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On Adaptive Confidence Sets for the Wasserstein Distances

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In the density estimation model, we investigate the problem of constructing *adaptive honest confidence sets* with diameter measured in Wasserstein distance W_p , $p \geq 1$, and for densities with unknown regularity measured on a Besov scale. As sampling domains, we focus on the d -dimensional torus \mathbb{T}^d , in which case $1 \leq p \leq 2$, and \mathbb{R}^d , for which $p = 1$. We identify necessary and sufficient conditions for the existence of adaptive confidence sets with diameters of the order of the regularity-dependent W_p -minimax estimation rate. Interestingly, it appears that the possibility of such adaptation of the diameter depends on the dimension of the underlying space. In low dimensions, $d \leq 4$, adaptation to any regularity is possible. In higher dimensions, adaptation is possible if and only if the underlying regularities belong to some interval of width at least $d/(d-4)$. This contrasts with the usual L_p -theory where, independently of the dimension, adaptation occurs only if regularities lie in a small fixed-width window. For configurations allowing these adaptive sets to exist, we explicitly construct confidence regions via the method of risk estimation. These are the first results in a statistical approach to adaptive uncertainty quantification with Wasserstein distances. Our analysis and methods extend to weak losses such as Sobolev norms with negative smoothness indices.

Keywords: Wasserstein distance; Uncertainty Quantification; Nonparametric confidence sets

1. Introduction

The construction of confidence sets is one of the fundamental problems of statistical inference, along with parameter estimation and hypothesis testing. Consider a model $\{P_f : f \in \mathcal{F}\}$, indexed by a family of functions \mathcal{F} , and observe (some quantity n of) data from the true distribution P_{f_0} , where $f_0 \in \mathcal{F}$. For most applications, having a single point estimate \hat{f}_n of the true parameter f_0 is not enough, and one desires to evaluate its performance in terms of a loss function, that is, to know how far it lies from f_0 . Producing a random set $C_n \subset \mathcal{F}$ from the data containing f_0 with a prescribed high probability $1 - \alpha$ achieves this aim. In this work, we investigate the existence of *adaptive honest confidence sets*. Since f_0 is unknown, we must insist that C_n possesses the previous property not just for f_0 , but for all $f \in \mathcal{F}$: we say that the confidence set C_n is *honest* if, at least for all sufficiently large n ,

$$\inf_{f \in \mathcal{F}} P_f(f \in C_n) \geq 1 - \alpha.$$

Furthermore, we desire the diameter of the set C_n to shrink in n as quickly as possible; however, typically the precise speed of this shrinkage depends on aspects of the unknown density f_0 such as its regularity, and so we find ourselves in an adaptation problem.

We work in a *density estimation model*: consider observations X_1, \dots, X_n independent and identically distributed (i.i.d.) from a probability measure P_{f_0} with probability density f_0 . The sample space

of the X_i 's will either be the d -dimensional torus \mathbb{T}^d or \mathbb{R}^d . We then study procedures in a representative ‘two-class adaptation problem’, where f_0 belongs to one of two classes $\mathcal{F}(r)$ and $\mathcal{F}(s)$ (to be precisely defined below), indexed by regularity parameters $r < s$, such that $\mathcal{F}(s) \subset \mathcal{F}(r)$. An adaptive honest confidence set C_n should satisfy the above honest coverage condition, and also have a diameter that shrinks at the minimax estimation rate of whichever class f_0 belongs to (typically the rate is faster for the smaller class $\mathcal{F}(s)$). The construction of such a confidence set involves assessing the accuracy with which one can estimate f_0 , which turns out to be more challenging than point estimation, as qualitative aspects of the parameter need to be identified. This problem has primarily been studied for L_p or related distances [3, 6, 7, 20, 21, 26, 35]. In L_2 loss, adaptive honest confidence sets exist only if the regularity parameters of interest lie in some ‘small’ interval ([3, 6, 21, 35]). More troublesome is the case of pointwise or L_∞ loss, where no such procedures exist ([20, 26]). This starkly contrasts the situation of adaptive estimation, where (perhaps at the cost of a logarithmic factor) it is possible to construct estimators which adapt to any regularity parameter ([14, 25]). Informally, these negative results come from the fact that, in L_2 loss, a related testing problem is easier (admits a faster convergence rate) than estimation, whereas for L_∞ loss, the testing and estimation problems are equally difficult ([3, 20]). This distinction highlights how the existence of adaptive honest confidence sets depends on the geometry induced by the loss function (see [18, Chapter 8] for an overview of these results).

Arising from the ideas of Optimal Transport [22, 29], Wasserstein distances W_p , $p \geq 1$, between probability measures have recently been studied in a wide array of fields such as optimization, machine learning, and statistics. For $p \geq 1$, the p -Wasserstein distance between μ and ν , probability measures on a metric space (\mathcal{X}, d) , is defined as

$$W_p(\nu, \mu) := \inf_{\pi \in \Pi(\nu, \mu)} \left(\int_{\mathcal{X} \times \mathcal{X}} d(x, y)^p d\pi(x, y) \right)^{1/p},$$

with the infimum ranging over the set $\Pi(\nu, \mu)$ of measures on $\mathcal{X} \times \mathcal{X}$ with given marginals ν and μ . It quantifies the minimal cost, as measured by the metric d , to morph the distribution μ into ν . For measures P_f and P_g dominated by a common measure and with densities f and g , this also entails a distance between those densities, with $W_p(f, g) := W_p(P_f, P_g)$.

Not only do these distances possess desirable theoretical properties ([39]), as they take into account the geometry of the underlying sample space, but recent numerical developments ([32]) have led to increased use in practical applications. They therefore now play a prominent role in statistics (see, for example, the review [31]). The convergence of the empirical distribution in W_p -distance is a well-studied problem (it stretches back to [15]), with definitive results on limit theorems for the \mathbb{R} sample space in [13]; for state-of-the-art results, see [16, 40]). In dimensions $d \geq 3$, the convergence rate of the empirical distribution (without further structural assumptions) is $n^{-1/d}$, demonstrating that convergence in W_p suffers from the curse of dimensionality. When measures have densities, a result in [41] states that, for certain classes of densities, W_p compares with Besov norms of smoothness -1 , a classical result for the W_1 distance due to the Kantorovich-Rubinstein duality formula. The convergence rates they obtain for regular densities using this comparison result, which lie closer to the parametric rate $n^{-1/2}$, highlight the importance of regularity of the signal in high-dimensional settings: to some extent, the curse of dimensionality can be mitigated by smoothness.

In addition, these rates are faster than the standard s -smooth nonparametric convergence rate $n^{-\frac{s}{2s+d}}$ for L_p loss, $1 \leq p < \infty$, reflecting the fact that Wasserstein distances are weaker than L_p distances. In this paper, we obtain similar quantitative improvements for testing separation rates of nonparametric statistical hypotheses. From this, on the bounded sample space \mathbb{T}^d we deduce new *qualitative phenomena regarding the existence and non-existence of adaptive honest confidence sets* when using the loss functions W_p , $1 \leq p \leq 2$. Surprisingly, in dimensions $d \leq 4$ we construct confidence sets that can

adapt to *any* set of regularities. This contrasts significantly with the fundamental limitations of adaptive confidence sets in L_p . In higher dimensions $d > 4$, adaptation is still possible for regularities belonging to a certain interval, which is wider than in the L_p case. The reason for this phenomenon is that while both the testing and estimation rates are faster than for L_p , the testing rate accelerates more, leaving ‘more space’ for adaptation to occur than in the analogous problem for L_p loss. As for densities on an unbounded sample space such as \mathbb{R}^d , the same phenomenon occurs, though we currently only have results for the W_1 distance.

From the general theory of confidence sets, it is known that such impossibility results may be circumvented if one is willing to remove certain ‘troublesome’ portions of the parameter space ([18, Proposition 8.3.7]). Recent works have focused on describing maximal sets of densities for which adaptation is possible, by introducing further structural constraints on the model. In [4], an L_2 -adaptive confidence set is shown to exist if one discards all densities within some positive radius of the smoother subclass; this radius converges to 0 as $n \rightarrow \infty$. Self-similarity conditions, which roughly speaking describe functions that are as regular at small scales as at larger scales, have been employed in the regression setting in [30, 33], as well as in density estimation [2, 10, 17]; see also [1]. In the study of adaptive Bayesian credible sets, self-similarity conditions were deployed in [34], and slightly more general polished tail assumptions were used in [36, 37]. We refer the interested reader to the review [27] for a more complete picture of the literature on uncertainty quantification in density estimation. In this paper, we do not pursue such a programme for the Wasserstein distances, instead leaving this problem for future work.

The paper is organized as follows. Section 2 formalizes our problem on the potential existence of adaptive honest confidence sets, and states our main results. The construction of such sets, whenever possible, and non-existence results are presented in Section 3 for the bounded sample space \mathbb{T}^d and Section 4 for the unbounded sample space \mathbb{R}^d . Proofs are deferred to Appendices B and C.

2. Main Results

2.1. Setting and Definitions

Initially, we assume that f_0 is a density on the d -dimensional torus, \mathbb{T}^d , which may be identified with $(0, 1]^d$. Our results also apply to the case of the unit cube $[0, 1]^d$ (and hence any bounded rectangular subset of \mathbb{R}^d), which is the focus of [41]; see Section A.3 below. For our loss function, we take the distance W_2 ; as described in Remark 2, this distance dominates W_p for $1 \leq p < 2$, in particular the important case of W_1 . Later, we consider the situation where f_0 is a density on the whole of \mathbb{R}^d ; while a study for $W_p, p > 1$ is beyond the scope of the present work, we obtain some definitive results for the loss function W_1 in Section 4.

