \frac{1}{n} \right\}, \quad \text{where} \quad \zeta_n D n^2 = B_{\zeta_n}^2. \quad (5)$$

While (5) is difficult to simplify or express in a closed form in general, it is quite simple to compute given the forms of $a$ and $b$. In this sense, (5) might be considered as an analogue of the Le Cam equation [Yang and Barron, 1999] (which gives a similar implicit formula for the minimax rate of nonparametric density estimation in terms of covering numbers) for estimating inner products and related quantities. It is easy to check that, in the Sobolev case (where $a_z = \| z \|^{-s}$ and $b_z = \| z \|^{-t}$ decay polynomially), (5) recovers the previously known rate (4). Moreover, our assumptions are also satisfied by other rates of interest, such as exponential (where $a_z = e^{-s\| z \|_1}$ and $b_z = e^{-t\| z \|_1}$) and Gaussian (where $a_z = e^{-s\| z \|_2^2}$ and $b_z = e^{-t\| z \|_2^2}$) rates, for which we are the first to identify minimax rates. As in the Sobolev case, the rates here exhibit the so-called “elbow” phenomenon, where the convergence rates is “parametric” (i.e., of order $\simeq 1/n$) when $t$ is sufficiently large relative to $s$, and slower otherwise. However, for rapidly decaying $b$ such as in the exponential case, the location of this elbow no longer depends directly on the dimension $D$; the parametric rate is achieved as soon as $t \geq 2s$.

We note that, in all of the above cases, the minimax rate (5) is achieved by a simple bilinear estimator:

$$\hat{S}_{\zeta_n} := \sum_{\| z \| \leq \zeta_n} \frac{\hat{\phi}_P(z) \hat{\phi}_Q(z)}{a_z^2},$$

where

$$\hat{\phi}_P(z) := \frac{1}{n} \sum_{i=1}^n \psi_z(X_i) \quad \text{and} \quad \hat{\phi}_Q(z) := \frac{1}{n} \sum_{i=1}^n \psi_z(Y_i)$$

are linear estimates of $\phi_P(z)$ and $\phi_Q(z)$, and $\zeta_n \geq 0$ is a tuning parameter. We also show that, in many cases, a rate-optimal $\zeta_n$ can be chosen adaptively (i.e., without knowledge of the space $H_b$ in which $P$ and $Q$ lie).

### 1.1. Motivating Examples

Here, we briefly present some examples of products $\langle \cdot, \cdot \rangle_a$ and spaces $H_a$ of the form (2) that are commonly encountered in statistical theory and functional analysis. In the following examples, the base measure on $\mathcal{X}$ is taken to be the Lebesgue measure $\mu$, and “probability densities” are with respect to $\mu$. Also, for any integrable function $f \in L^1(\mathcal{X})$, we use $\hat{f}_z = \int_{\mathcal{X}} f \psi_z d\mu$ to denote the $z^{th}$ Fourier coefficient of $f$ (where $\psi_z$ is the $z^{th}$ Fourier basis element as in (1)).

The simplest example is the standard $L^2$ inner product:
Example 1. In the “unweighted” case where $a_z = 1$ for all $z \in \mathbb{Z}$, $\mathcal{H}_a$ includes the usual space $L^2(\mathcal{X})$ of square-integrable probability densities on $\mathcal{X}$, and, for $P$ and $Q$ with square-integrable densities $p, q \in L^2(\mathcal{X})$, we have

$$\langle p, q \rangle_a = \int_{\mathcal{X}} p(x)q(x) \, dx.$$ 

Typically, however, we are interested in weight sequences such that $a_z \to 0$ as $\|z\| \to \infty$ and $\mathcal{H}_a$ will be strictly smaller than $L^2(\mathcal{X})$ to ensure that $\langle \cdot, \cdot \rangle_a$ is finite-valued; this corresponds intuitively to requiring additional smoothness of functions in $\mathcal{H}$. Here are two examples widely used in statistics:

Example 2. If $\mathcal{H}_K$ is a reproducing kernel Hilbert space (RKHS) with a symmetric, translation-invariant kernel $K(x, y) = \kappa(x - y)$ (where $\kappa \in L^2(\mathcal{X})$), one can show via Bochner’s theorem (see, e.g., Theorem 6.6 of [Wendland, 2005]) that the semi-inner product induced by the kernel can be written in the form

$$\langle f, g \rangle_{\mathcal{H}_K} := \sum_{z \in \mathbb{Z}} \bar{z}^2 \bar{f}_z \bar{g}_z.$$ 

Hence, setting each $a_z = \langle \kappa, \psi_z \rangle = \bar{\kappa}_z$, $\mathcal{H}_a$ contains any distributions $P$ and $Q$ on $\mathcal{X}$ with densities $p, q \in \mathcal{H}_K = \{ p \in L^2 : \langle p, p \rangle_{\mathcal{H}_K} < \infty \}$, and we have $\langle P, Q \rangle_a = \langle p, q \rangle_{\mathcal{H}_K}$.

Example 3. For $s \in \mathbb{N}$, $\mathcal{H}^s$ is the $s$-order Sobolev space

$$\mathcal{H}^s := \left\{ f \in L^2(\mathcal{X}) : f \text{ is } s\text{-times weakly differentiable with } f^{(s)} \in L^2(\mathcal{X}) \right\},$$ 

endowed with the semi-inner product of the form

$$\langle p, q \rangle_{\mathcal{H}^s} := \left\langle \left( p^{(s)}, q^{(s)} \right) \right\rangle_{L^2(\mathcal{X})} = \sum_{z \in \mathbb{Z}} |z|^{2s} \bar{f}_z \bar{g}_z \quad (6)$$

where the last equality follows from Parseval’s identity. Indeed, (6) is commonly used to generalize $\langle f, g \rangle_{\mathcal{H}^s}$, for example, to non-integer values of $s$. Thus, setting $a_z = |z|^{-s}$, $\mathcal{H}_a$ contains any distributions $P, Q \in \mathcal{P}$ with densities $p, q \in \mathcal{H}^s$, and, moreover, we have $\langle P, Q \rangle_a = \langle p, q \rangle_{\mathcal{H}^s}$. Note that, when $s \geq D/2$, one can show via Bochner’s theorem that $\mathcal{H}^s$ is in fact also an RKHS, with symmetric, translation-invariant kernel defined as above by $\kappa(x) = \sum_{z \in \mathbb{Z}} z^{-s} \psi_z$.

Paper Organization

The remainder of this paper is organized as follows: In Section 2, we provide notation needed to formally state our estimation problem, given in Section 3. Section 4 reviews related work on estimation of functionals of probability densities, as well as some applications of this work. Sections 5 and 6 present our main theoretical results, with upper
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bounds in Sections 5 and minimax lower bounds in Section 6; proofs of all results are given in Appendix 9. Section 7 expands upon these general results in a number of important special cases. Finally, we conclude in Section 8 with a discussion of broader consequences and avenues for future work.

2. Notation

We assume the sample space $\mathcal{X} \subseteq \mathbb{R}^D$ is a compact subset of $\mathbb{R}^D$, and we use $\mu$ to denote the usual Lebesgue measure on $\mathcal{X}$. We use $\{\psi_z\}_{z \in \mathbb{Z}^D}$ to denote the standard orthonormal Fourier basis of $L_2(\mathcal{X})$, indexed by $D$-tuples of integer frequencies $z \in \mathbb{Z}^D$. For any function $f \in L_2(\mathcal{X})$ and $z \in \mathbb{Z}^D$, we use

$$\tilde{f}_z := \int_{\mathcal{X}} f(x) \psi_z(x) \, d\mu(x)$$

to denote the $z^{th}$ Fourier coefficient of $f$ (i.e., the projection of $f$ onto $\psi_z$), and for any probability distribution $P \in \mathcal{P}$, we use the same notation

$$\phi_P(z) := \mathbb{E}_{X \sim P}[\psi_z(X)] = \int_{\mathcal{X}} \psi_z(x) \, dP(x)$$

to denote the characteristic function of $P$.

We will occasionally use the notation $\|z\|$ for indices $z \in \mathbb{Z}$. Due to equivalence of finite dimensional norms, the exact choice of norm affects only constant factors; for concreteness, one may take the Euclidean norm.

For certain applications, it is convenient to consider only a subset $Z \subseteq \mathbb{Z}^D$ of indices of interest (for example, Sobolev seminorms are indexed only over $Z = \{z \in \mathbb{Z}^D : z_1, ..., z_D \neq 0\}$). The subset $Z$ may be considered arbitrary but fixed in our work.

Given two $(0, \infty)$-valued sequences $a = \{a_z\}_{z \in Z}$ and $b = \{b_z\}_{z \in Z}$, we are interested in products of the form

$$\langle f, g \rangle_a := \sum_{z \in Z} \tilde{f}_z \overline{g}_z a_z^2,$$

and their induced (semi)norms $\|f\|_a = \sqrt{\langle f, f \rangle_a}$ over spaces of the form $^5$

$$\mathcal{H}_a = \{ f \in L_2(\mathcal{X}) : \|f\|_a < \infty \}$$

(and similarly when replacing $a$ by $b$). Typically, we will have $a_z, b_z \to 0$ and $\frac{b_z}{a_z} \to 0$ whenever $\|z\| \to \infty$, implying the inclusion $\mathcal{H}_b \subseteq \mathcal{H}_a \subseteq L^2(\mathcal{X})$.

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4A more proper mathematical term for $a$ and $b$ would be net.

5Specifically, we are interested in probability densities, which lie in the simplex $\mathcal{P} := \{ f \in L_1(\mathcal{X}) : f \geq 0, \int_{\mathcal{X}} f \, d\mu = 1 \}$, so that we should write, e.g., $p, q \in \mathcal{H} \cap \mathcal{P}$. Henceforth, “density” refers to any function lying in $\mathcal{P}$.
3. Formal Problem Statement

Suppose we observe $n$ i.i.d. samples $X_1, \ldots, X_n \sim P$ and $n$ i.i.d. samples $Y_1, \ldots, Y_n \sim Q$, where $P$ and $Q$ are (unknown) distributions lying in the (known) space $\mathcal{H}_a$. We are interested in the problem of estimating the inner product (2), along with the closely related (squared) seminorm and pseudometric given by

$$\|P\|_a^2 := \langle P, P \rangle_a \quad \text{and} \quad \|P - Q\|_a^2 := \|P\|_a^2 + \|Q\|_a^2 - 2\langle P, Q \rangle_a.$$ (7)

We assume $P$ and $Q$ lie in a (known) smaller space $\mathcal{H}_b \subseteq \mathcal{H}_a$, and we are specifically interested in identifying, up to constant factors, the minimax mean squared (i.e., $L^2$) error $M(a, b)$ of estimating $\langle P, Q \rangle_a$ over $P$ and $Q$ lying in a unit ellipsoid with respect to $\| \cdot \|_b$; that is, the quantity

$$M(a, b) := \inf_{\hat{S}} \sup_{\|P\|_b, \|Q\|_b \leq 1} \mathbb{E}_{X_1, \ldots, X_n \sim P, Y_1, \ldots, Y_n \sim Q} \left[ \left| \hat{S} - \langle P, Q \rangle_a \right|^2 \right],$$ (8)

where the infimum is taken over all estimators (i.e., all functions $\hat{S} : \mathbb{R}^{2n} \to \mathbb{C}$ of the data $X_1, \ldots, X_n, Y_1, \ldots, Y_n$).