2.1.1. Parameter Spaces

Here we define the classes of probability densities on \mathbb{T}^d we consider; definitions for \mathbb{R}^d are similar but deferred to Section 4. Let $\{\phi \equiv 1, \psi_{lk} : l \geq 0, 0 \leq k < 2^{ld}\}$ be an S -regular periodised Daubechies wavelet basis of $L_2(\mathbb{T}^d)$; see Appendix A for further details. We denote by $\langle f, g \rangle = \int_{\mathbb{T}^d} fg$ the usual inner product on L_2 . For any $f \in L_p(\mathbb{T}^d)$, $1 \leq p < \infty$, the wavelet expansion

$$f = \langle f, 1 \rangle + \sum_{l \geq 0} \sum_{k=0}^{2^{ld}-1} \langle f, \psi_{lk} \rangle \psi_{lk} \quad (1)$$

converges in L_p , and if f is continuous then the expansion converges uniformly on \mathbb{T}^d . We write $K_j(f)$ for the projection of f onto the first j resolution levels, i.e.

$$K_j(f) = \langle f, 1 \rangle + \sum_{l < j} \sum_{k=0}^{2^{ld}-1} \langle f, \psi_{lk} \rangle \psi_{lk}. \quad (2)$$

To define the parameter classes, we use the scale of *Besov spaces*, B_{pq}^s , $1 \leq p, q \leq \infty$, $s \geq 0$ as defined in Appendix A. The index s should be interpreted as a smoothness or regularity parameter. Using the definition of the Besov norm (32) and the embedding $\ell_q \subset \ell_\infty$, for $f \in B_{pq}^s(\mathbb{T}^d)$ we have that

$$\|\langle f, \psi_l \cdot \rangle\|_p \leq \|f\|_{B_{pq}^s} 2^{-l(s + \frac{d}{2} - \frac{d}{p})}. \quad (3)$$

Thus $f \in B_{pq}^s$ if its wavelet coefficients decay sufficiently fast as l grows, as measured by s .

The use of subsets of Besov spaces as parameter spaces in nonparametric statistics is well-established, and the scale contains several of the regularity classes usually considered in such settings: for example, the Sobolev spaces ($H^s = B_{22}^s$) and the Hölder spaces (for $s \notin \mathbb{N}$, $C^s = B_{\infty\infty}^s$, and for $s \in \mathbb{N}$, $C^s \subsetneq B_{\infty\infty}^s$). See [18, Section 4.3] for further discussion on this subject.

In standard loss functions such as L_2 or L_∞ , it is typically assumed that f lies in some norm-ball in B_{pq}^s , for some choice of s, p, q . Here we slightly restrict the function class, insisting that the densities under consideration are bounded and bounded away from 0. In particular, the lower bound condition facilitates the faster minimax estimation rates of Proposition 2; it is shown in [41] that removing this condition results in slower rates for most parameter configurations.

Definition 1. Let $1 \leq p, q \leq \infty$, $s \geq 0$, $B \geq 1$, $M \geq 1 \geq m > 0$. Define the function class

$$\mathcal{F}_{s,p,q}(B; m, M) = \left\{ f \in B_{pq}^s : \int_{\mathbb{T}^d} f = 1, \quad \|f\|_{B_{pq}^s} \leq B, \quad m \leq f \leq M \text{ a.e.} \right\}; \quad (4)$$

Note that we always have $1 \in \mathcal{F}_{s,p,q}(B; m, M)$, and so the class is non-empty. Henceforth we fix $p = 2$ and consider q, B, m, M to be given. Define

$$\mathcal{F}(s) := \mathcal{F}_{s,2,q}(B; m, M).$$

For large s and smaller values of $B \geq 1$, the condition $f \leq M$ is superfluous. However, the imposition of the uniform lower bound $f \geq m > 0$ means that $\mathcal{F}(s)$ is a strict subset of the more typical parameter space $\{f \in B_{2q}^s : f \geq 0, \int f = 1, \|f\|_{B_{2q}^s} \leq B\}$. Also, it is clear from the definition (32) that the continuous embedding $B_{pq}^s \subset B_{pq}^r$ holds with operator norm 1, so $\mathcal{F}(s) \subset \mathcal{F}(r)$ for $r \leq s$.

2.1.2. Notation

For a probability density f , let P_f and E_f denote respectively the probability and expectation when $X_1, \dots, X_n \stackrel{\text{i.i.d.}}{\sim} f$. For real numbers a, b , we write $a \wedge b = \min(a, b)$ and $a \vee b = \max(a, b)$. Given sequences (a_n) and (b_n) , we write $a_n \lesssim b_n$ if there exists a constant $C > 0$ that is independent of n such that for all n , $a_n \leq C b_n$; we also write $a_n \simeq b_n$ if $a_n \lesssim b_n$ and $b_n \lesssim a_n$. Given any subset A of a metric space (\mathcal{A}, d) , we write $|A|_d$ for the d -diameter of A , defined by

$$|A|_d := \sup_{x, y \in A} d(x, y).$$

Given a subset $B \subset \mathcal{A}$ and a point $a \in \mathcal{A}$, we define the distance of a to B as

$$d(a, B) := \inf_{b \in B} d(a, b).$$

2.2. Description of the Problem

Suppose initially that $f \in \mathcal{F}(r)$ for some given $r \geq 0$. We wish to construct a confidence set C_n for the unknown density f ; informally, we would like C_n to contain f with (some chosen) high probability. Specifically, given $\alpha \in (0, 1)$, we require any confidence set $C_n = C_n(\alpha, X_1, \dots, X_n)$ to have *honest coverage* at level $1 - \alpha$ over the class $\mathcal{F}(s)$, that is, there exists $n_0 \in \mathbb{N}$ such that for all $n \geq n_0$,

$$\inf_{f \in \mathcal{F}(r)} P_f(f \in C_n) \geq 1 - \alpha. \quad (5)$$

The ‘honesty’ refers to the uniformity over $\mathcal{F}(r)$. We remark that in the minimax paradigm, one must necessarily insist on honesty, since the true density f_0 is unknown: ‘dishonest’ adaptive confidence sets exist (see [18, Corollary 8.3.10]), but the index n_0 from which coverage is valid depends on the unknown f , so such procedures produce questionable guarantees in practice.

It is clear that the smaller the set C_n , the more informative it is; otherwise one could just take C_n to be the whole parameter space $\mathcal{F}(r)$. Thus we desire the W_2 -diameter of our set C_n to shrink as quickly as possible in n . Suppose C_n satisfies the honest coverage condition (5) for some $\alpha \in (0, 1)$, and let r_n be a positive sequence such that for some $\beta > \alpha$ and every $n \geq n_0$, we have

$$\inf_{\tilde{f}_n} \sup_{f \in \mathcal{F}(r)} P_f(W_2(\tilde{f}_n, f) \geq r_n) \geq \beta. \quad (6)$$

Here, the infimum is taken over all *estimators* (i.e. measurable functions) $\tilde{f}_n = \tilde{f}_n(X_1, \dots, X_n)$. Then by Lemma 2 in [35], the W_2 -diameter of C_n satisfies, for $n \geq n_0$,

$$\sup_{f \in \mathcal{F}(r)} P_f(|C_n|_{W_2} \geq r_n) \geq \beta - \alpha;$$

in particular, its diameter cannot shrink faster than r_n with high probability. We define the *minimax estimation rate* (in probability) over $\mathcal{F}(s)$, denoted $r_n^*(s)$, to be the ‘slowest’ sequence (i.e. the largest such sequence up to a multiplicative prefactor) r_n such that (6) is satisfied for some $\beta > 0$ and some $n_0 \geq 1$. Usually this rate depends on the smoothness parameter s .

Remark 1. The term ‘minimax estimation rate’ is often reserved for any sequence \bar{r}_n such that

$$\inf_{\tilde{f}_n} \sup_{f \in \mathcal{F}(r)} E_f W_2(\tilde{f}_n, f) \simeq \bar{r}_n.$$

By Markov’s inequality, we have that $r_n^* \lesssim \bar{r}_n$. In fact, as shown by Proposition 2 below, in this problem the rates r_n^* and \bar{r}_n coincide (possibly up to a logarithmic factor when $d = 2$).

In general, it is unrealistic to assume that the regularity r is known. Thus we find ourselves in an adaptation problem, where we wish to construct procedures that do not depend on the unknown smoothness r , but which result in (near-)optimal performance for a range of values of r . In order to highlight the main ideas, let us consider the two class adaptation problem, where for some fixed $s > r \geq 0$ we consider the model $\mathcal{F}(r)$, but also seek optimal performance over the smoother subclass

$\mathcal{F}(s) \subset \mathcal{F}(r)$. We discuss after Theorem 4 how one might construct confidence sets adapting to a continuous window of smoothnesses $[r, R]$ or even all $r \geq 0$ simultaneously.

Definition 2. We say that $C_n = C_n(\alpha, \alpha', X_1, \dots, X_n)$ is a *near-optimal adaptive W_2 confidence set* over $\mathcal{F}(s) \cup \mathcal{F}(r)$, $s > r$, if it satisfies the following properties, for given $\alpha, \alpha' \in (0, 1)$:

- (i) **Honest Coverage:** for all n sufficiently large,

$$\inf_{f \in \mathcal{F}(r)} P_f(f \in C_n) \geq 1 - \alpha; \quad (7)$$

- (ii) **Diameter Shrinkage:** there exists a constant $K = K(\alpha') > 0$ such that

$$\sup_{f \in \mathcal{F}(r)} P_f(|C_n|_{W_2} > K R_n(r)) \leq \alpha' \quad (8)$$

and

$$\sup_{f \in \mathcal{F}(s)} P_f(|C_n|_{W_2} > K R_n(s)) \leq \alpha', \quad (9)$$

for n large enough, where the rate sequences $R_n(r)$ and $R_n(s)$ satisfy

$$R_n(r) \leq a_n r_n^*(r) \quad \text{and} \quad R_n(s) \leq a_n r_n^*(s),$$

for a_n some power of $\log n$, and $r_n^*(r)$ and $r_n^*(s)$ the minimax rates of estimation over $\mathcal{F}(r)$ and $\mathcal{F}(s)$ respectively (these are given in Proposition 2 for the case of \mathbb{T}^d and Theorem 6 for the case of \mathbb{R}^d).

Typically, for optimal adaptive confidence sets one insists that the rates $R_n(r), R_n(s)$ in (8) and (9) are equal up to constants to the minimax estimation rates $r_n^*(r), r_n^*(s)$. Our definition of ‘near-optimal’ allows for $R_n(t)$ to equal $r_n^*(t)$, $t = r, s$, up to a logarithmic factor in n , and is thus a slight relaxation. Admitting this relaxation does not alter the (existence and) non-existence results of [3, 7, 18, 20], since these results are due to a polynomial discrepancy between minimax estimation and testing rates; see Section 3.3 below.

We only consider the problem of adaptation in the smoothness parameter and do not address the question of adaptation to other parameters in the definition of the class $\mathcal{F}(s)$, such as the Besov norm bound B . See Remark 5 below for a discussion of this issue.

2.3. Adaptive W_2 Confidence Sets on \mathbb{T}^d

Our first theorem exhaustively classifies the parameter configurations for which adaptive honest confidence sets exist for W_2 loss; in the cases where such confidence sets do exist, an explicit construction is given in Theorem 4 below.

Theorem 1. Fix $1 \leq q \leq \infty$, $B \geq 1$, $M \geq 1 \geq m > 0$. Consider the two class adaptation problem for confidence sets as defined by (7)-(9).

- (i) Let $d \leq 4$ and $s > r \geq 0$. Then for any $\alpha, \alpha' > 0$, there exists a near-optimal adaptive W_2 confidence set.
- (ii) Let $d > 4$ and $0 \leq r < s \leq \frac{2d-4}{d-4}r + \frac{d}{d-4}$. Then for any $\alpha, \alpha' > 0$, there exists a near-optimal adaptive W_2 confidence set.

(iii) Let $d > 4$ and $0 \leq r < s$ with $s > \frac{2d-4}{d-4}r + \frac{d}{d-4}$. Then for any $\alpha, \alpha' > 0$ such that $2\alpha + \alpha' < 1$, no near-optimal adaptive W_2 confidence set exists.

Remark 2. We have focussed on the particular choice of W_2 ; by Jensen's inequality, this distance dominates W_p for $1 \leq p < 2$. Since the minimax estimation rates in these problems are independent of p (c.f. Proposition 2), this means that the above existence results hold for W_p , $1 \leq p \leq 2$, in particular for the important case of W_1 . Moreover, in the case of W_1 , one may remove the lower bound condition in the definition of $\mathcal{F}(s)$; see Remark 3 below.

Theorem 1 says that in low dimensions, $d \leq 4$, there exists a confidence set which adapts optimally in W_2 -diameter to any two smoothnesses $s > r \geq 0$. As the construction does not depend on s , in fact adaptation occurs simultaneously for all $s \geq r$ (strictly speaking, $r \leq s \leq S$ where S is the regularity of the wavelet basis used), where r is a chosen 'baseline' smoothness. Contrast this to the case of L_p loss, $2 \leq p \leq \infty$: for $p < \infty$, in any dimension, there exists a (near-)optimal adaptive confidence set if and only if $s \leq \frac{p}{p-1}r$ [3, 7]; for L_∞ loss, adaptive confidence sets do not exist for any choice of $s > r \geq 0$ [20, 26]. See [18, Section 8.3] for a complete account of the L_2 and L_∞ theory.

In higher dimensions $d > 4$, Theorem 1 (together with the same confidence set as constructed in the case $d \leq 4$) gives a continuous 'window' of smoothnesses for which adaptation occurs simultaneously, in a similar vein to the case of L_p , $p < \infty$. However, for the W_2 loss this window is significantly wider; moreover, regardless of how small we choose the minimal smoothness $r \geq 0$, this window has width at least $\frac{d}{d-4}$, whereas for L_p , $2 \leq p < \infty$, the window is of width $\frac{r}{p-1} \leq r$, which will be very narrow for small values of r .

These results are related to the fact that W_2 is a weaker loss function than L_p : specifically, Proposition 1 and (12) show that on the class $\mathcal{F}(s)$, W_2 is comparable to a Sobolev (or Besov) norm of smoothness -1 . In very low dimensions $d = 1, 2$, the estimation rate is independent of the smoothness parameter s , meaning that any confidence set satisfying (8) automatically satisfies the faster shrinkage condition (9) (with a possibly enlarged constant K). In low dimensions $d = 3, 4$, one finds a very fast minimax testing separation rate, which is at least as fast as the parametric rate of estimation $n^{-1/2}$ (this is implied by the above existence results and Lemma 2 below). Even in higher dimensions, there is a substantial acceleration in the testing separation rate as compared to L_2 loss. Meanwhile, although there is also some acceleration in the estimation rates, the effect is not so pronounced. This explains the wider window of adaptation seen in Theorem 1 for W_2 loss, as compared to L_p loss: the greater discrepancy between testing and estimation rates gives more room for adaptation to take place.

Theorem 1 is proved in Section 3; we outline the arguments now. For the existence result, we use the method of constructing confidence sets via risk estimation as in [6, 21, 35]; see [18, Section 6.4] for a concise summary of these ideas. These methods require the loss function under consideration to be a Hilbert space norm. Accordingly, we upper bound W_2 by a suitable Sobolev-type norm for which one can perform risk estimation with fast convergence rates; moreover, the estimation rates for this dominating norm differ from those for W_2 by only a logarithmic factor. In particular, the notions of near-optimal adaptive confidence sets for these two loss functions are equivalent. The non-existence result is obtained using a testing argument as in [3], [20] and others, together with a lower bound for the minimax separation rate in a related testing problem. Moreover, the precise characterisation of the separation rate identifies a certain small subset of $\mathcal{F}(r)$ consisting of 'problematic' densities which, once removed, permit the existence of confidence sets (with honesty relative to a smaller set of densities), as in the previous two references. We discuss the existence of these more general confidence sets after Theorem 5. These theoretical results and constructions extends more generally to the study of adaptive honest confidence sets with negative Sobolev norm distances, and we discuss them in Section 2.5. For $p > 2$, [7] develops a construction of adaptive L_p -confidence sets whose radii are selected

via testing. Though an extension of these ideas to W_p -confidence sets should be possible, we do not pursue it here as the methodology greatly differs from the one used in the present paper.

2.4. Adaptive W_1 Confidence Sets on \mathbb{R}^d

The case of densities on \mathbb{R}^d is also of great interest; there are several situations in which it is unrealistic to assume compact support of the density f . Accordingly, let X_1, \dots, X_n be an i.i.d. sample drawn from some unknown density f on \mathbb{R}^d . We take the Wasserstein-1 distance W_1 to be our loss function. We generalise our methods from the case of \mathbb{T}^d to produce adaptive confidence sets for f which adapt over similar function classes $\mathcal{G}(s)$, defined in (21) below and involving a constant L which uniformly bounds the exponential moments of the densities in $\mathcal{G}(s)$. The discussion following Theorem 1 is relevant in this context as well: in particular, since the confidence sets constructed in cases (i) and (ii) do not depend on s , adaptation in fact takes place for the full range of possible values of s (i.e. $s \geq r$ when $d \leq 4$ and s in some given window when $d > 4$).

Theorem 2. *Fix $1 \leq q \leq \infty$, $B \geq 1$, $M \geq 1 \geq m > 0$. Consider the two class adaption problem for confidence sets defined by (7)-(9), with function classes \mathcal{F} replaced by \mathcal{G} and W_2 in place of W_1 .*

- (i) *Let $d \leq 4$ and $s > r \geq 0$. Then for any $\alpha, \alpha' > 0$, there exists a near-optimal adaptive W_1 confidence set.*
- (ii) *Let $d > 4$ and $0 \leq r < s \leq \frac{2d-4}{d-4}r + \frac{d}{d-4}$. Then for any $\alpha, \alpha' > 0$, there exists a near-optimal adaptive W_1 confidence set.*
- (iii) *Let $d > 4$, L be large enough and $0 \leq r < s$ with $s > \frac{2d-4}{d-4}r + \frac{d}{d-4}$. Then for any $\alpha, \alpha' > 0$ such that $2\alpha + \alpha' < 1$, no near-optimal adaptive W_1 confidence set exists.*

The bound L on exponential moments in (21) is a technical condition which allows us to construct adaptive estimators and confidence sets via the method of risk minimization (see Section 4). We are naturally interested in the existence of confidence sets for large L , i.e. on larger classes of densities. Moreover, small values of L may lead to empty classes (see the discussion after Definition 4 below) for which the theory of confidence sets is superfluous.