4. Related Work

This section reviews previous studies on special cases of the problem we study, as well as work on estimating related functionals of probability distributions, and a few potential applications of this work in statistics and machine learning.

4.1. Prior work on special cases

While there has been substantial work on estimating unweighted $L^2$ norms and distances of densities [Schweder, 1975, Anderson et al., 1994, Giné and Nickl, 2008], to the best of our knowledge, most work on the more general problem of estimating weighted inner products or norms has been on estimating Sobolev quantities (see Example 3 in Section 1) by Bickel and Ritov [1988], Donoho and Nussbaum [1990], and Singh et al. [2016]. Bickel and Ritov [1988] considered the case of integer-order Sobolev norms, which have the form

$$\|f\|_{H^s}^2 = \|f^{(s)}\|^2_{L^2(X)} = \int \left( f^{(s)}(x) \right)^2 dx,$$ (9)

for which they upper bounded the error of an estimator based on plugging a kernel density estimate into (9) and then applying an analytic bias correction. They also derived matching minimax lower bounds for this problem.\(^6\) Singh et al. [2016] proved rate-matching

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\(^6\)Bickel and Ritov [1988] actually make Hölder assumptions on their densities (essentially, an $L_\infty$ bound on the derivatives of the density), rather than our slightly milder Sobolev assumption (essentially, an $L_2$ bound on the derivative). However, as we note in Section 8, these assumptions are closely related such that the results are comparable up to constant factors.
upper bounds on the error of a much simpler inner product estimator (generalizing an estimator proposed by Donoho and Nussbaum [1990]), which applies for arbitrary \( s \in \mathbb{R} \). Our upper and lower bounds are strict generalizations of these results. Specifically, relative to this previous work on the Sobolev case, our work makes advances in three directions:

1. We consider estimating a broader class of inner product functionals \( \langle p, q \rangle_z \), for arbitrary sequences \( \{a_z\}_{z \in \mathbb{Z}} \). The Sobolev case corresponds to \( a_z = \|z\|^{-s} \) for some \( s > 0 \).
2. We consider a broader range of assumptions on the true data densities, of the form \( \|p\|_b, \|q\|_b < \infty \), for arbitrary sequences \( \{b_z\}_{z \in \mathbb{Z}} \). The Sobolev case corresponds to \( b_z = \|z\|^{-t} \) for some \( t > 0 \).
3. We prove lower bounds that match our upper bounds, thereby identifying minimax rates. For many cases, such as Gaussian or exponential RKHS inner products or densities, these results are the first concerning minimax rates, and, even in the Sobolev case, our lower bounds address some previously open cases (namely, non-integer \( s \) and \( t \), and \( D > 1 \)).

The closely related work of Fan [1991] also generalized the estimator of Donoho and Nussbaum [1990], and proved (both upper and lower) bounds on \( M(a, b) \) for somewhat more general sequences, and also considered norms with exponent \( p \neq 2 \) (i.e., norms not generated by an inner product, such as those underlying a broad class of Besov spaces). However, his analysis placed several restrictions on the rates of \( a \) and \( b \); for example, it requires

\[
\sup_{Z \subseteq \mathbb{Z}} \frac{|Z| \sup_{z \in \mathbb{Z}} a_z^{-2}}{\sum_{z \in \mathbb{Z}} a_z^{-2}} < \infty \quad \text{and} \quad \sup_{Z \subseteq \mathbb{Z}} \frac{|Z| \sup_{z \in \mathbb{Z}} b_z^{-2}}{\sum_{z \in \mathbb{Z}} b_z^{-2}} < \infty.
\]

This holds when \( a \) and \( b \) decay polynomially, but fails in many of the cases we consider, such as exponential decay. The estimation of norms with \( p \neq 2 \) and \( a \) and \( b \) decaying non-polynomially, therefore, remains an important unstudied case, which we leave for future work.

Finally, we note that, except Singh et al. [2016], all the above works have considered only \( D = 1 \) (i.e., when the sample space \( \mathcal{X} \subseteq \mathbb{R} \)), despite the fact that \( D \) can play an important role in the convergence rates of the estimators. The results in this paper hold for arbitrary \( D \geq 1 \).

### 4.2. Estimation of related functionals

There has been quite a large amount of recent work [Nguyen et al., 2010, Liu et al., 2012, Moon and Hero, 2014b, Singh and Póczos, 2014a,b, Krishnamurthy et al., 2014, Moon and Hero, 2014a, Krishnamurthy et al., 2015, Kandasany et al., 2015, Gao et al., 2015a,b, Mukherjee et al., 2015, 2016, Moon et al., 2016, Singh and Póczos, 2016, Berrett et al., 2016, Gao et al., 2017a,b, Jiao et al., 2017, Han et al., 2017, Noshad et al., 2017, Wisler et al., 2017, Singh and Póczos, 2017, Noshad and Hero III, 2018, Bulinski and Dimitrov, 2018]
on practical estimation of nonlinear integral functionals of probability densities, of the form
\[ F(p) = \int_X \phi(p(x)) \, dx, \tag{10} \]
where \( \phi : [0, \infty) \to \mathbb{R} \) is nonlinear but smooth. Whereas minimax optimal estimators have been long established, their computational complexity typically scales as poorly as \( O(n^3) \) [Birgé and Massart, 1995, Laurent et al., 1996, Kandasamy et al., 2015]. Hence, this recent work has focused on analyzing more computationally efficient (but less statistically efficient) estimators, as well as on estimating information-theoretic quantities such as variants of entropy, mutual information, and divergence, for which \( \phi \) can be locally non-smooth (e.g., \( \phi = \log \)), and can hence follow somewhat different minimax rates.

As discussed in detail by Laurent et al. [1996], under Sobolev smoothness assumptions on \( p \), estimation of quadratic functionals (such as those considered in this paper) is key to constructing minimax rate-optimal estimators for general functionals of the form (10). The reason for this is that minimax rate-optimal estimators of \( F(p) \) can often be constructed by approximating a second-order Taylor (a.k.a., von Mises [Kandasamy et al., 2015]) expansion of \( F \) around a density estimate \( \hat{p} \) of \( p \) that is itself minimax rate-optimal (with respect to integrated mean squared error). Informally, if we expand \( F(p) \) as
\[ F(p) = F(\hat{p}) + \langle \nabla F(\hat{p}), p - \hat{p} \rangle_{L^2} + \langle p - \hat{p}, (\nabla^2 F(\hat{p}))p - \hat{p} \rangle_{L^2} + O \left( \|p - q\|_{L^2}^3 \right), \tag{11} \]
where \( \nabla F(\hat{p}) \) and \( \nabla^2 F(\hat{p}) \) are the first and second order Frechet derivatives of \( F \) at \( \hat{p} \). In the expansion (11), the first term is a simple plug-in estimate, and the second term is linear in \( p \), and can therefore be estimated easily by an empirical mean. The remaining term is precisely a quadratic functional of the density, of the type we seek to estimate in this paper. Indeed, to the best of our knowledge, this is the approach taken by all estimators that are known to achieve minimax rates [Birgé and Massart, 1995, Laurent et al., 1996, Krishnamurthy et al., 2014, Kandasamy et al., 2015, Mukherjee et al., 2015, 2016] for general functionals of the form (10).

Interestingly, the estimators studied in the recent papers above are all based on either kernel density estimators [Singh and Póczos, 2014a,b, Krishnamurthy et al., 2014, 2015, Kandasamy et al., 2015, Moon et al., 2016, Mukherjee et al., 2015, 2016] or \( k \)-nearest neighbor methods [Moon and Hero, 2014a,b, Singh and Póczos, 2016, Berrett et al., 2016, Gao et al., 2017b]. This contrasts with our approach, which is more comparable to orthogonal series density estimation; given the relative efficiency of computing orthogonal series estimates (e.g., via the fast Fourier transform), it may be desirable to try to adapt our estimators to these classes of functionals.

When moving beyond Sobolev assumptions, only estimation of very specific functionals has been studied. For example, under RKHS assumptions, only estimation of maximum mean discrepancy (MMD) [Gretton et al., 2012, Ramdas et al., 2015, Tolstikhin et al., 2016], has received much attention. Hence, our work significantly expands our understanding of minimax functional estimation in this setting. More generally, our work begins to provide a framework for a unified understanding of functional estimation across different types of smoothness assumptions.
Along a different line, there has also been some work on estimating $L^p$ norms for regression functions, under similar Sobolev smoothness assumptions [Lepski et al., 1999]. However, the problem of norm estimation for regression functions turns out to have quite different statistical properties and requires significantly different estimators and analysis, compared to norm estimation for density functions. Generally, the problem for densities is statistically easier in terms of having a faster convergence rate under a comparable smoothness assumption; this is most obvious when $p = 1$, since the $L^1$ norm of a density is always 1, while the $L^1$ norm of a regression function is less trivial to estimate. However, this is true more generally as well. For example, Lepski et al. [1999] showed that, under $s$-order Sobolev assumptions, the minimax rate for estimating the $L^2$ norm of a 1-dimensional regression function (up to log factors) is $\asymp n^{-\frac{1}{2s+1}}$, whereas the corresponding rate for estimating the $L^2$ norm of a density function is $\asymp n^{-\min\{\frac{1}{2s+1},1\}}$, which is parametric when $s \geq 1/4$. To the best of our knowledge, there has been no work on the natural question of estimating Sobolev or other more general quadratic functionals of regression functions.

4.3. Applications

Finally, although this paper focuses on estimation of general inner products from the perspective of statistical theory, we mention a few of the many applications that motivate the study of this problem.

Estimates of quadratic functionals can be directly used for nonparametric goodness-of-fit, independence, and two-sample testing [Anderson et al., 1994, Dumbgen, 1998, Ingster and Suslina, 2012, Goria et al., 2005, Pardo, 2005, Chwialkowski et al., 2015]. They can also be used to construct confidence sets for a variety of nonparametric objects [Li, 1989, Baraud, 2004, Genovese and Wasserman, 2005], as well as for parameter estimation in semi-parametric models [Wolsztynski et al., 2005].

In machine learning, Sobolev-weighted distances can also be used in transfer learning [Du et al., 2017] and transduction learning [Quadrianto et al., 2009] to measure relatedness between source and target domains, helping to identify when transfer can benefit learning. Semi-inner products can be used as kernels over probability distributions, enabling generalization of a wide variety of statistical learning methods from finite-dimensional vectorial inputs to nonparametric distributional inputs [Sutherland, 2016]. This distributional learning approach has been applied to many diverse problems, including image classification [Póczos et al., 2011, Póczos et al., 2012], galaxy mass estimation [Ntampaka et al., 2015], ecological inference [Flaxman et al., 2015, 2016], aerosol prediction in climate science [Szabó et al., 2015], and causal inference [Lopez-Paz et al., 2015]. Finally, it has recently been shown that the losses minimized in certain implicit generative models can be approximated by Sobolev and related distances [Liang, 2017]. Further applications of these quantities can be found in [Principe, 2010].
5. Upper Bounds

In this section, we provide upper bounds on minimax risk. Specifically, we propose estimators for semi-inner products, semi-norms, and pseudo-metrics, and bound the risk of the semi-inner product estimator; identical bounds (up to constant factors) follow easily for semi-norms and pseudo-metrics.