2.5. Extension to negative Sobolev norm distances

To better understand the phenomena in Theorems 1 and 2, it is elucidating to consider negative order Sobolev norm loss, $H^{-t} = B_{22}^{-t}$, $t > 0$ (see Appendix A for definitions), since the W_2 distance is dominated by such a norm (see (12) below). One finds that the minimax estimation rate for $t \geq d/2$ is (up to a log factor) $n^{-1/2}$, so no meaningful adaptation is required and one constructs a confidence set which ‘adapts’ over all smoothnesses as in Proposition 3 below. When $t < d/2$, computations analogous to those in Section 3 show that the gap between testing and estimation rates are wider for larger t , enabling adaptation over a larger window of regularities (see Remark 8 below). Here, one finds a continuous transition as t increases from 0 (which is the L_2 case) to $d/2$, at which point confidence sets can adapt to any two smoothnesses. However, the specific geometry of the parameter space induced by the loss function is crucial, rather than how weak the loss function is *per se*: if instead we consider $B_{\infty\infty}^{-t}$ loss, when $t < d/2$ the minimax estimation and testing rates can be shown to coincide; meanwhile, the estimation rate is independent of the smoothness parameter when $t \geq d/2$. So in the case of $B_{\infty\infty}^{-t}$ loss, when $t < d/2$ no adaptive confidence sets exist for any two smoothnesses by Lemma 2 below, but for $t \geq d/2$ they trivially exist.

Whenever they exist, the construction of confidence sets in Section 3 below extends easily to the case of negative order Sobolev norms H^{-t} , $t > 0$, and other Besov norms using norm embeddings as in [18, Section 4.3]; see Remark 8 below.

3. Proof of Theorem 1

3.1. A Hilbert Norm Upper Bound for W_2

We wish to construct confidence sets by performing risk estimation. The inner product structure of Hilbert space norms makes them particularly amenable to risk estimation, and so we seek some Hilbert norm which upper bounds the W_2 distance.

For this, we introduce the *logarithmic Sobolev norm* ([18, Section 4.4]; see [8], [9] for another statistical application of such norms).

Definition 3. Define the $H^{-1,\delta}$ norm of $f \in L_2(\mathbb{T}^d)$ as

$$\|f\|_{H^{-1,\delta}} = |\langle f, 1 \rangle| + \left(\sum_{l \geq 0} 2^{-2l} \max(l, 1)^{2\delta} \|\langle f, \psi_l \rangle\|_2^2 \right)^{1/2}.$$

Note the similarity to the definition of the $B_{22}^{-1} = H^{-1}$ norm given by (32); indeed, when $\delta = 0$ the two norms coincide with the Sobolev norm of regularity -1. We refer to this as a ‘logarithmic’ Sobolev space because the parameter δ measures the smoothness of f on a logarithmic scale.

We require the following comparison inequality from [41].

Proposition 1 (Theorem 3, [41]). *Let $1 \leq p < \infty$. Let f, g be two densities in $L_p(\mathbb{T}^d)$, and assume that for almost every $x \in \mathbb{T}^d$, $M \geq \max(f(x), g(x)) \geq m > 0$, for real numbers M and m . Then*

$$M^{-1/p'} \|f - g\|_{B_{p\infty}^{-1}} \lesssim W_p(f, g) \lesssim m^{-1/p'} \|f - g\|_{B_{p1}^{-1}}, \quad (10)$$

where $\frac{1}{p} + \frac{1}{p'} = 1$, and the constants depend only on d, p and the wavelet basis. Moreover, when $p = 1$, one may choose $m = 0$ (with the convention $0^0 = 1$).

This result is an extension of the celebrated Kantorovich-Rubinstein duality formula, which states that for two probability measures μ, ν on \mathbb{T}^d ,

$$W_1(\mu, \nu) = \sup_{h \in \text{Lip}_1(\mathbb{T}^d)} \int h \, d(\mu - \nu), \quad (11)$$

where the supremum is taken over all functions $h : \mathbb{T}^d \rightarrow \mathbb{R}$ with Lipschitz constant bounded by 1. We may relate this to (10) using the sequence of norm-continuous embeddings ([18, Section 4.3])

$$B_{11}^{-1} \subset \left(B_{\infty\infty}^1 \right)^* \subset BL(\mathbb{T}^d)^* \subset \left(B_{\infty 1}^1 \right)^* \subset B_{1\infty}^{-1},$$

where $BL(\mathbb{T}^d)$ is the space of bounded Lipschitz functions on \mathbb{T}^d (note that any Lipschitz function on \mathbb{T}^d is bounded, so $BL(\mathbb{T}^d)$ and $\text{Lip}_1(\mathbb{T}^d)$ coincide). However, in order to generalise this to $W_p, p > 1$,

one must impose that the probability measures have densities which are bounded and bounded away from zero; indeed, for densities not bounded below, no norm provides a similar comparison to W_p ([41, Theorem 7]), and convergence rates are slower than those in Proposition 2. Thus the restriction from the usual choices of Besov norm-balls to the classes $\mathcal{F}(s)$, $s \geq 0$ is necessary.

A simple application of the Cauchy-Schwarz inequality confirms that $H^{-1,\delta} \subset B_{21}^{-1}$ as soon as $\delta > 1/2$. Thus in conjunction with the upper bound in Proposition 1, we have that, for $r \geq 0$, $f \in \mathcal{F}(r)$ and \tilde{f}_n any estimator of f ,

$$W_2(f, \tilde{f}_n) \lesssim \|f - \tilde{f}_n\|_{B_{21}^{-1}} \lesssim \|f - \tilde{f}_n\|_{H^{-1,\delta}}, \quad (12)$$

where the first constant depends on the parameters of the class $\mathcal{F}(r)$, but the second constant depends only on the wavelet basis and d .

Remark 3. When using W_1 loss, one may consider the class $\mathcal{F}(s)$ with the choice $m = 0$, i.e. densities are not required to be bounded away from zero. Then the $H^{-1,\delta}$ norm still provides an upper bound for W_1 for densities in $\mathcal{F}(s)$ due to the upper bound in (10) and the sequence of continuous embeddings $H^{-1,\delta} \subset B_{21}^{-1} \subset B_{11}^{-1}$, where the second embedding follows from Jensen's inequality (with operator norm 1).

For the remainder of this section, we work in $H^{-1,\delta}$ risk; as soon as $\delta > 1/2$, this provides a Hilbert norm upper bound for the W_2 risk. In particular, any coverage guarantee for a $H^{-1,\delta}$ ball is automatically inherited by the W_2 ball with the same centre and radius scaled by the embedding constant from (12). Of course, by constructing confidence sets for a stronger loss function, we may not be able to attain near-optimal diameter shrinkage, but we shall see that this is not the case.

3.2. Construction of Confidence Sets

We first give the minimax estimation rates for the problem under consideration. These are important for two reasons: firstly, they provide the benchmark for the 'size' of an optimal confidence set. Moreover, our confidence sets are centred at a suitable estimator of f , which must perform well for the resulting confidence set to also have good performance. In the density estimation problem, the estimation rates for W_2 loss are as follows:

Proposition 2. *Let $s \geq 0$ and let $r_n^*(s)$ denote the minimax rate of estimation over $\mathcal{F}(s)$. Then*

$$r_n^*(s) \lesssim \begin{cases} n^{-1/2}, & d = 1, \\ n^{-1/2} \log n, & d = 2, \\ n^{-\frac{s+1}{2s+d}}, & d \geq 3, \end{cases}$$

where the constant depends on the parameters of the class $\mathcal{F}(s)$ and the wavelet basis. Moreover, for any $s \geq 0$,

$$r_n^*(s) \gtrsim \begin{cases} n^{-1/2}, & d = 1, 2 \\ n^{-\frac{s+1}{2s+d}}, & d \geq 3, \end{cases}$$

where the infimum is over all estimators \tilde{f}_n based on a sample of size n .

The upper bounds follow from Theorem 1 in [41] and Remark 1. The lower bounds are proved as in Theorem 6.3.9 in [18], where one ensures the existence of a suitable W_2 -separated set using the lower bound in Proposition 1. See also Theorem 2 in [41].

We centre our confidence sets at an estimator \hat{f}_n of f which has near-optimal convergence over the classes $\mathcal{F}(s)$ and $\mathcal{F}(r)$. The theory of adaptive estimation is relatively complete, and in the vast majority of cases it is possible to construct adaptive estimators which converge at the minimax estimation rate (perhaps up to a logarithmic factor) over a wide range of smoothnesses - we mention only the classical references [14] and [25].

The choice of Wasserstein loss adds a minor complication to the usual case of ‘norm-type’ loss functions. The Wasserstein distance $W_p(f, \tilde{f}_n)$ is only well-defined if \tilde{f}_n is also a density, and thus we ought to insist that any estimator we define is indeed a density almost surely. To achieve this, given any wavelet-based estimator of the form

$$\tilde{f}_n = \tilde{f}_{-1} + \sum_{l \geq 0} \sum_{k=0}^{2^{ld}-1} \tilde{f}_{lk} \psi_{lk}$$

where \tilde{f}_{lk} are the wavelet coefficients of the estimator, we insist that $\tilde{f}_{-1} = 1$. This ensures that $\int_{\mathbb{T}^d} \tilde{f}_n = 1$. The problem of non-negativity is more subtle. In [41], it was addressed by projecting \tilde{f}_n onto the class of densities $\mathcal{F}(r)$ with respect to the B_{p1}^{-1} norm, where r is the smallest regularity to which we want to adapt. However, this projection step makes the estimator essentially intractable. Instead, we use the well-known L_∞ consistency of the adaptive estimators considered below (c.f. [14], for example) together with the fact that the densities in $\mathcal{F}(r)$ are uniformly bounded away from 0 to conclude that for sufficiently large n , with high probability \tilde{f}_n is in fact a probability density. Whenever \tilde{f}_n fails to be non-negative, we simply replace it with an arbitrary choice of density (e.g. uniform); as $n \rightarrow \infty$, this event occurs with vanishing probability.