5.1. Proposed Estimators

Our proposed estimator \( \hat{S}_Z \) of \( \langle P, Q \rangle_a \) consists of simply plugging estimates of \( \phi_P \) and \( \tilde{Q} \) into a truncated version of the summation in Equation (2). Specifically, since

\[
\phi_P(z) = \mathbb{E}_{X \sim P} \left[ \psi_z(X) \right],
\]

we estimate each \( \phi_P(z) \) by \( \hat{\phi}_P(z) := \frac{1}{n} \sum_{i=1}^{n} \psi_z(X_i) \) and each \( \phi_Q(z) \) by \( \hat{\phi}_Q(z) := \frac{1}{n} \sum_{i=1}^{n} \psi_z(Y_i) \). Then, for some finite set \( Z \subseteq \mathbb{Z} \) (a tuning parameter to be chosen later) our estimator \( \hat{S}_Z \) for the product (2) is

\[
\hat{S}_Z := \sum_{z \in Z} \frac{\hat{\phi}_P(z) \hat{\phi}_Q(z)}{a_z^2}. \tag{12}
\]

To estimate the squared semi-norm \( \|P\|_a^2 \) from a single sample \( X_1, \ldots, X_n \overset{i.i.d.}{\sim} P \), we use

\[
\hat{N}_Z := \sum_{z \in Z} \frac{\hat{\phi}_P(z) \hat{\phi}_P(z)'}{a_z^2}. \tag{13}
\]

where \( \hat{\phi}_P(z) \) is estimated using the first half \( X_1, \ldots, X_{[n/2]} \) of the sample, \( \hat{\phi}_P(z)' \) is estimated using the second half \( X_{[n/2]+1}, \ldots, X_n \) of the sample. While it is not clear that sample splitting is optimal in practice, it allows us to directly apply convergence results for the semi-inner product, which assume the samples from the two densities are independent.

To estimate the squared pseudo-metric \( \|P - Q\|_a^2 \) from two samples \( X_1, \ldots, X_n \overset{i.i.d.}{\sim} P \) and \( Y_1, \ldots, Y_n \overset{i.i.d.}{\sim} Q \), we combine the above inner product and norm estimators according to the formula (7), giving

\[
\hat{\rho}_Z = \hat{N}_Z + \hat{M}_Z - 2\hat{S}_Z,
\]

where \( \hat{M}_Z \) denotes the analogue of the norm estimator (13) applied to \( Y_1, \ldots, Y_n \).
5.2. Bounding the risk of $\hat{S}_Z$

Here, we state upper bounds on the bias, variance, and mean squared error of the semi-inner product estimator $\hat{S}_Z$, beginning with an easy bound on the bias of $\hat{S}_Z$ (proven in Appendix 9.1):

**Proposition 1** (Upper bound on bias of $\hat{S}_Z$). Suppose $P,Q \in H_b$. Then,

$$|\mathbb{E}[\hat{S}_Z]| \leq \|P\|_b \|Q\|_b \sup_{z \in Z \setminus Z} \frac{b_z^2}{a_z^2},$$

(14)

where $\mathbb{E}[\hat{S}_Z] := \mathbb{E}[\hat{S}_Z] - \langle P,Q \rangle_a$ denotes the bias of $\hat{S}_Z$.

Note that for the above bound to be non-trivial, we require $b_z \to 0$ faster than $a_z$ as $\|z\| \to \infty$ which ensures that $\sup_{z \in Z \setminus Z} \frac{b_z}{a_z} < \infty$. While (14) does not explicitly depend on the sample size $n$, in practice, the parameter set $Z$ will be chosen to grow with $n$, and hence the supremum over $Z \setminus Z$ will decrease monotonically with $n$. Next, we provide a bound on the variance of $\hat{S}_Z$, whose proof, given in Appendix 9.2, is more involved.

**Proposition 2** (Upper bound on variance of $\hat{S}_Z$). Suppose $P,Q \in H_b$. Then,

$$\mathbb{V}[\hat{S}_Z] \leq \frac{2\|P\|_2\|Q\|_2^2}{n^2} \sum_{z \in Z} \frac{1}{a_z^2} + \frac{\|P\|_b^2\|Q\|_b^2 + \|P\|_b^2\|Q\|_b^2}{n} R_{a,b,Z} + \frac{2\|P\|_a^2\|Q\|_a^2}{n},$$

(15)

where $\mathbb{V}$ denotes the variance operator and

$$R_{a,b,Z} := \left( \sum_{z \in Z} \frac{b_z^4}{a_z^4} \right)^{1/4} \left( \sum_{z \in Z} \left( \frac{b_z}{a_z^2} \right)^8 \right)^{1/8} \left( \sum_{z \in Z} b_z^8 \right)^{1/8}.$$  

(16)

Having bounded the bias and variance of the estimator $\hat{S}_Z$, we now turn to the mean squared error (MSE). Via the usual decomposition of MSE into (squared) bias and variance, Propositions 1 and 2 together immediately imply the following bound:

**Theorem 3** (Upper bound on MSE of $\hat{S}_Z$). Suppose $P,Q \in H_b$. Then,

$$\text{MSE} \left[ \hat{S}_Z \right] \leq \|P\|_2^2\|Q\|_2^2 \sup_{z \in Z \setminus Z} \frac{b_z^4}{a_z^4} + \frac{2\|P\|_2\|Q\|_2^2}{n^2} \sum_{z \in Z} \frac{1}{a_z^2}$$

$$+ \frac{\|Q\|_b^2\|P\|_b + \|P\|_b^2\|Q\|_b}{n} R_{a,b,Z} + \frac{2\|P\|_a^2\|Q\|_a^2}{n},$$

(17)

where $R_{a,b,Z}$ is as defined in (16).
Corollary 4 (Norm estimation). In the particular case of norm estimation (i.e., when $Q = P$), this simplifies to:

$$\text{MSE}\left(\hat{S}_Z\right) \leq \|P\|_b^4 \sup_{z \in Z \setminus Z} \frac{b_z^4}{a_z^2} + \frac{2\|P\|_b^2}{n^2} \sum_{z \in Z} \frac{1}{a_z^2} + \frac{2\|P\|_b^2}{n} R_{a,b,Z} + \frac{2\|P\|_b^4}{n}. \tag{18}$$

5.3. Discussion of Upper Bounds

Two things might stand out that distinguish the above variance bound from many other nonparametric variance bounds: First, the rate depends on the smoothness of $P, Q \in \mathcal{H}_b$. Smoothness assumptions in nonparametric statistics are usually needed only to bound the bias of estimators [Tsybakov, 2008]. The reason the smoothness appears in this variance bound is that the estimand in Equation (2) includes products of the Fourier coefficients of $P$ and $Q$. Hence, the estimates $\hat{\phi}_P(z)$ of $\phi_P(z)$ are scaled by $\hat{\phi}_Q(z)$, and vice versa, and as a result, the decay rates of $\phi_P(z)$ and $\phi_Q(z)$ affect the variance of the tails of $\hat{S}_Z$.

One consequence of this is that the convergence rates exhibit a phase transition, with a parametric convergence rate when the tails of $\phi_P$ and $\hat{Q}$ are sufficiently light, and a slower rate otherwise.

Second, the bounds are specific to the Fourier basis (as opposed to, say, any uniformly bounded basis, e.g., one with $\sup_{z \in Z, x \in X} |\psi_z(x)| \leq 1$). The reason for this is that, when expanded, the variance includes terms of the form $E_{X \sim P} |\phi_y(x)\psi_z(X)|$, for some $y \neq z \in Z$. In general, these covariance-like terms are difficult to bound tightly; for example, the uniform boundedness assumption above would only give a bound of the form $E_{X \sim P} |\phi_y(x)\psi_z(X)| \leq \min\{\phi_P(y), \phi_P(z)\}$. For the Fourier basis, however, the recurrence relation $\phi_y\psi_z = \phi_{y+z}$ allows us to bound $E_{X \sim P} |\phi_y(x)\psi_z(X)| = E_{X \sim P} |\phi_{y+z}(X)| = \phi_P(y+z)$ in terms of assumptions on the decay rates of the coefficients of $P$. It turns out that $\phi_P(y+z)$ decays significantly faster than $\min\{\phi_P(y), \phi_P(z)\}$, and this tighter bound is needed to prove optimal convergence rates.

More broadly, this suggests that convergence rates for estimating inner products in terms of weights in a particular basis may depend on algebraic properties of that basis. For example, another common basis, the Haar wavelet basis, satisfies a different recurrence relation: $\phi_y \psi_z \in \{0, \phi_y, \psi_z\}$, depending on whether (and how) the supports of $\phi_y$ and $\psi_z$ are nested or disjoint. We leave investigation of this and other bases for future work.

Clearly, $\sup_{z \in Z} R_{a,b,Z} < \infty$ if and only if $\sum_{z \in Z} b_z^4/a_z^8$ is summable (i.e., $\sum_{z \in Z} b_z^4/a_z^8 < \infty$). Thus, assuming $|Z| = \infty$, this already identifies the precise condition required for the minimax rate to be parametric. When it is the case that

$$\frac{R_{a,b,Z}}{n} \in O \left( \sup_{z \in Z \setminus Z} \frac{b_z^4}{a_z^2} + \frac{1}{n^2} \sum_{z \in Z} \frac{1}{a_z^2} \right),$$

the third term in (17) will be dominated by the first and third terms, and so the upper
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bound simplifies to order

\[ \text{MSE} \left[ \hat{S}_Z \right] \lesssim \frac{1}{n} + \min_{Z \subseteq \mathbb{Z}} \sup_{z \in \mathbb{Z} \setminus Z} \left[ \frac{b_z^4}{a_z^4} + \frac{1}{n^2} \sum_{z \in \mathbb{Z}} \frac{1}{a_z^4} \right]. \tag{19} \]

This happens for every choice of \( a_z \) and \( b_z \) we consider in this paper, including the Sobolev (polynomial decay) case and the RKHS case. However, simplifying the bound further requires some knowledge of the form of \( a \) and/or \( b \), and we develop this in several cases in Section 7. In Section 8, we also consider some heuristics for approximately simplifying (19) in certain settings.

6. Lower Bounds

In this section, we provide a lower bound on the minimax risk of the estimation problems described in Section 3. Specifically, we use a standard information theoretic framework to lower bound the minimax risk for semi-norm estimation; bounds of the same rate follow easily for inner products and pseudo-metrics. In a wide range of cases, our lower bound matches the MSE upper bound (Theorem 3) presented in the previous section.