Theorem 3. *Let $d \geq 2$. Then there exists an estimator \hat{f}_n of f such that for all $n \geq n_0(B)$ and all $s \geq 0$,*

$$\sup_{f \in \mathcal{F}(s)} E_f \|f - \hat{f}_n\|_{H^{-1,\delta}}^2 \lesssim (\log n)^{2\delta} \left(\frac{n}{\log n} \right)^{-\frac{2(s+1)}{2s+d}},$$

where the constant depends on B, d and the wavelet basis.

The definition of \hat{f}_n and proof of Theorem 3 can be found in Appendix B, and follows from the classical ideas of [14].

Next, we introduce a U -statistic to perform risk estimation. Recall that given any estimator \tilde{f}_n of f such that $\langle \tilde{f}_n, 1 \rangle = 1$, the $H^{-1,\delta}$ loss can be expressed as

$$\|f - \tilde{f}_n\|_{H^{-1,\delta}}^2 = \sum_{l \geq 0} 2^{-2l} (l \vee 1)^{2\delta} \sum_{k=0}^{2^{ld}-1} \langle f - \tilde{f}_n, \psi_{lk} \rangle^2.$$

To estimate this loss, we use the approach of sample splitting. Suppose we have a sample of size $2n$ which we divide into two subsamples: $\mathcal{S}^1 = (X_1, \dots, X_n)$, $\mathcal{S}^2 = (X_{n+1}, \dots, X_{2n})$. Denote expectation with respect to sample i by $E^{(i)}$; we denote variances and probabilities accordingly. We compute our estimator $\tilde{f}_n = \tilde{f}_n(X_1, \dots, X_n)$ based on \mathcal{S}^1 and, for $j \geq 0$, define the U -statistic based on the

sample \mathcal{S}^2 as

$$U_{n,j}(\tilde{f}_n) = \frac{2}{n(n-1)} \sum_{i < i', i, i' \in \mathcal{S}^2} \sum_{l < j} 2^{-2l} (l \vee 1)^{2\delta} \sum_{k=0}^{2^{ld}-1} \left(\psi_{lk}(X_i) - \langle \psi_{lk}, \tilde{f}_n \rangle \right) \left(\psi_{lk}(X_{i'}) - \langle \psi_{lk}, \tilde{f}_n \rangle \right). \quad (13)$$

Since the sample is i.i.d., we see that

$$E_f^{(2)} U_{n,j}(\tilde{f}_n) = \sum_{l < j} 2^{-2l} (l \vee 1)^{2\delta} \sum_{k=0}^{2^{ld}-1} \langle \psi_{lk}, f - \tilde{f}_n \rangle^2 = \|K_j(f - \tilde{f}_n)\|_{H^{-1,\delta}}^2.$$

Thus $U_{n,j}(\tilde{f}_n)$ is an unbiased estimator of the j^{th} resolution level approximation of the loss $\|f - \tilde{f}_n\|_{H^{-1,\delta}}$. The key idea behind the U -statistic is that the removal of the diagonal in the outermost sum in (13) eliminates the highest variance terms. Thus by averaging over $O(n^2)$ terms with small variance, we expect the U -statistic to have very small variance (as in Theorem 6.4.6 of [18]). This is confirmed by the next lemma.

Lemma 1. *Assume $f \in L^\infty(\mathbb{T}^d)$ is a probability density, and \tilde{f}_n is an estimator for f based on the subsample \mathcal{S}^1 . Then*

$$\begin{aligned} \text{Var}^{(2)}(U_{n,j}(\tilde{f}_n)) &\leq \frac{4\|f\|_\infty}{n} \left(\max_{l \geq -1} 4^{-l} (l \vee 1)^{2\delta} \right) \|K_j(f - \tilde{f}_n)\|_{H^{-1,\delta}}^2 \\ &\quad + \frac{2\|f\|_\infty^2}{n(n-1)} \sum_{l \leq j-1} 2^{l(d-4)} (l \vee 1)^{4\delta} \\ &=: \kappa_{n,j,\delta}^2(f). \end{aligned} \quad (14)$$

This result is analogous to Theorem 4.1 in [35]; for completeness, we give a proof in Appendix B.

With the adaptive estimator \hat{f}_n and the U -statistic $U_{n,j}(\hat{f}_n)$ in hand, we are now ready to give the construction of optimal confidence sets for the two-class adaptation problem.

We first note that for $d = 1, 2$, the minimax rates of estimation from Proposition 2 do not depend on the smoothness parameter s ; in particular, the two diameter shrinkage conditions (8) and (9) become a single condition. Thus in these dimensions, defining an adaptive confidence set is very easy; indeed, there is no meaningful adaptation which needs to take place.

When $d = 1$, the empirical measure is a minimax optimal estimator of the sampling measure (see, for instance, [16] or [40]). When $d = 2$, we centre at the adaptive estimator from Theorem 3 in place of the empirical measure P_n , as P_n is no longer minimax optimal, and standard kernel or wavelet projection estimators require choices of tuning parameters depending on the smoothness parameter to attain optimal rates.

Proposition 3. (i) *Let $d = 1$. Consider the two-class adaptation problem over $\mathcal{F}(s) \cup \mathcal{F}(r)$ where $s > r \geq 0, q \in [1, \infty], B \geq 1, M \geq 1 \geq m > 0$ are all fixed. Then given any $\alpha \in (0, 1)$, the confidence set based on a sample X_1, \dots, X_n defined by*

$$C_n = \left\{ g \in \mathcal{F}(r) : W_2(P_g, P_n) \leq D\alpha^{-1/2} n^{-1/2} \right\}$$

is an optimal adaptive W_2 confidence set, where $P_n = n^{-1} \sum_{i=1}^n \delta_{X_i}$ is the n -sample empirical measure and the constant D depends on B, m and the wavelet basis.

- (ii) Let $d = 2$. Consider the two-class adaptation problem over $\mathcal{F}(s) \cup \mathcal{F}(r)$ where $s > r \geq 0, q \in [1, \infty], B \geq 1, M \geq 1 \geq m > 0$ are all fixed. Then given any $\alpha \in (0, 1)$, the confidence set based on a sample X_1, \dots, X_n defined by

$$C_n = \left\{ g \in \mathcal{F}(r) : W_2(g, \hat{f}_n) \leq D\alpha^{-1/2}n^{-1/2}(\log n)^{2+\delta} \right\}$$

is a near-optimal adaptive W_2 confidence set, where \hat{f}_n is the adaptive estimator from Theorem 3 and the constant D depends on B, m and the wavelet basis.

The diameter shrinkage conditions are met trivially, while honest coverage follows from Chebyshev's inequality in a standard fashion.

When $d \geq 3$, the minimax rates depend on the smoothness parameter and so the diameter shrinkage condition differs between $\mathcal{F}(r)$ and $\mathcal{F}(s)$, $r \neq s$. In particular, this precludes any confidence set C_n with deterministic radius, as used above. Instead, we centre at the adaptive estimator \hat{f}_n from Theorem 3, and use the estimate of its loss provided by the U -statistic $U_{j,n}(\hat{f}_n)$ as defined in (13) to determine the radius. We write $U_j := U_{j,n}(\hat{f}_n)$ in the sequel.

Theorem 4. Let $d \geq 3$. Fix $B \geq 1, M \geq 1 \geq m > 0, 1 \leq q \leq \infty$, and let $s > r \geq 0$. If $d > 4$, assume additionally that $s \leq \frac{2d-4}{d-4}r + \frac{d}{d-4}$. Fix $\alpha \in (0, 1)$, and $\delta > 1/2$. Consider the confidence set based on a sample of size $2n$, $\mathcal{S}^1 \cup \mathcal{S}^2$ given by

$$C_n = \left\{ g \in \mathcal{F}(r) : \|g - \hat{f}_n^T\|_{H^{-1}, \delta} \leq \sqrt{z_\alpha \kappa_{n,j_n, \delta}(g) + U_{j_n} + G(j_n)} \right\} \quad (15)$$

where \hat{f}_n^T is computed on \mathcal{S}^1 , U_{j_n} is computed on \mathcal{S}^2 and:

- $\kappa_{n,j,\delta}^2(g) := \frac{4\|g\|_\infty}{n} \|K_j(g - \hat{f}_n^T)\|_{H^{-1}, \delta}^2 + \frac{2\|g\|_\infty^2}{n(n-1)} \sum_{l \leq j-1} 2^{l(d-4)} (l \vee 1)^{4\delta}$;
- j_n is such that $2^{j_n} \simeq \left(\frac{n}{\log n} \right)^{\frac{1}{2r+d/2}}$;
- $G(j_n) = j_n^{2\delta} 2^{-2j_n(r+1)} \log n$;
- $z_\alpha = (\alpha/2)^{-1/2}$.

Then for all $n \geq n_0(B)$, C_n satisfies (7), as well as (8) and (9) for a suitable constant $K > 0$ depending on r, s, α, α' and the parameters of the class $\mathcal{F}(r)$ with the rates

$$R_n(r) = (\log n)^{\delta + \frac{r+1}{2r+d}} n^{-\frac{r+1}{2r+d}}, \quad R_n(s) = (\log n)^{\delta + \frac{s+1}{2s+d}} n^{-\frac{s+1}{2s+d}}.$$

In particular, C_n is a near-optimal adaptive W_2 confidence set over $\mathcal{F}(s) \cup \mathcal{F}(r)$.

Remark 4 (Adaptation over ranges of classes). Note that the construction of C_n is completely independent of s , and \hat{f}_n adapts simultaneously over all $s \geq 0$. So when $d \leq 4$, C_n adapts simultaneously over all $s \geq r$, and when $d > 4$, C_n adapts simultaneously over the full window of admissible values of s .

Remark 5 (Adaptation to other parameters). We note that the construction of the confidence set in Theorem 4 does not depend on B or m , and so in fact this particular confidence set is also adaptive over $B \geq 1$ and $m > 0$, in the sense that any dependence of the minimax rates $r_n^*(r), r_n^*(s)$ on B or m are eventually accounted for by the logarithmic term in $R_n(r), R_n(s)$. (Note however that the constants in our theoretical guarantees explode as $B \rightarrow \infty$ or $m \rightarrow 0$.) However, the construction of C_n does depend on M . See [3] for more discussion on the role of M .

Remark 6 (Adapting to wider ranges of smoothnesses in high dimensions). In the $d > 4$ case, following the ideas in [3], one may still obtain adaptation over a window of the form $[0, R]$ for arbitrary $R > 0$ at the cost of removing certain troublesome portions of the classes $\mathcal{F}(r), r \in [0, R]$. In this restricted model, one can identify the smoothness of the unknown density within a window of the form $\left[r, \frac{2d-4}{d-4}r + \frac{d}{d-4}\right]$ using tests as in [3] or [30]. Once this window is identified, in particular the relevant value of r , one can use the associated confidence set as constructed in Theorem 4.

Remark 7. (Necessity of log-factors) One may ask whether it is possible to remove the log-factors in the shrinkage rates and construct a confidence set with $R_n(r) = r_n^*(r), R_n(s) = r_n^*(s)$. These log factors fundamentally arise from the use of the embedding $H^{-1,\delta} \hookrightarrow B_{21}^{-1}$ for $\delta > 1/2$. For confidence sets constructed via risk estimation we conjecture that this is a necessary step, as it is precisely the accelerated risk estimation for Hilbert space norms which enables the adaptivity of the confidence set. However, it is conceivable that another approach, such as the testing method of [7], could be used to construct W_2 confidence sets with sharp diameter shrinkage rates (although such an approach will not generalise beyond the two class problem).

Remark 8 (Weak Sobolev norms $H^{-t}, t > 0$). Our methods extend to the use of negative order Sobolev norms $H^{-t} = B_{22}^{-t}, t > 0$ as loss functions in place of $H^{-1,\delta}$ (see Appendix A for definitions). The analysis of the estimator \hat{f}_n is completely analogous, and one must suitably augment the U -statistic $U_{n,j}$ to estimate the H^{-t} loss. One finds that the resulting confidence set \tilde{C}_n adapts to any two smoothnesses $0 \leq r < s < \infty$ when $t \geq d/4$; if instead $t < d/4$, adaptation is possible over a window of smoothnesses $0 \leq r < s \leq \frac{d}{d-4t}t + \frac{2d-4t}{d-4t}r$. Moreover, in this latter case, the arguments of Section 3.3 below can be augmented to show that if s does not lie in this window, then no such confidence set can exist.

The proof of this theorem proceeds similarly to that of Proposition 2.1 in [35], and is given in Appendix B.

The confidence sets constructed above prove statements (i) and (ii) of Theorem 1.

3.3. Testing rates and non-existence of Confidence Sets

We turn now to proving the impossibility result (iii) in Theorem 1.

The question of existence of adaptive confidence sets is closely related to a composite hypothesis testing problem. This connection was identified in the first works on adaptive confidence sets; for a complete decision-theoretic overview, see [18, Chapter 8]. For $\rho \geq 0$ and $s > r \geq 0$, define the separated function class

$$\tilde{\mathcal{F}}(r, \rho) := \{f \in \mathcal{F}(r) : W_2(f, \mathcal{F}(s)) \geq \rho\}$$

We may have $\rho = 0$, in which case $\tilde{\mathcal{F}}(r, 0) = \mathcal{F}(r)$. However, if $\rho > 0$ then $\tilde{\mathcal{F}}(r, \rho)$ is a strict subset of $\mathcal{F}(r)$, disjoint from $\mathcal{F}(s)$. The testing problem we consider is

$$H_0 : f \in \mathcal{F}(s) \quad \text{vs.} \quad H_1 : f \in \tilde{\mathcal{F}}(r, \rho). \quad (16)$$

As the usefulness of a test is naturally assessed by the sum of its Type I and Type II errors, the minimax rate of testing for the problem (16) is defined as any sequence $(\rho_n^*)_{n \geq 1}$ such that

- For any $\beta' > 0$, there exists a constant $L = L(\beta')$ and a measurable test $\Psi_n : (\mathbb{T}^d)^n \rightarrow \{0, 1\}$ such that

$$\sup_{f \in \mathcal{F}(s)} \mathbb{E}_f[\Psi_n] + \sup_{f \in \tilde{\mathcal{F}}(r, L\rho_n^*)} \mathbb{E}_f[1 - \Psi_n] \leq \beta'. \quad (17)$$

- There exists some $\beta > 0$ such that for all $\rho_n = o(\rho_n^*)$,

$$\liminf_{n \rightarrow \infty} \inf_{\Psi_n} \left[\sup_{f \in \mathcal{F}(s)} \mathbb{E}_f[\Psi_n] + \sup_{f \in \tilde{\mathcal{F}}(r, \rho_n)} \mathbb{E}_f[1 - \Psi_n] \right] \geq \beta, \quad (18)$$

where the infimum ranges over the set of tests Ψ_n .

The following result characterises the role of the minimax testing rate ρ_n^* in the existence and non-existence of confidence sets. Essentially, it says ρ_n^* provides a ‘speed limit’ on how quickly the confidence set can shrink when f is in the smoother submodel $\mathcal{F}(s)$:

Lemma 2 (Proposition 8.3.6, [18]). *Let ρ_n^* be the minimax testing rate for (16), and $\tilde{r}_n(s), \tilde{r}_n(r)$ be two sequences such that $\tilde{r}_n(s) = o(\rho_n^*)$ and $\tilde{r}_n(r) = o(\tilde{r}_n(r))$. Let $\alpha, \alpha' > 0$. Then, for any $\rho_n = o(\rho_n^*)$ and $L > 0$, there does not exist any set $C_n(\alpha, X_1, \dots, X_n)$ satisfying*

- $\liminf_{n \rightarrow \infty} \inf_{f \in \mathcal{F}(s) \cup \tilde{\mathcal{F}}(r, \rho_n)} P_f(f \in C_n) \geq 1 - \alpha$,
- $\limsup_{n \rightarrow \infty} \sup_{f \in \tilde{\mathcal{F}}(r, \rho_n)} P_f(|C_n|_{W_2} > L\tilde{r}_n(r)) \leq \alpha'$,
- $\limsup_{n \rightarrow \infty} \sup_{f \in \mathcal{F}(s)} P_f(|C_n|_{W_2} > L\tilde{r}_n(s)) \leq \alpha'$,

as long as α, α' are such that $0 < 2\alpha + \alpha' < \beta$, with β as in (18).

This non-existence phenomenon occurs because any C_n satisfying the conditions of the Lemma induces a test

$$\Psi_n = 1\{C_n \cap \tilde{\mathcal{F}}(r, \rho_n') \neq \emptyset\}$$

which is uniformly consistent for the separation rate ρ_n' in the sense of (17) whenever $\rho_n = o(\rho_n')$. If we were able to choose ρ_n' to be $o(\rho_n^*)$, this would contradict the definition of the minimax testing rate ρ_n^* ; thus no such confidence set can exist. Note that the argument works for any rate $\tilde{r}_n(s) = o(\rho_n^*)$, not just the minimax rate of estimation; in particular, we can multiply the minimax estimation rate by a poly-logarithmic factor so long as there is a polynomial gap between the testing and estimation rates.

It remains to determine the minimax rate of testing for the problem (16); this is done in the following theorem.

Theorem 5. *Assume $s > r \geq 0$ and $d > 4$. Let ρ_n^* be the minimax rate of testing for the problem (16). Then there exist a constant $c > 0$ depending on the parameters of the class $\mathcal{F}(s)$ and the wavelet basis, and $n_0 = n_0(B, M)$ such that for all $n \geq n_0$,*

$$\rho_n^* \geq cn^{-\frac{r+1}{2r+d/2}}.$$

Also, (18) holds for any $\beta < 1$.

The proof of Theorem 5 is given in Appendix B, and follows a multiple-testing lower bound. Assume now that $d > 4$ and $s > \frac{2d-4}{d-4}r + \frac{d}{d-4}$. Then the minimax rate of testing ρ_n^* is slower than the minimax estimation rate $r_n^*(s)$ by a polynomial factor; in light of Lemma 2, this means there is no near-optimal

adaptive W_2 confidence set over $\mathcal{F}(s) \cup \mathcal{F}(r)$ for any practical choice of α, α' (for such a set to exist, we would require $2\alpha + \alpha' \geq 1$). This proves statement (iii) of Theorem 1. However, this does not rule out the existence of confidence sets satisfying weaker conditions than those in Definition 2, namely those listed in Lemma 2 for some $\rho_n \geq L\rho_n^*$, $L > 0$. Such sets actually exist in view of Proposition 8.3.7 of [18] and Theorem 3.

Moreover, the confidence set C_n constructed in Theorem 4 in conjunction with the argument used to prove Lemma 2 shows that the lower bound of Theorem 5 is sharp up to a poly-logarithmic factor.

4. Extension of the Theory to \mathbb{R}^d

Having provided a fairly complete resolution of the problem of adaptive W_2 confidence sets when the sample space is \mathbb{T}^d , we extend our results to the case of the unbounded sample space \mathbb{R}^d with W_1 loss. The key tool is the Kantorovich-Rubinstein duality formula ([23])

$$W_1(f, g) = \sup_{h \in \text{Lip}_1(\mathbb{R}^d)} \int_{\mathbb{R}^d} h(x)(f(x) - g(x)) \, dx, \quad (19)$$

where $\text{Lip}_1(\mathbb{R}^d)$ is the set of 1-Lipschitz functions on \mathbb{R}^d .