**Theorem 5** (Lower Bound on Minimax MSE). Suppose \( \mathbf{X} \) has finite base measure \( \mu(\mathbf{X}) = 1 \) and suppose the basis \( \{ \psi_z \}_{z \in \mathbb{Z}} \) contains the constant function \( \phi_0 = 1 \) and is uniformly bounded (i.e., \( \sup_{z \in \mathbb{Z}} \| \psi_z \|_\infty < \infty \)). Define \( Z_{\zeta_n} := \{ z \in \mathbb{Z}^D : \| z \|_\infty \leq \zeta_n \}, A_{\zeta_n} := \sum_{z \in Z_{\zeta_n}} a_z^{-2} \) and \( B_{\zeta_n} := \sum_{z \in Z_{\zeta_n}} b_z^{-2} \). If \( B_{\zeta_n} \in \Omega \left( \zeta_n^2 D^2 n \right) \), then we have the minimax lower bound

\[
\inf_{\hat{S}} \sup_{\| h \|_b \leq 1} \mathbb{E} \left[ \left( \hat{S} - \| h \|_a^2 \right)^2 \right] \in \Omega \left( \max \left\{ \frac{A_{\zeta_n}^2}{B_{\zeta_n}^2}, n^{-1} \right\} \right),
\]

where \( \zeta_n \) is chosen to satisfy \( B_{\zeta_n}^2 \gg \zeta_n^D n^2 \). Also, if \( B_{\zeta_n} \in o \left( \zeta_n^2 D^2 n \right) \), then we have the (looser) minimax lower bound

\[
\inf_{\hat{S}} \sup_{\| h \|_b \leq 1} \mathbb{E} \left[ \left( \hat{S} - \| h \|_a^2 \right)^2 \right] \in \Omega \left( \max \left\{ \frac{A_{\zeta_n}^2 n^{2D}}{n^{D/2}}, n^{-1} \right\} \right).
\]

**Remark 6.** The uniform boundedness assumption permits the Fourier basis, our main case of interest, but also allows other bases (see, e.g., the “generalized Fourier bases” used in Corollary 2.2 of Liang [2017]).

**Remark 7.** The condition that \( B_{\zeta_n} \in \Omega \left( \zeta_n^2 D^2 \right) \) is needed to ensure that the “worst-case” densities we construct in the proof of Theorem 5 are indeed valid probability densities (specifically, that they are non-negative). Hence, this condition would no longer be necessary if we proved results in the simpler Gaussian sequence model, as in many
previous works on this problem (e.g., [Cai, 1999, Cai et al., 2005]). However, when $B_{\zeta_n} \in o(\zeta_n^{2D})$, density estimation, and hence the related problem of norm estimation, become asymptotically easier than the analogous problems under the Gaussian sequence model.

Remark 8. Intuitively, the ratio $A_{\zeta_n}/B_{\zeta_n}$ measures the relative strengths of the norms $\| \cdot \|_a$ and $\| \cdot \|_b$. As expected, consistent estimation is possible if and only if $\| \cdot \|_b$ is a stronger norm than $\| \cdot \|_a$.

7. Special Cases

In this section, we develop our lower and upper results for several special cases of interest. The results of this section are summarized in Table 1.

Notation: Here, for simplicity, we assume that the estimator $\hat{S}_Z$ uses a choice of $Z$ that is symmetric across dimensions; in particular, $Z = \prod_{j=1}^D \{\phi_{-\zeta_n}, \ldots, \phi_0, \ldots, \phi_{\zeta_n}\}$ (for some $\zeta_n \in \mathbb{N}$ depending on $n$) is the Cartesian product of $D$ sets of the first $2\zeta_n + 1$ integers. Throughout this section, we use $\lesssim$ and $\gtrsim$ to denote inequality up to log $n$ factors. Although we do not explicitly discuss estimation of $L_2$ norms, it appears as a special case of the Sobolev case with $s = 0$.

7.1. Sobolev

For some $s, t \geq 0$, $a_z = \|z\|^{-s}$ and $b_z = \|z\|^{-t}$.

Upper Bound: By Proposition 1, $\mathbb{E}[\hat{S}_Z] \lesssim \zeta_n^{2(s-t)}$, and, by Proposition 2,

$$\mathbb{V}[\hat{S}_Z] \lesssim \frac{\zeta_n^{4s+D}}{n^2} + \frac{\zeta_n^{4s-3t+D/2}}{n} + \frac{1}{n}.$$ 

Thus,

$$\text{MSE}[\hat{S}_Z] \lesssim \frac{\zeta_n^{4s+D}}{n^2} + \frac{\zeta_n^{4s-3t+D/2}}{n} + \frac{1}{n}.$$

One can check that $\zeta_n^{4s-t} + \frac{\zeta_n^{4s+D}}{n^2}$ is minimized when $\zeta_n \asymp n^{\frac{s}{s-t}}$, and that, for this choice of $\zeta_n$, the $\frac{\zeta_n^{4s-3t+D/2}}{n}$ term is of lower order, giving the convergence rate

$$\text{MSE}[\hat{S}_Z] \asymp n^{\frac{s(4s-t)}{4s-t+D}}.$$ 

Lower Bound: Note that $A_{\zeta_n} \asymp \zeta_n^{2s+D}$ and $B_{\zeta_n} \asymp \zeta_n^{2t+D}$. Solving $B_{\zeta_n}^2 = \zeta_n^{D} n^2$ gives $\zeta_n \asymp n^{\frac{D}{4s-t+D}}$. Thus, Theorem 5 gives a minimax lower bound of

$$\inf_{\hat{S}} \sup_{\|p\|_a, \|q\|_b \leq 1} \mathbb{E} \left[ \left( \hat{S} - \langle p, q \rangle_b \right)^2 \right] \gtrsim \frac{A_{\zeta_n}^2}{B_{\zeta_n}^2} = \zeta_n^{4(s-t)} = n^{\frac{4s-t}{4s-t+D}},$$

matching the upper bound. Note that the rate is parametric ($\asymp n^{-1}$) when $t \geq 2s + D/4$, and slower otherwise.
7.2. Gaussian RKHS

For some $t \geq s \geq 0$, $a_z = e^{-s\|z\|^2}$ and $b_z = e^{-t\|z\|^2}$.

**Upper Bound:** By Proposition 1, $\mathbb{E}[\tilde{S}_Z] \lesssim e^{2(s-t)\zeta_n^2}$. If we use the upper bound

$$\sum_{z \in Z} e^{\theta \|z\|^2} \leq C_\theta \zeta_n^D e^{\theta \zeta_n^2},$$

for any $\theta > 0$ and some $C_\theta > 0$, then Proposition 2 gives

$$\mathbb{V}[\tilde{S}_Z] = \frac{\zeta_n^{4s^2} e^{2s^2}}{n^2} + \frac{\zeta_n^{89D/20} e^{(4s-3t)\zeta_n^2}}{n} + \frac{1}{n}.$$

Thus,

$$\text{MSE}[\tilde{S}_Z] \lesssim e^{4(s-t)\zeta_n^2} + \frac{\zeta_n^{89D/20} e^{(4s-3t)\zeta_n^2}}{n} + \frac{1}{n}.$$

One can check that $e^{4(s-t)\zeta_n^2} + \frac{\zeta_n^{89D/20} e^{(4s-3t)\zeta_n^2}}{n}$ is minimized when $\zeta_n \approx \sqrt{\frac{\log n}{2t}}$, and that, for this choice of $\zeta_n$, the $\zeta_n^{89D/20} e^{(4s-3t)\zeta_n^2}$ term is of lower order, giving an MSE convergence rate of

$$\text{MSE}[\tilde{S}_Z] \lesssim n^{2(\frac{s-t}{t})} = n^{2(s/t-1)}.$$

**Lower Bound:** Again, we use the bound

$$A_{\zeta_n} = \sum_{z \in Z_{\zeta_n}} e^{2s\|z\|^2} \lesssim \zeta_n^{D} e^{2s\zeta_n^2},$$

as well as the trivial lower bound $B_{\zeta_n} = \sum_{z \in Z_{\zeta_n}} e^{2s\|z\|^2} \geq e^{2s\zeta_n^2}$. Solving $B_{\zeta_n} = \zeta_n^{D} n^2$ gives $\zeta_n \approx \sqrt{\frac{\log n}{2t}}$ up to log log $n$ factors. Thus, ignoring log $n$ factors, Theorem 5 gives a minimax lower bound of

$$\inf_{\hat{S}} \sup_{\|p\|_b, \|q\|_b \leq 1} \mathbb{E} \left[ \left( \hat{S} - \langle p, q \rangle_b \right)^2 \right] \gtrsim n^{\frac{2(s-t)}{t}},$$

for some $C > 0$, matching the upper bound rate. Note that the rate is parametric when $t \geq 2s$, and slower otherwise.

7.3. Exponential RKHS

For some $t \geq s \geq 0$, $a_z = e^{-s\|z\|^2}$ and $b_z = e^{-t\|z\|^2}$.

**Upper Bound:** By Proposition 1, $\mathbb{E}[\tilde{S}_Z] \lesssim e^{2(s-t)\zeta_n}$. Since, for fixed $D$,

$$\sum_{z \in Z} e^{r\|z\|^2} \approx e^{r\zeta_n+D} \gtrsim e^{r\zeta_n},$$

we have

$$\mathbb{V}[\tilde{S}_Z] = \frac{\zeta_n^{4s^2} e^{2s^2}}{n^2} + \frac{\zeta_n^{89D/20} e^{(4s-3t)\zeta_n^2}}{n} + \frac{1}{n}.$$
by Proposition 2, we have
\[ \mathbb{V} [\hat{S}_Z] \propto \frac{e^{4s\zeta_n}}{n^2} + \frac{e^{4s-3t}\zeta_n}{n} + \frac{1}{n}, \]
giving a mean squared error bound of
\[ \text{MSE} [\hat{S}_Z] \propto \frac{e^{4(s-t)\zeta_n}}{n^2} + \frac{e^{4s-3t}\zeta_n}{n} + \frac{1}{n}. \]
One can check that \( e^{4(s-t)\zeta_n} \) is minimized when \( \zeta_n = \frac{\log n}{2t} \), and that, for this choice of \( \zeta_n \), the \( t = \frac{4s-t\zeta_n}{n} \) term is of lower order, giving an MSE convergence rate of
\[ \text{MSE} [\hat{S}_Z] \lesssim n^{2(s-t)-1} = n^{2(s/t-1)}. \]

**Lower Bound:** Note that \( A_{\zeta_n} \approx e^{2s\zeta_n} \) and \( B_{\zeta_n} = e^{2t\zeta_n} \). Solving \( B_{\zeta_n} = \zeta_n D n^2 \) gives, up to \( \log \log n \) factors, \( \zeta_n \approx \frac{\log n}{2t} \). Thus, Theorem 5 gives a minimax lower bound of
\[ \inf_S \sup_{\|p\|,\|q\| \leq 1} \mathbb{E} \left[ \left( \hat{S} - \langle p, q \rangle b \right)^2 \right] \gtrsim n^{2(s-t)}, \]
for some \( C > 0 \), matching the upper bound rate. Note that the rate is parametric when \( t \geq 2s \), and slower otherwise.

### 7.4. Logarithmic decay

For some \( t \geq s \geq 0 \), \( a_z = (\log \|z\|)^{-s} \) and \( b_z = (\log \|z\|)^{-t} \). Note that, since our lower bound requires \( B_{\zeta_n} \in \Omega(\zeta_n D) \), we will only study the upper bound for this case.

**Upper Bound:** By Proposition 1, \( \mathbb{E} [\hat{S}_Z] \lesssim (\log \zeta_n)^{2(s-t)} \). By the upper bound
\[ \sum_{z \in \mathbb{Z}_n} (\log \|z\|)^\theta \leq C_\theta \zeta_n D (\log \zeta_n)^\theta, \]
for any \( \theta > 0 \) and some \( C_\theta > 0 \), Proposition 2 gives
\[ \mathbb{V} [\hat{S}_Z] = \frac{\zeta_n^D (\log \zeta_n)^{4s}}{n^2} + \frac{\zeta_n^{89D/20} (\log \zeta_n)^{4s-3t}}{n} + \frac{1}{n}, \]
giving a mean squared error bound of
\[ \text{MSE} [\hat{S}_Z] \lesssim (\log \zeta_n)^{4(s-t)} + \frac{\zeta_n^D (\log \zeta_n)^{4s}}{n^2} + \frac{\zeta_n^{89D/20} (\log \zeta_n)^{4s-3t}}{n} + \frac{1}{n}. \]
One can check that \( (\log \zeta_n)^{4(s-t)} + \frac{\zeta_n^{89D/20} (\log \zeta_n)^{4s-3t}}{n} \) is minimized when \( \zeta_n^{89D/20} (\log \zeta_n)^{4t+D} \approx n \), and one can check that, for this choice of \( \zeta_n \), the \( \frac{\zeta_n^D (\log \zeta_n)^{4s}}{n^2} \) term is of lower order.

Thus, up to \( \log n \) factors, \( \zeta_n \approx n^{2/D} \), and so, up to \( \log \log n \) factors,
\[ (\log \zeta_n)^{4(s-t)} \approx (\log n)^{4(s-t)}. \]
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\[ b_z = \log^{-s} \|z\| \leq (\log n)^{4(s-1)} \max \left\{ n^{-1}, n^{\frac{4(s-1)}{n+2}} \right\} \]

\[ a_z = \|z\|^{-s} \leq n^{-1} \]

\[ a_z = e^{-s\|z\|} \leq n^{-1} \]

\[ a_z = e^{-s\|z\|} \leq n^{-1} \]

\[ a_z = e^{-s\|z\|} \leq n^{-1} \]

Table 1. Minimax convergence rates for different combinations of \(a_z\) and \(b_z\). Results are given up to \(\log n\) factors, except the case when both \(a_z\) and \(b_z\) are logarithmic, which is given up to \(\log \log n\) factors. Note that, in this last case, only the upper bound is known. A value of \(\infty\) indicates that the estimand itself may be \(\infty\) and consistent estimation is impossible.

7.5. Sinc RKHS

For any \(s \in (0, \infty)^D\), the sinc kernel, defined by

\[ K_{\text{sinc}}^s(x, y) = \frac{\prod_{j=1}^d s_j^s \sin \left( \frac{x_j - y_j}{s_j} \right)}{\pi}, \]

where

\[ \sin(x) = \begin{cases} \frac{\sin(x)}{x} & \text{if } x \neq 0 \\ 1 & \text{else} \end{cases}, \]

generates the RKHS \( \mathcal{H}_{\text{sinc}}^s = \{ f \in L^2 : \|f\|_{K_{\text{sinc}}^s} < \infty \} \), of band-limited functions, where the norm is generated by the inner product \( \langle f, g \rangle_{K_{\text{sinc}}^s} = \langle f, g \rangle_\alpha \), where \( a_z = 1_{\{\|z\| \leq s\}} \) (with the convention that \( \frac{n}{n} = 0 \)). If we assume that \( p \in \mathcal{H}_{\text{sinc}}^t \), where \( t \leq s \), then fixing \( Z := \{ z \in \mathbb{Z}^D : \|z\| \leq s \} \), by Proposition 1, \( \mathbb{E}[\hat{S}_Z] = 0 \), and, by Proposition 2, one can easily check that \( \mathbb{V} [\hat{S}_Z] \leq n^{-1} \). Thus, without any assumptions on \( P \), we can always estimate \( \|P\|_{K_{\text{sinc}}^s} \) at the parametric rate.

8. Discussion

In this paper, we focused on the case of inner product weights and density coefficients in the Fourier basis, which play well-understood roles in widely used spaces such as Sobolev spaces and reproducing kernel Hilbert spaces with translation-invariant kernels.

For nearly all choices of weights \( \{a_z\}_{z \in \mathcal{Z}} \) and \( \{b_z\}_{z \in \mathcal{Z}} \), ignoring the parametric \( 1/n \) term that appears in both the upper and lower bounds, the upper bound boils down to

\[ \min_{\kappa_n \in \mathbb{N}} \frac{b_{2,\kappa_n}^4}{a_{2,\kappa_n}^4} + \frac{\sum_{z \in \mathcal{Z}_{\kappa_n}} a_z^{-4}}{n^2}, \]

or, equivalently,

\[ \frac{b_{2,\kappa_n}^4}{a_{2,\kappa_n}^4} \quad \text{where} \quad \frac{b_{\kappa_n}^4}{a_{\kappa_n}^4} = \frac{\sum_{z \in \mathcal{Z}_{\kappa_n}} a_z^{-4}}{n^2} \]
and the lower bound boils down to

\[ \left( \frac{\sum_{z \in Z_{\xi_n}} a_{z}^{-2}}{\sum_{z \in Z_{\xi_n}} b_{z}^{-2}} \right)^2, \quad \text{where} \quad \left( \sum_{z \in Z_{\xi_n}} b_{z}^{-2} \right)^2 = \zeta_n^D n^2. \]

These rates match if

\[ \frac{a_{\xi_n}^{-4}}{b_{\xi_n}^{-4}} \leq \left( \frac{\sum_{z \in Z_{\xi_n}} a_{z}^{-2}}{\sum_{z \in Z_{\xi_n}} b_{z}^{-2}} \right)^2 \quad \text{and} \quad \frac{b_{\xi_n}^4 \left( \sum_{z \in Z_{\xi_n}} b_{z}^{-2} \right)^2}{a_{\xi_n}^4 \sum_{z \in Z_{\xi_n}} a_{z}^{-4}} \leq \zeta_n^D \]  

Furthermore, if the equations in (20) hold modulo logarithmic factors, then the upper and lower bounds match modulo logarithmic factors. This holds almost automatically if \( b_{z} \) decays exponentially or faster, since, then, \( \zeta_{n} \) grows logarithmically with \( n \). Noting that the lower bound requires \( B_{\xi_n} \in \Omega (\zeta_n^D) \), this also holds automatically if \( b_{z} = |z|^t \) with \( t \geq D/2 \).

Table 1 collects the derived minimax rates for various standard choices of \( a \) and \( b \). For entries below the diagonal, \( b_{z}/a_{z} \to \infty \) as \( ||z|| \to \infty \), and so \( \mathcal{H}_b \not\subseteq \mathcal{H}_a \). As a result, consistent estimation is not possible in the worst case. The diagonal entries of Table 1, for which \( a \) and \( b \) have the same form, are derived in Section 7 directly from our upper and lower bounds on \( M(a,b) \). These cases exhibit a phase transition, with convergence rates depending on the parameters \( s \) and \( t \). When \( t \) is sufficiently larger than \( s \), the variance is dominated by the low-order terms of the estimand (2), giving a convergence rate of \( \asymp n^{-1} \). Otherwise, the variance is dominated by the tail terms of (2), in which case minimax rates depend smoothly on \( s \) and \( t \). This manifests in the \( \max \{ n^{-1}, n^{R(s,t)} \} \) form of the minimax rates, where \( R \) is non-decreasing in \( s \) and non-increasing in \( t \).

Notably, the data dimension \( D \) plays a direct role in the minimax rate only in the Sobolev case when \( t < 2s + D/4 \). Otherwise, the role of \( D \) is captured entirely within the assumption that \( p,q \in \mathcal{H}_b \). This is consistent with known rates for estimating other functionals of densities under strong smoothness assumptions such as the RKHS assumption [Gretton et al., 2012, Ramdas et al., 2015].

Finally, we note some consequences for more general (non-Hilbert) Sobolev spaces \( W^{s,p} \), defined for \( s \geq 0, p \geq 1 \) as the set of functions in \( \mathcal{L}^p \) having weak \( s \text{th} \) derivatives in \( \mathcal{L}^p \). The most prominent example is that of the Hölder spaces \( W^{s,\infty} \) of essentially bounded functions having essentially bounded \( s \text{th} \) weak derivatives; Hölder spaces are used widely in nonparametric statistics [Bickel and Ritov, 1988, Tsybakov, 2008]. Recall that, for \( p \leq q \) and any \( s \geq 0 \), these spaces satisfy the embedding \( W^{s,q} \subseteq W^{s,p} \) [Villani, 1985], and that \( W^{s,2} = \mathcal{H}^s \). Then, for \( P,Q \in W^{s,p} \), our upper bound in Theorem 3 implies an identical upper bound when \( p \geq 2 \), and our lower bound in Theorem 5 implies an identical lower bound when \( p \leq 2 \).

Further work is needed to verify tightness of these bounds for \( p \neq 2 \). Moreover, while this paper focused on the Fourier basis, it is also interesting to consider other bases, which may be informative in other spaces. For example, wavelet bases are more natural representations in a wide range of Besov spaces [Donoho and Johnstone, 1995]. It is also
of interest to consider non-quadratic functionals as well as non-quadratic function classes. In these cases simple quadratic estimators such as those considered here may not achieve the minimax rate, but it may be possible to correct this with simple procedures such as thresholding, as done, for example, by Cai et al. [2005] in the case of $\mathcal{L}_p$ balls with $p < 2$. Finally, the estimators considered here require some knowledge of the function class in which the true density lies. It is currently unclear whether and how the various strategies for designing adaptive estimators, such as block-thresholding [Cai, 1999] or Lepski’s method [Lepski and Spokoiny, 1997], which have been applied to estimate quadratic functionals over $\mathcal{L}_p$ balls and Besov spaces [Efroimovich et al., 1996, Cai et al., 2006], may confer adaptivity when estimating functionals over general quadratically weighted spaces.
9. Proofs

In this section, we present the proofs of main results.