Our techniques do not extend to the distances W_p , $p > 1$, due to the dependence on the lower bound m in Proposition 1 (which is the analogue of (19) for $p > 1$): any density on \mathbb{R}^d must decay to 0 at infinity, so using this result yields suboptimal convergence rates, even under favourable tail conditions.

In this section, it is assumed that we observe $X_1, \dots, X_n \stackrel{\text{i.i.d.}}{\sim} f_0$ for some density f_0 on \mathbb{R}^d , and we wish to perform inference on f_0 using W_1 as the loss function.

4.1. Parameter Spaces

We use an S -regular tensor product wavelet basis of $L^2(\mathbb{R}^d)$ of the form

$$\left\{ \phi_k, \psi_{lk} : k \in \mathbb{Z}^d, l \geq 0 \right\}$$

as introduced in Appendix A (we index the ψ_{lk} using only k, l by a slight abuse of notation). We write $K_j(f)$ for the projection of f onto the first j resolution layers, as in (2). Besov norms on \mathbb{R}^d , also defined in Appendix A, are defined analogously to those on \mathbb{T}^d , and the relation (3) holds.

Our goal is to construct an adaptive confidence set for the true density f_0 using risk estimation, where the adaptation occurs with respect to the smoothness parameter s . We shall consider functions in B_{2q}^s . Unlike our previous classes $\mathcal{F}(s)$ on \mathbb{T}^d , we need not assume that our densities are bounded away from zero, or something analogous such as sufficiently slow decay in the tails. However, in order to deal with the unboundedness of the sample space \mathbb{R}^d , we must impose a moment condition.

For $\alpha, \beta > 0$, define the α, β -exponential moment of a density f as

$$\mathcal{E}_{\alpha, \beta}(f) := \int_{\mathbb{R}^d} \exp(\beta \|x\|^\alpha) f(x) \, dx = E_f \left(e^{\beta \|X\|^\alpha} \right). \quad (20)$$

Definition 4. Let $1 \leq p, q \leq \infty$, $s \geq 0$, $B \geq 1$, $M > 0$, $\alpha, \beta > 0$ and $L \geq 1$. Define the function class

$$\mathcal{G}_{s,p,q}(B, M; \alpha, \beta, L) = \left\{ f \in B_{pq}^s(\mathbb{R}^d) : \int_{\mathbb{R}^d} f = 1, \|f\|_{B_{pq}^s} \leq B, 0 \leq f \leq M \text{ a.e., } \mathcal{E}_{\alpha, \beta}(f) \leq L \right\}. \quad (21)$$

Henceforth, we fix $p = 2$ and consider $q, B, M, \alpha, \beta, L$ to be given. Define

$$\mathcal{G}(s) := \mathcal{G}_{s,2,q}(B, M; \alpha, \beta, L).$$

Observe that for M close to 0 and L close to 1, the class $\mathcal{G}(s)$ is empty. We therefore assume in the sequel that L is sufficiently large (depending on M, B) for $\mathcal{G}(s)$ to be non-empty.

The focus on $p = 2$ is quite natural in view of the material developed in the previous section, relying on risk estimation to compute the diameter of confidence sets. Combining the exponential moment condition and the bound on the B_{2q}^s -norm, we prove in Lemma 8 that densities in $\mathcal{G}(s)$ also have their B_{1q}^s -norm bounded by a constant depending on the class parameters.

4.2. Estimation Upper Bounds for W_1

As before, we should insist on our estimator \tilde{f}_n being a density almost surely. Indeed, the fact that \tilde{f}_n has total mass 1 is vital to the proof of Proposition 4 below. However, we note that there is no intrinsic requirement in (19) that f and g should be nonnegative, and so we will allow our estimators to take negative values. If a genuine density is required, one can just take the positive part of the estimator and renormalize.

The following proposition gives an upper bound on the W_1 distance which is convenient for wavelet estimators.

Proposition 4. *For any probability density f with a finite first moment and any estimator \tilde{f}_n of f which has a finite first moment almost surely, we have that*

$$W_1(\tilde{f}_n, f) \lesssim \sum_{k \in \mathbb{Z}^d} \|k\| |\langle f - \tilde{f}_n, \phi_k \rangle| + \sum_{l \geq 0} 2^{-l(\frac{d}{2}+1)} \sum_{k \in \mathbb{Z}^d} |\langle f - \tilde{f}_n, \psi_{lk} \rangle|, \quad (22)$$

where the constant depends only on the wavelet basis.

Remark 9. Let \hat{f}_n be some estimator of f , not necessarily with total mass 1. We obtain an estimator which integrates to 1 almost surely, which we call \tilde{f}_n , by renormalising the first wavelet layer of \hat{f}_n , that is, renormalising $\hat{f}_0 := K_0(\hat{f}_n)$. Then we set

$$\tilde{f}_n = \frac{\hat{f}_0}{\int \hat{f}_0(x) dx} + \sum_{l \geq 0} \sum_{k \in \mathbb{Z}^d} \langle \hat{f}_n, \psi_{lk} \rangle \psi_{lk}.$$

Note that while one can perform this procedure for any estimator \hat{f}_n , it is particularly simple for wavelet-based estimators. Assuming L_1 -consistency of \hat{f}_n , $\hat{f}_0 \rightarrow K_0(f)$ and thus $K_0(\hat{f}_n) \rightarrow K_0(f)$ in L_1 . Moreover, for the wavelet estimators we use below, this convergence occurs very fast, at the rate $n^{-\frac{S}{2S+d}}$, where S is the regularity of the wavelet basis. Thus it suffices to consider the un-normalised estimator \hat{f}_n in the decomposition (22) whenever $s \leq S - 1$, which we do in the sequel.

We first establish an upper bound for the estimation rate over the class $\mathcal{G}(s)$.

Theorem 6. *For any $s \geq 0$, there exists an estimator \hat{f}_n such that for all sufficiently large n ,*

$$\sup_{f \in \mathcal{G}(s)} E_f W_1(\hat{f}_n, f) \lesssim \begin{cases} (\log n)^{\frac{\gamma_d}{2}+1} n^{-1/2}, & d = 2, \\ (\log n)^{\frac{\gamma_d}{2}} n^{-\frac{s+1}{2s+d}}, & d \geq 3. \end{cases}$$

where γ is a constant depending on α and β only, and the constant depends on the parameters of the class $\mathcal{G}(s)$ and the wavelet basis. For $d = 1$, the empirical measure P_n satisfies

$$\sup_{f \in \mathcal{G}(s)} E_f W_1(P_n, P_f) \lesssim n^{-1/2}.$$

Remark 10. These rates are sharp up to a logarithmic factor so long as L is sufficiently large: one uses a reduction to a multiple testing problem as in the proof of the lower bounds in Proposition 2, and then uses an analogous collection of well-separated densities defined on some common compact set. For large enough L , the compact support ensures that these densities have suitable exponential moments and so belong to $\mathcal{G}(s)$.

Remark 11. An inspection of the proof reveals that in fact it suffices to assume a suitable polynomial moment, depending on s ; however, for convenience we assume an exponential moment which works for all $s \geq 0$.

The proofs of Proposition 4 and Theorem 6 are given in Appendix C. The estimator \hat{f}_n is simply a wavelet projection estimator which is zero outside of a growing compact set; the risk outside of the compact is controlled using the moment assumption.

As in the case of \mathbb{T}^d , we require an adaptive estimator.

Theorem 7. Let $d \geq 2$, and let $\gamma > 0$ be as in Theorem 6. Then there exists an estimator \hat{f}_n of f such that for all $n \geq n_0(B)$ and all $s \geq 0$,

$$\sup_{f \in \mathcal{G}(s)} E_f W_1(\hat{f}_n, f) \lesssim (\log n)^{\frac{\gamma d}{2}} \left(\frac{n}{\log n} \right)^{-\frac{s+1}{2s+d}},$$

where the constant depends on the parameters of the class $\mathcal{G}(s)$ and the wavelet basis.

The definition of \hat{f}_n and proof of Theorem 7 are given in Appendix C.

4.3. Construction of Confidence Sets

Let us now concretely state the two-class adaptation problem we wish to solve. Fix two smoothnesses $s > r \geq 0$ and consider the model $\mathcal{G}(r) = \mathcal{G}(r) \cup \mathcal{G}(s)$. Given $\alpha \in (0, 1)$, we seek a confidence set C_n which has honest coverage at level $1 - \alpha$, that is, for all n sufficiently large,

$$\inf_{f \in \mathcal{G}(r)} P_f(f \in C_n) \geq 1 - \alpha, \quad (23)$$

as well as the two diameter shrinkage conditions: for all $\alpha' > 0$ there exists a constant $K = K(\alpha') > 0$ such that

$$\sup_{f \in \mathcal{G}(r)} P_f(|C_n|_{W_1} > K R_n(r)) \leq \alpha', \quad (24)$$

$$\sup_{f \in \mathcal{G}(s)} P_f(|C_n|_{W_1} > K R_n(s)) \leq \alpha', \quad (25)$$

where $R_n(r)$ and $R_n(s)$ equal the convergence rates in Theorem 6 up to a poly-logarithmic factor.

As discussed previously, the $d = 1$ and $d = 2$ cases are straightforward given the existence of the estimator from Theorem 7, since here the convergence rates do not depend on the smoothness r . We thus restrict our attention to the case $d \geq 3$.