9.1. Proof of Proposition 1

We first bound the bias \(|\mathbb{E} \left[ \hat{S}_Z \right] - \langle P, Q \rangle_a|\), where randomness is over the data \(X_1, \ldots, X_n \text{ i.i.d.}\) \(P\), and \(Y_1, \ldots, Y_n \text{ i.i.d.} \sim Q\). Since 
\[
\hat{S}_Z = \sum_{z \in Z} \frac{\hat{\phi}_P(z) \hat{\phi}_Q(z)}{a_z^2},
\]
is bilinear in \(\hat{P}\) and \(\hat{Q}\), which are independent, and 
\[
\hat{\phi}_P(z) = \frac{1}{n} \sum_{i=1}^{n} \psi(z)(X_i) \quad \text{and} \quad \hat{\phi}_Q(z) = \frac{1}{n} \sum_{i=1}^{n} \psi(z)(Y_i)
\]
are unbiased estimators of \(\phi_P(z) = \mathbb{E}_{X \sim P} \left[ \psi(z)(X) \right]\) and \(\phi_Q(z) = \mathbb{E}_{Y \sim Q} \left[ \psi(z)(Y) \right]\), respectively, we have that 
\[
\mathbb{E} \left[ \hat{S}_Z \right] = \sum_{z \in Z} \frac{\mathbb{E} \left[ \hat{\phi}_P(z) \right] \mathbb{E} \left[ \hat{\phi}_Q(z) \right]}{a_z^2} = \sum_{z \in Z} \frac{\phi_P(z) \phi_Q(z)}{a_z^2}.
\]

Hence, the bias is 
\[
\mathbb{E} \left[ \hat{S}_Z \right] - \langle P, Q \rangle_a = \sum_{z \in Z \setminus Z} \frac{\phi_P(z) \phi_Q(z)}{a_z^2}.
\]

If \(p, q \in \mathcal{H}_b \subset \mathcal{H}_a \subseteq L^2\) defined by 
\[
\mathcal{H}_b := \left\{ f \in L^2 : \|f\|_b := \sum_{z \in Z} \frac{f(z)^2}{b_z} < \infty \right\},
\]
then, applying Cauchy-Schwarz followed by Hölder’s inequality, we have 
\[
\mathbb{E} \left[ \hat{S}_Z \right] - \langle P, Q \rangle_a = \sum_{z \in Z \setminus Z} \frac{\phi_P(z) \phi_Q(z)}{a_z^2} \leq \sqrt{\sum_{z \in Z \setminus Z} \frac{\phi_P(z)^2}{a_z^2} \sum_{z \in Z \setminus Z} \frac{\phi_Q(z)^2}{a_z^2}} = \sqrt{\sum_{z \in Z \setminus Z} \frac{b_z^2 \phi_P(z)^2}{a_z^2} \sum_{z \in Z \setminus Z} \frac{b_z^2 \phi_Q(z)^2}{b_z^2} \leq \|P\|_b \|Q\|_b \sup_{z \in Z \setminus Z} \frac{b_z^2}{a_z^2}}.
\]
Note that this recovers the bias bound of Singh et al. [2016] in the Sobolev case: If \( a_z = z^{-s} \) and \( b_z = z^{-t} \) with \( t \geq s \), then

\[
\left| \mathbb{E} \left[ \hat{S}_Z \right] - \langle P, Q \rangle_a \right| \leq \|P\|_b \|Q\|_b |Z|^{2(s-t)},
\]

where \(|Z|\) denotes the cardinality of the index set \( Z \).

9.2. Proof of Proposition 2

In this section, we bound the variance of \( \mathbb{V}[S_Z] \), where, again, randomness is over the data \( X_1, ..., X_n, Y_1, ..., Y_n \). The setup and first several steps of our proof are quite general, applying to arbitrary bases. However, without additional assumptions, our approach eventually hits a roadblock. Thus, to help motivate our assumptions and proof approach, we begin by explaining this general setup in Section 9.2.1, and then proceed with steps specific to the Fourier basis in Section 9.2.2.

9.2.1. General Proof Setup

Our bound is based on the Efron-Stein inequality [Efron and Stein, 1981]. For this, suppose that we draw extra independent samples \( X'_1 \sim p \) and \( Y'_1 \sim q \), and let \( \hat{S}'_Z \) and \( \hat{S}''_Z \) denote the estimator given in Equation (12) when we replace \( X_1 \) with \( X'_1 \) and when we replace \( Y_1 \) with \( Y'_1 \), respectively, that is

\[
\hat{S}'_Z := \sum_{z \in Z} \frac{\hat{\phi}_P(z') \hat{\phi}_Q(z)}{a_j^2} \quad \text{and} \quad \hat{S}''_Z := \sum_{z \in Z} \frac{\hat{\phi}_P(z) \hat{\phi}_Q(z)'}{a_j^2},
\]

where

\[
\hat{\phi}_P(z') := \frac{1}{n} \left( \psi_z(X'_1) + \sum_{i=2}^n \psi_z(X_i) \right), \quad \text{and} \quad \hat{\phi}_Q(z') := \frac{1}{n} \left( \psi_z(Y'_1) + \sum_{i=2}^n \psi_z(Y'_i) \right).
\]

Then, since \( X_1, ..., X_n \) and \( Y_1, ..., Y_n \) are each i.i.d., the Efron-Stein inequality [Efron and Stein, 1981] gives

\[
\mathbb{V} \left[ \hat{S}_Z \right] \leq \frac{n}{2} \left( \mathbb{E} \left[ \left| \hat{S}_Z - \hat{S}'_Z \right|^2 \right] + \mathbb{E} \left[ \left| \hat{S}_Z - \hat{S}''_Z \right|^2 \right] \right). \tag{21}
\]

We now study just the first term as the analysis of the second is essentially identical. Expanding the definitions of \( \hat{S}_Z \) and \( \hat{S}'_Z \), and leveraging the fact that all terms in \( \hat{\phi}_P(z) - \)
\( \hat{\phi}_P(z)' \) not containing \( X_1 \) or \( X'_1 \) cancel,

\[
\mathbb{E} \left[ \left( \tilde{S}_Z - \tilde{S}_Z' \right)^2 \right] = \mathbb{E} \left[ \sum_{z \in Z} \left( \frac{\left( \hat{\phi}_P(z) - \hat{\phi}_P(z)' \right) \phi_Q(z)}{a_z^2} \right)^2 \right]
\]

\[
= \mathbb{E} \left[ \sum_{z \in Z} \left( \frac{\left( \hat{\phi}_P(z) - \hat{\phi}_P(z)' \right) \phi_Q(z)}{a_z^2} \right) \left( \frac{\left( \hat{P}_w - \hat{P}_w' \right) \hat{Q}_w}{a_w^2} \right) \right]
\]

\[
= \frac{1}{n^2} \sum_{z \in Z} \sum_{w \in Z} \mathbb{E} \left[ \hat{Q}_w \phi_Q(z) \left( \phi_w(X_1) - \phi_w(X'_1) \right) \left( \phi_w(X_1) - \phi_w(X'_1) \right) \right]
\]

\[
= \frac{1}{n^2} \sum_{z \in Z} \sum_{w \in Z} \mathbb{E} \left[ \phi_Q(z) \hat{Q}_w \right] \mathbb{E} \left[ \left( \phi_w(X_1) - \phi_w(X'_1) \right) \left( \phi_w(X_1) - \phi_w(X'_1) \right) \right]
\]

\[
= \frac{2}{n^2} \sum_{z \in Z} \sum_{w \in Z} \mathbb{E} \left[ \phi_Q(z) \hat{Q}_w \right] \mathbb{E} \left[ \phi_w(X) \hat{Q}_w \right]
\]

Expanding the \( \mathbb{E} \left[ \phi_Q(z) \hat{Q}_w \right] \) term, we have

\[
\mathbb{E} \left[ \phi_Q(z) \hat{Q}_w \right] = \frac{1}{n^2} \sum_{i=1}^{n} \mathbb{E} \left[ \psi_z(Y_i) \phi_w(Y_j) \right]
\]

\[
= \frac{1}{n^2} \sum_{i=1}^{n} \mathbb{E} \left[ \psi_z(Y_i) \phi_w(Y_i) \right] + \frac{1}{n^2} \sum_{i=1}^{n} \mathbb{E} \left[ \psi_z(Y_i) \right] \mathbb{E} \left[ \phi_w(Y_i) \right]
\]

\[
= \frac{1}{n} \mathbb{E} \left[ \psi_z(Y) \phi_w(Y) \right] + \frac{n-1}{n} \phi_Q(z) \hat{Q}_w,
\]

which combined with Equation (22) yields

\[
\mathbb{E} \left[ \left( \tilde{S}_Z - \tilde{S}_Z' \right)^2 \right] = \frac{2}{n^3} \sum_{z \in Z} \sum_{w \in Z} \left( \mathbb{E} \left[ \psi_z(Y) \phi_w(Y) \right] + (n-1) \phi_Q(z) \hat{Q}_w \right)
\]

\[
\times \mathbb{E} \left[ \phi_w(X) \phi_w(X) - \phi_P(z) \hat{P}_w \right].
\](23)
thornormal basis, it is difficult to argue more than that, via Cauchy-Schwarz,
\[ \mathbb{E} \left[ \psi_z(X) \phi_w(X) \right] \leq \sqrt{\mathbb{E} \left[ |\psi_z(X)|^2 \right] \mathbb{E} \left[ |\phi_w(X)|^2 \right]}. \]

However, considering, for example, the very well-behaved case when \( P \) is the uniform density on \( \mathcal{X} \), we would have (since \( \{ \psi_z \}_{z \in \mathcal{Z}} \) is orthonormal) \( \mathbb{E} \left[ |\psi_z(X)|^2 \right] = \mathbb{E} \left[ |\phi_w(X)|^2 \right] = \frac{1}{\mu(\mathcal{X})} \), which does not decay as \( \|z\|, \|w\| \to \infty \). If we were to follow this approach, the Efron-Stein inequality would eventually give a variance bound on \( \hat{S}_Z \) that includes a term of the form
\[ \frac{(n-1)}{n^2 \mu(\mathcal{X})} \sum_{z,w \in \mathcal{Z}} \frac{\phi_Q(z)\phi_w}{a_z^2 a_w^2} = \frac{(n-1)}{n^2 \mu(\mathcal{X})} \left( \sum_{z \in \mathcal{Z}} \phi_Q(z) a_z^2 \right)^2 \leq \frac{1}{n \mu(\mathcal{X})} \|q\|^2 \sum_{z \in \mathcal{Z}} b_z^2. \]

While relatively general, this bound is loose, at least in the Fourier case. Hence, we proceed along tighter analysis that is specific to the Fourier basis.

9.2.2. Variance Bounds in the Fourier Basis
In the case that \( \{ \psi_z \}_{z \in \mathcal{Z}} \) is the Fourier basis, the identities \( \overline{\psi_z} = \phi_z \) and \( \psi_z \phi_w = \psi_{z+w} \) imply that \( \mathbb{E}[\psi_z(X)\phi_w(X)] = \hat{P}_{z-w} \) and \( \mathbb{E}[\phi_w(Y)\psi_z(Y)] = \hat{Q}_{z-w}, \) thus, the expression (23) simplifies to
\[ \mathbb{E} \left[ \hat{S}_Z - \hat{S}_Z \right] = \frac{2}{n^3 \mathcal{Z}} \sum_{z \in \mathcal{Z}} \sum_{w \in \mathcal{Z}} \left( \hat{Q}_{z-w} + (n-1)\hat{Q}_{z-w} - \hat{Q}_{z-w} \right) \frac{\hat{P}_{z-w} - \phi_P(z)\hat{P}_{z-w}}{a_z^2 a_w^2} \]
\[ = \frac{2}{n^3 \mathcal{Z}} \sum_{z \in \mathcal{Z}} \sum_{w \in \mathcal{Z}} \frac{\hat{Q}_{z-w} \hat{P}_{z-w} - \hat{Q}_{z-w} \phi_P(z)\hat{P}_{z-w} + (n-1)\hat{Q}_{z-w} \hat{P}_{z-w} - (n-1)\hat{Q}_{z-w} \phi_P(z)\hat{P}_{z-w}}{a_z^2 a_w^2}. \]

This contains four terms to bound, but they are dominated by the following three main terms:
\[ \frac{2}{n^3 \mathcal{Z}} \sum_{z \in \mathcal{Z}} \sum_{w \in \mathcal{Z}} \frac{\hat{Q}_{z-w} \hat{P}_{z-w}}{a_z^2 a_w^2}, \quad (24) \]
\[ \frac{2(n-1)}{n^3 \mathcal{Z}} \sum_{z \in \mathcal{Z}} \sum_{w \in \mathcal{Z}} \frac{\phi_Q(z)\hat{Q}_w \hat{P}_{z-w}}{a_z^2 a_w^2}, \quad (25) \]
and
\[ \frac{2(n-1)}{n^3 \mathcal{Z}} \sum_{z \in \mathcal{Z}} \sum_{w \in \mathcal{Z}} \frac{\phi_Q(z)\hat{Q}_w \phi_P(z)\hat{P}_{z-w}}{a_z^2 a_w^2}, \quad (26) \]

Bounding (24): Applying the change of variables \( k = z - w \) gives
\[ \left| \frac{2}{n^3} \sum_{z \in \mathcal{Z}} \sum_{w \in \mathcal{Z}} \frac{\hat{P}_{z-w} \hat{Q}_{z-w}}{a_z^2 a_w^2} \right| = \frac{2}{n^3} \sum_{k \in \mathcal{Z}} \left| \hat{P}_k \hat{Q}_{-k} \sum_{z \in \mathcal{Z}} \frac{1}{a_z^2 a_z^{-k}} \right| \leq \frac{2}{n^3} \sum_{k \in \mathcal{Z}} \left| \hat{P}_k \hat{Q}_{-k} \right| \sum_{z \in \mathcal{Z}} \frac{1}{a_z^2} \]
\[ \leq \frac{2}{n^3} \sum_{k \in \mathcal{Z}} \left| \hat{P}_k \hat{Q}_{-k} \right| \sum_{z \in \mathcal{Z}} \frac{1}{a_z^2} \leq \frac{2 \|P\|_2 \|Q\|_2}{n^3} \sum_{z \in \mathcal{Z}} \frac{1}{a_z^2}. \quad (27) \]
where in (*), we use the fact that
\[ f_Z(k) := \sum_{z \in \mathbb{Z}} \frac{1}{a_z^2 a_{z-k}^2} \]
is the convolution (over \( \mathbb{Z} \)) of \( \{a_z^{-2}\}_{z \in \mathbb{Z}} \) with itself, which is always maximized when \( k = 0 \).

**Bounding (25):** Applying Cauchy-Schwarz inequality twice, yields
\[
\left| \sum_{z \in \mathbb{Z}} \sum_{w \in \mathbb{Z}} \frac{\phi_Q(z)\tilde{Q}_w\tilde{P}_{z-w}}{a_z^2 a_w^2} \right| = \left| \sum_{z \in \mathbb{Z}} \frac{\phi_Q(z)}{b_z} \sum_{w \in \mathbb{Z}} \frac{b_w\tilde{Q}_w\tilde{P}_{z-w}}{a_z^2 a_w^2} \right|
\leq \|Q\|_b \left( \sum_{z \in \mathbb{Z}} \left( \sum_{w \in \mathbb{Z}} \frac{b_z\tilde{Q}_w\tilde{P}_{z-w}}{a_z^2 a_w^2} \right)^2 \right)^{1/2}
\leq \|Q\|_b \left( \sum_{z \in \mathbb{Z}} \frac{b_z^2}{a_z^4} \sum_{w \in \mathbb{Z}} \tilde{Q}_w\tilde{P}_{z-w} \right)^{1/2}
\leq \|Q\|_b \left( \sum_{z \in \mathbb{Z}} \frac{b_z^4}{a_z^8} \right)^{1/4} \left( \sum_{z \in \mathbb{Z}} \sum_{w \in \mathbb{Z}} \tilde{Q}_w\tilde{P}_{z-w} \right)^{1/4}. \tag{28}
\]

Note that now we can view the expression
\[
\left( \sum_{z \in \mathbb{Z}} \sum_{w \in \mathbb{Z}} \frac{\tilde{Q}_w\tilde{P}_{z-w}}{a_z^2 a_w^2} \right)^{4/4} = \left\| \frac{\tilde{Q}}{a^2} \ast \tilde{P} \right\|_4
\]
as the \( L_4 \) norm of the convolution between the sequence \( \tilde{Q}/a^2 \) and the sequence \( \tilde{P} \). To proceed, we apply (a discrete variant of) Young’s inequality for convolutions [Beckner, 1975], which states that, for constants \( \alpha, \beta, \gamma \geq 1 \) satisfying \( 1 + 1/\gamma = 1/\alpha + 1/\beta \) and arbitrary functions \( f \in L^\alpha(\mathbb{R}^D), g \in L^\beta(\mathbb{R}^D) \),
\[
\|f \ast g\|_\gamma \leq \|f\|_\alpha \|g\|_\beta.
\]

Applying Young’s inequality for convolutions with powers\(^7\) \( \alpha = \beta = 8/5 \) (so that \( \alpha, \beta \geq 1 \) and \( 1/\alpha + 1/\beta = 1 + 1/4 \)), gives
\[
\left( \sum_{z \in \mathbb{Z}} \sum_{w \in \mathbb{Z}} \frac{\tilde{Q}_w\tilde{P}_{z-w}}{a_z^2 a_w^2} \right)^{4} \leq \left( \sum_{z \in \mathbb{Z}} \frac{\phi_Q(z)^\alpha}{a_z^{2\alpha}} \right)^{1/\alpha} \left( \sum_{z \in \mathbb{Z}} \phi_P(z)^\beta \right)^{1/\beta}
= \left( \sum_{z \in \mathbb{Z}} \frac{\phi_Q(z)^\alpha b_z^2}{a_z^{2\alpha}} \right)^{1/\alpha} \left( \sum_{z \in \mathbb{Z}} \frac{\phi_P(z)^\beta b_z^\beta}{b_z^{2\beta}} \right)^{1/\beta}.
\]

\(^7\)This seemingly arbitrary choice of \( \alpha \) and \( \beta \) arises from analytically minimizing the final bound.
Since $2/\alpha = 2/\beta \geq 1$, we can now apply Hölder’s inequality to each of the above summations, with powers $(2/\alpha, 2\beta/(2-\alpha)) = (2/\beta, 2\beta - \beta) = (\frac{5}{4}, \frac{1}{8})$. This gives

$$\left( \sum_{z \in Z} \frac{\phi_Q(z)^{\alpha}}{b^2_z} \frac{b_z^\alpha}{a^2_z} \right)^{1/\alpha} \leq \|b\|_b \left( \sum_{z \in Z} \frac{b_z}{a^2_z} \right)^{\frac{2\alpha}{2-\alpha}} = \|b\|_b \left( \sum_{z \in Z} \left( \frac{b_z}{a^2_z} \right)^8 \right)^{1/8}$$

and

$$\left( \sum_{z \in Z} \frac{\phi_P(z)^{\beta}}{b^2_z} \frac{b_z^\beta}{a^2_z} \right)^{1/\beta} \leq \|b\|_b \left( \sum_{z \in Z} \frac{b_z^{2\beta}}{a^2_z} \right)^{\frac{2\beta}{2-\beta}} = \|b\|_b \left( \sum_{z \in Z} b^8_z \right)^{1/8}.$$ 

Combining these inequalities with inequality (28) gives

$$\left| \sum_{z \in Z} \sum_{w \in Z} \frac{\phi_Q(z)\tilde{Q}_w P_{z-w}}{a^2_z a^2_w} \right| \leq \|Q\|_b^2 \|P\|_b R_{a,b,Z},$$

where $R_{a,b,Z}$ is as in (16).

**Bounding (26):** Applying Cauchy-Schwarz yields

$$\frac{2(n-1)}{n^3} \sum_{z \in Z} \sum_{w \in Z} \frac{\tilde{Q}_w \phi_Q(z) \phi_P(z) P_w}{a^2_z a^2_w} = \frac{2(n-1)}{n^3} \left( \sum_{z \in Z} \frac{\phi_Q(z)^2}{a^2_z} \right) \left( \sum_{w \in Z} \frac{\tilde{Q}_w P_w}{a^2_w} \right) \leq 2 \left( \sum_{z \in Z} \frac{\phi_Q(z)^2}{a^2_z} \right) \left( \sum_{z \in Z} \frac{\phi_P(z)^2}{a^2_z} \right) = \frac{2\|P\|_b^2 \|Q\|_b^2}{n^2}.$$ 

Plugging these into Efron-Stein yields the result.

### 9.3. Proof of Theorem 5

**Proof.** The $\Omega(n^{-1})$ term of the lower bound, reflecting parametric convergence when the tails of the estimand (2) are light relative to the first few terms, follows from classic information bounds [Bickel and Ritov, 1988]. We focus on deriving the $\Omega(A^2/B_\zeta^2)$ term, reflecting slower convergence when the estimand is dominated by its tail. To do this, we consider the uniform density $\psi_0$ and a family of $2|Z_\zeta|$ small perturbations of the form

$$g_{\zeta,\tau} = \psi_0 + c_\zeta \sum_{z \in Z_\zeta} \tau_z \psi_z,$$

where $\zeta \in \mathbb{N}$, $\tau \in \{-1, 1\}^{Z_\zeta}$, and $c_\zeta = B_\zeta^{-1/2}$.

We now separately consider the “smooth” case, in which $B_\zeta \in \Omega(\zeta^{2D})$, and the “unsmooth” case, in which $B_\zeta \in o(\zeta^{2D})$.

**The smooth case** ($B_\zeta \in \Omega(\zeta^{2D})$): By Le Cam’s Lemma (see, e.g., Section 2.3 of Tsybakov [2008]), it suffices to prove four main claims about the family of $g_{\zeta,\tau}$ functions defined in Equation (29):
1. Each $\|g_{\zeta,\tau}\|_b \leq 1$.
2. Each
   \[
   \inf_{\tau \in \{-1,1\}^{2\zeta}} \|g_{\zeta,\tau}\|_a - \|\psi_0\|_a \geq \frac{A_{\zeta}}{B_{\zeta}}.
   \]
3. Each $g_{\zeta,\tau}$ is a density function (i.e., $\int_{\mathcal{X}} g_{\zeta,\tau} = 1$ and $g_{\zeta,\tau} \geq 0$).
4. $\zeta$ and $c_{\zeta}$ are chosen (depending on $n$) such that
   \[
   DT_{TV}\left(\psi_0^\perp, \frac{1}{2|\zeta|^{1/2}} \sum_{\tau \in \{-1,1\}^{2\zeta}} g_{\zeta,\tau}^{\perp}\right) \leq \frac{1}{2}.
   \]

For simplicity, for now, suppose $\mathcal{Z} = \mathbb{N}^D$ and $Z_{\zeta} = [\zeta]^D$. For any $\tau \in \{-1,1\}^{2\zeta}$, let

\[
g_{\zeta,\tau} = \psi_0 + c_{\zeta} \sum_{z \in \mathbb{Z}_\zeta} \tau_z \psi_z.
\]

By setting $c_{\zeta} = B_{\zeta}^{-1/2} = \left(\sum_{z \in \mathbb{Z}_\zeta} b_z^{-2}\right)^{-1/2}$, we automatically ensure the first two claims:

\[
\|g_{\zeta,\tau}\|_b^2 = c_{\zeta}^2 \sum_{z \in \mathbb{Z}_\zeta} b_z^{-2} = 1,
\]

and

\[
\inf_{\tau \in \{-1,1\}^{2\zeta}} \|g_{\zeta,\tau}\|_a^2 - \|\psi_0\|_a^2 = c_{\zeta}^2 \sum_{z \in \mathbb{Z}_\zeta} a_z^{-2} = \frac{A_{\zeta}}{B_{\zeta}}.
\]

To verify that each $g_{\zeta,\tau}$ is a density, we first note that, since, for $z \neq 0$, $\int_{\mathcal{X}} \psi_z = 0$, and so

\[
\int_{\mathcal{X}} g_{\zeta,\tau} = \int_{\mathcal{X}} \psi_0 = 1.
\]

Also, since $\psi_0$ is constant and strictly positive and the supremum is taken over all $\tau \in \{-1,1\}^{2\zeta}$, the condition that all $g_{\zeta,\tau} \geq 0$ is equivalent to

\[
\sup_{\tau \in \{-1,1\}^{2\zeta}} B_{\zeta}^{-1/2} \left\| \sum_{z \in \mathbb{Z}_\zeta} \tau_z \psi_z \right\|_\infty = \sup_{\tau \in \{-1,1\}^{2\zeta}} \|g_{\zeta,\tau} - \psi_0\|_\infty \leq \|\psi_0\|_\infty.
\]

For the Fourier basis, each $\|\psi_z\|_\infty = 1$,\footnote{This is the only step in the proof that uses any properties specific to the Fourier basis.} and so

\[
\sup_{\tau \in \{-1,1\}^{2\zeta}} \left\| \sum_{z \in \mathbb{Z}_\zeta} \tau_z \psi_z \right\|_\infty \asymp \sup_{\tau \in \{-1,1\}^{2\zeta}} \sum_{z \in \mathbb{Z}_\zeta} \|\psi_z\|_\infty \asymp |Z_{\zeta}| = \zeta^D.
\]

Thus, we precisely need $B_{\zeta} \in \Omega(\zeta^{2D})$, and it is sufficient, for example, that $b_z \in O(\|z\|^{-D/2})$. 
Finally, we show that

\[ D_{TV}\left(\psi^n_0, \frac{1}{2^{\left|Z_\zeta\right|}} \sum_{\tau \in \{-1,1\}^{2\zeta}} g^n_{\zeta,\tau} \right) \leq \frac{1}{2} \]  

(30)

(where \(h^n : \mathcal{X}^n \to [0, \infty)\) denotes the joint likelihood of \(n\) IID samples). For any particular \(\tau \in \{-1,1\}^{2\zeta}\) and \(x_1, \ldots, x_n \in \mathcal{X}\), the joint likelihood is

\[ g^n_{\zeta,\tau}(x_1, \ldots, x_n) = \prod_{i=1}^{n} \left(1 + c_\zeta \sum_{z \in Z_\zeta} \tau_z \psi_z(x_i) \right) \]

\[ = 1 + \sum_{\ell=1}^{n} \sum_{i_1, \ldots, i_\ell \in \left[\frac{n}{2}\right]} \sum_{z_1, \ldots, z_\ell \in Z_\zeta} \prod_{k=1}^{\ell} \tau_{z_k} \psi_{z_k}(x_{i_k}) \]

Thus, the likelihood of the uniform mixture over \(\tau \in \{-1,1\}^{2\zeta}\) is

\[ \frac{1}{2^{\left|Z_\zeta\right|}} \sum_{\tau \in \{-1,1\}^{2\zeta}} g^n_{\zeta,\tau}(x_1, \ldots, x_n) \]

\[ = 1 + \frac{1}{2^{\left|Z_\zeta\right|}} \sum_{\tau \in \{-1,1\}^{2\zeta}} \sum_{\ell=1}^{\left|\frac{n}{2}\right|} \sum_{i_1, \ldots, i_\ell \in \left[\frac{n}{2}\right]} \sum_{z_1, \ldots, z_\ell \in Z_\zeta} \prod_{k=1}^{\ell} \tau_{z_k} \psi_{z_k}(x_{i_k}) \]

\[ = 1 + \sum_{\ell=1}^{\left|\frac{n}{2}\right|} c_\zeta \sum_{i_1, \ldots, i_\ell \in \left[\frac{n}{2}\right]} \sum_{z_1, \ldots, z_\ell \in Z_\zeta} \prod_{k=1}^{\ell} \psi_{z_k}(x_{i_{2k-1}}) \psi_{z_k}(x_{i_{2k}}) \]

where \(\lfloor a \rfloor\) denotes the largest integer at most \(a \in [0, \infty)\). This equality holds because, within the sum over \(\tau \in \{-1,1\}^{2\zeta}\), any term in which any \(\tau_z\) appears an odd number of times will cancel. The remaining terms each appear \(2^{\left|Z_\zeta\right|}\) times. Thus, the total variation
distance is

\[
D_{TV} \left( \frac{1}{2^n} \sum_{\tau \in \{-1,1\}^n} g_{\zeta,\tau} n \right) = \frac{1}{2} \left\| \psi_0^n - \frac{1}{2^n} \sum_{\tau \in \{-1,1\}^n} g_{\zeta,\tau} \right\|_1
\]

\[
= \frac{1}{2} \int_{X^n} \left| \sum_{i_1, \ldots, i_{2\ell} \in [n]} \sum_{z_1, \ldots, z_{2\ell} \in Z_{\zeta}} \prod_{k=1}^\ell \psi_{z_k}(x_{i_{2k-1}}) \psi_{z_k}(x_{i_{2k}}) \right| \, d(x_1, \ldots, x_n)
\]

\[
\leq \frac{1}{2} \sum_{\ell=1}^{\lfloor n/2 \rfloor} c_{\zeta}^{2\ell} \int_{X^n} \left| \sum_{i_1, \ldots, i_{2\ell} \in [n]} \sum_{z_1, \ldots, z_{2\ell} \in Z_{\zeta}} \prod_{k=1}^\ell \psi_{z_k}(x_{i_{2k-1}}) \psi_{z_k}(x_{i_{2k}}) \right|^2 \, d(x_1, \ldots, x_n),
\]

where we used the triangle inequality. By Jensen’s inequality (since \( X = [0,1] \)),

\[
\int_{X^n} \left( \sum_{i_1, \ldots, i_{2\ell} \in [n]} \sum_{z_1, \ldots, z_{2\ell} \in Z_{\zeta}} \prod_{k=1}^\ell \psi_{z_k}(x_{i_{2k-1}}) \psi_{z_k}(x_{i_{2k}}) \right)^2 \, d(x_1, \ldots, x_n)
\]

\[
\leq \int_{X^n} \left( \sum_{i_1, \ldots, i_{2\ell} \in [n]} \sum_{z_1, \ldots, z_{2\ell} \in Z_{\zeta}} \prod_{k=1}^\ell \psi_{z_k}(x_{i_{2k-1}}) \psi_{z_k}(x_{i_{2k}}) \right)^2 \, d(x_1, \ldots, x_n).
\]

Since \( \{ \psi_z \}_{z \in Z_{\zeta}} \) is an orthogonal system in \( L^2(X) \), we can pull the summations outside the square, so

\[
\int_{X^n} \left( \sum_{i_1, \ldots, i_{2\ell} \in [n]} \sum_{z_1, \ldots, z_{2\ell} \in Z_{\zeta}} \prod_{k=1}^\ell \psi_{z_k}(x_{i_{2k-1}}) \psi_{z_k}(x_{i_{2k}}) \right)^2 \, d(x_1, \ldots, x_n)
\]

\[
= \sum_{i_1, \ldots, i_{2\ell} \in [n]} \sum_{z_1, \ldots, z_{2\ell} \in Z_{\zeta}} \int_{X^n} \left( \prod_{k=1}^\ell \psi_{z_k}(x_{i_{2k-1}}) \psi_{z_k}(x_{i_{2k}}) \right)^2 \, d(x_1, \ldots, x_n)
\]

\[
= \sum_{i_1, \ldots, i_{2\ell} \in [n]} \sum_{z_1, \ldots, z_{2\ell} \in Z_{\zeta}} 1 = \left( \frac{n}{2\ell} \right)^{\ell} \zeta^{D\ell} \leq \frac{n^{2\ell} \zeta^{D\ell}}{(2\ell)!^2},
\]

since

\[
\left( \frac{n}{2\ell} \right) = \frac{n!}{(2\ell)!(n-2\ell)!} \leq \frac{n^{2\ell}}{(2\ell)!^2} \leq \frac{n^{2\ell}}{(2\ell)!^2}.
\]
Combining this with inequalities (31) and (32) gives

\[
D_{\text{TV}} \left( \psi_0^n, \frac{1}{2|Z_\zeta|} \sum_{\tau \in \{-1,1\}^2 \zeta} g_{\zeta,\tau}^0 \right) \leq \frac{1}{2} \sum_{\ell=1}^{|n/2|} \frac{(\ell c_\zeta D/2)}{\ell!} \leq \exp \left( \frac{nc_\zeta D}{2} \right) - 1, \tag{33}
\]

where we used the fact that the exponential function is greater than any of its Taylor approximations on \([0, \infty)\). The last expression in inequality (33) vanishes if \(nc_\zeta D/2 \to 0\).

Recalling now that we set \(c_\zeta = B_\zeta^{-1/2}\), for some constant \(C > 0\), the desired bound (30) holds by choosing \(\zeta \) satisfying

\[
\zeta \leq Cn^{-2/3D}.
\]

**The unsmooth case \((B_\zeta \in o(\zeta^{2D}))\):** Finally, we consider the ‘highly unsmooth’ case, when \(B_\zeta \in o(\zeta^{2D})\). In this case, we must modify the above proof to ensure that the \(g_{\zeta,\tau}\) functions are all non-negative. In the Fourier case, we again wish to ensure

\[
c_\zeta \zeta D = c_\zeta |Z_\zeta| \approx c_\zeta \sup_{\tau \in \{-1,1\}^2 \zeta} \left\| \sum_{z \in Z_\zeta} \tau_z \psi_z \right\|_\infty \leq 1,
\]

but this is no longer guaranteed by setting \(c_\zeta = B_\zeta^{-1/2}\); instead, we use the smaller value \(c_\zeta = \zeta^{-D}\). Clearly, we still have \(\|g_{\zeta,\tau}\|_b^2 \leq 1\). Now, however, we have a smaller estimation error

\[
\inf_{\tau \in \{-1,1\}^2 \zeta} \|g_{\zeta,\tau}\|_a^2 - \|\psi_0\|_a^2 = c_\zeta^2 \sum_{z \in Z_\zeta} a_z^{-2} = \frac{A_\zeta}{\zeta^{2D}}. \tag{34}
\]

Also, the information bound (33) now vanishes when \(n\zeta^{-3D/2} = nc_\zeta D/2 \to 0\), so that, for some constant \(C > 0\), the desired bound (30) holds by choosing \(\zeta \) satisfying

\[
\zeta \leq Cn^{2/(3D)}.
\]

Plugging this into equation (34) gives

\[
\inf_{\tau \in \{-1,1\}^2 \zeta} \|g_{\zeta,\tau}\|_a^2 - \|\psi_0\|_a^2 \geq \frac{A_{n2/(3D)}}{n^{4/3}}.
\]

Finally, by Le Cam’s lemma, this implies the minimax rate

\[
\inf_{\hat{S}} \sup_{p,q \in \mathcal{H}_b} \mathbb{E} \left[ \left( \hat{S} - \langle p, q \rangle \right)^2 \right] \geq \left( \frac{A_{n2/(3D)}}{n^{4/3}} \right)^2.
\]

\[\square\]
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