Let X_1, \dots, X_{2n} be an i.i.d. sample from the unknown $f \in \mathcal{G}(r)$. We split the sample as before into two equal halves, indexed by $\mathcal{S}^1 = 1, \dots, n$ and $\mathcal{S}^2 = \{n+1, \dots, 2n\}$, and denote by $P^{(i)}, E^{(i)}$ probabilities and expectations taken over \mathcal{S}^i . We wish to construct a confidence set via risk estimation, centred at the adaptive estimator \hat{f}_n from Theorem 7, which we compute using \mathcal{S}^1 . Proposition 4 provides a natural upper bound for $W_1(f, \hat{f}_n)^2$ which we then decompose into several terms. Define the thresholds $\kappa_{-1n} = \kappa_{0n} \simeq (\log n)^\gamma$, $\kappa_{ln} = 2^l \kappa_{0n}$ for γ chosen as in Theorem 6. Applying the Cauchy-Schwarz inequality several times, we obtain the bound

$$\begin{aligned} W_1(f, \hat{f}_n)^2 \leq & 3 \left((\log n)^{\gamma(d+2)} \left[\sum_{\|k\|_\infty \leq \kappa_{-1n}} \langle f - \hat{f}_n, \phi_k \rangle^2 + j \sum_{l < j} 2^{-2l} \sum_{\|k\|_\infty \leq \kappa_{ln}} \langle f - \hat{f}_n, \psi_{lk} \rangle^2 \right] \right. \\ & + \left[\sum_{l \geq j} 2^{-l(\frac{d}{2}+1)} \sum_{\|k\|_\infty \leq \kappa_{ln}} |\langle f - \hat{f}_n, \psi_{lk} \rangle| \right]^2 \\ & \left. + \left[\sum_{\|k\|_\infty > \kappa_{-1n}} \|k\| |\langle f, \phi_k \rangle| + \sum_{l \geq 0} 2^{-l(\frac{d}{2}+1)} \sum_{\|k\|_\infty > \kappa_{ln}} |\langle f, \psi_{lk} \rangle| \right]^2 \right). \end{aligned} \quad (26)$$

The final term is controlled using the moment assumption on $f \in \mathcal{G}(r)$; indeed, from the proof of Theorem 6 we have that for all $f \in \mathcal{G}(r)$, this term is bounded above by

$$\Delta_n := C(d) L^2 (\log n)^{2\gamma} n^{-1}, \quad (27)$$

where $C(d)$ is a constant depending only on d and the wavelet basis.

We next consider the remaining terms in (26). We introduce pseudo-distances $\tilde{W}^{(n,j)}(f, g)$ defined as

$$\begin{aligned} \tilde{W}^{(n,j)}(f, g) = & \left[\sum_{\|k\|_\infty \leq \kappa_{-1n}} \langle f - g, \phi_k \rangle^2 + j \sum_{l < j} 2^{-2l} \sum_{\|k\|_\infty \leq \kappa_{ln}} \langle f - g, \psi_{lk} \rangle^2 \right]^{1/2} \\ & + \sum_{l \geq j} 2^{-l(\frac{d}{2}+1)} \sum_{\|k\|_\infty \leq \kappa_{ln}} |\langle f - g, \psi_{lk} \rangle|. \end{aligned} \quad (28)$$

Observe that for $f, g \in \mathcal{G}(r)$,

$$W_1(f, g) \leq \sqrt{3(\log n)^{\gamma(d+2)}} \cdot \tilde{W}^{(n,j)}(f, g) + \sqrt{3\Delta_n};$$

this is true uniformly over $r \geq 0$. Since $\sqrt{\Delta_n}$ converges (up to a logarithmic factor) at the parametric rate, this means that any diameter shrinkage condition with respect to $\tilde{W}^{(n,j)}$ provides an analogous shrinkage condition for W_1 , with only a slightly worse rate. Moreover, the first part of $\tilde{W}^{(n,j)}(f, g)$ is

well-suited to estimation using a U -statistic. To this end, define the U -statistic

$$V_{n,j} = V_{n,j}(\hat{f}_n) := \frac{2}{n(n-1)} \sum_{i < i', i, i' \in \mathcal{S}^2} \left[\sum_{\|k\|_\infty \leq \kappa_{-1n}} \left(\phi_k(X_i) - \langle \hat{f}_n, \phi_k \rangle \right) \left(\phi_k(X_{i'}) - \langle \hat{f}_n, \phi_k \rangle \right) \right. \\ \left. + j \sum_{l < j} 2^{-2l} \sum_{\|k\|_\infty \leq \kappa_{ln}} \left(\psi_{lk}(X_i) - \langle \hat{f}_n, \psi_{lk} \rangle \right) \left(\psi_{lk}(X_{i'}) - \langle \hat{f}_n, \psi_{lk} \rangle \right) \right]. \quad (29)$$

Clearly we have that $E_f^{(2)} V_{n,j}$ is equal to the square of the first term in (28) with f, \hat{f}_n in place of f, g . Analogously to Lemma 1, one shows that $V_{n,j}$ has small variance.

Lemma 3. *For $f \in L_\infty(\mathbb{R}^d)$, we have that, for some constant C_d depending only on d and the wavelet basis,*

$$\begin{aligned} \text{Var}_f^{(2)}(V_{n,j}) &\leq \frac{C_d}{2} \left(\frac{j^2 \|f\|_\infty^2 (\log n)^{\gamma_d}}{n(n-1)} \sum_{l < j} 2^{l(d-4)} \right. \\ &\quad \left. \dots + \frac{\|f\|_\infty}{n} \left[\sum_{\|k\|_\infty \leq \kappa_{-1n}} \langle f - \hat{f}_n, \phi_k \rangle^2 + j^2 \sum_{l < j} 2^{-4l} \sum_{\|k\|_\infty \leq \kappa_{ln}} \langle f - \hat{f}_n, \psi_{lk} \rangle^2 \right] \right) \\ &\leq C_d \left(\frac{j^2 \|f\|_\infty^2 (\log n)^{\gamma_d}}{n(n-1)} \sum_{l < j} 2^{l(d-4)} + \tilde{W}^{(n,j)}(f, \hat{f}_n)^2 \right) \\ &=: \lambda_{j,n}^2(f). \end{aligned}$$

For the second part of $\tilde{W}^{(n,j)}(f, \hat{f}_n)$, we use the concentration arguments from the proof of Theorem 7 to show that this term is suitably small with high probability uniformly over $f \in \mathcal{G}(r)$.

Given a sequence (j_n) , we write $\tilde{W}^{(n)}$ for $\tilde{W}^{(n,j_n)}$, and V_{j_n} for V_{n,j_n} .

Theorem 8. *Let $d \geq 3$. Fix $B \geq 1, M > 0, \alpha, \beta, L > 0, 1 \leq q \leq \infty$, and $s > r \geq 0$. Let $\gamma \geq 1$ be as in Theorem 6. If $d > 4$, assume additionally that $s \leq \frac{2d-4}{d-4}r + \frac{d}{d-4}$. Fix $\alpha \in (0, 1)$. Consider the confidence set based on a sample of size $2n$ given by*

$$C_n = \left\{ g \in \mathcal{G}(r) : \tilde{W}^{(n)}(g, \hat{f}_n) \leq C(d) \sqrt{z_\alpha \lambda_{n,j_n}(g) + V_{j_n} + G_{j_n}} \right\} \quad (30)$$

where \hat{f}_n is computed on \mathcal{S}^1 , V_{j_n} is computed on \mathcal{S}^2 , $C(d)$ is a constant depending on d and the wavelet basis, and:

- $\lambda_{n,j_n}(g)$ is as in Lemma 3;
- j_n is such that $2^{j_n} \simeq \left(\frac{n}{\log n} \right)^{\frac{1}{2r+d/2}}$;
- $G_{j_n} = (\log n)^{\gamma_d+1} 2^{-2j_n(r+1)}$;
- $z_\alpha = (\alpha/2)^{-1/2}$.

Then for all $n \geq n_0(B)$, C_n satisfies (23), as well as (24) and (25) for a suitable constant $K > 0$ with the rates

$$R_n(r) = (\log n)^{\gamma(d+1)} \left(\frac{n}{\log n} \right)^{-\frac{r+1}{2r+d}}, \quad R_n(s) = (\log n)^{\gamma(d+1)} \left(\frac{n}{\log n} \right)^{-\frac{s+1}{2s+d}}.$$

In particular, C_n is a near-optimal adaptive W_1 confidence set over $\mathcal{F}(s) \cup \mathcal{F}(r)$.

The proof is almost identical to that of Theorem 4; a more detailed argument can be found in Appendix C. In particular, this proves statements (i) and (ii) of Theorem 2.

4.4. Non-Existence of Confidence Sets

We now turn to the non-existence result (iii) in Theorem 2, a consequence of Lemma 2 (which holds in a general decision theoretic framework). We therefore require a lower bound on the minimax separation rate in the testing problem

$$H_0 : f \in \mathcal{G}(s) \quad \text{vs.} \quad H_1 : f \in \tilde{\mathcal{G}}(r, \rho), \quad (31)$$

where the separated alternative $\tilde{\mathcal{G}}(r, \rho)$ is defined analogously to before:

$$\tilde{\mathcal{G}}(r, \rho) := \{f \in \mathcal{G}(r) : W_1(f, \mathcal{G}(s)) \geq \rho\}.$$

Theorem 9. Assume that $d > 4$ and $s > r \geq 0$. Let ρ_n^* be the minimax rate of testing for the problem (31). Then, for L sufficiently large in (21), there exist a constant $c > 0$ depending on the parameters of the class $\mathcal{G}(s)$ and the wavelet basis, and $n_0 = n_0(B, M)$ such that for all $n \geq n_0$,

$$\rho_n^* \geq cn^{-\frac{r+1}{2r+d/2}}.$$

Also, (18) holds for any $\beta < 1$.

The proof is given in Appendix C, and is similar to the proof of Theorem 5. As before, this implies statement (iii) of Theorem 2.

Appendix A: Wavelets and Besov Spaces

Here we introduce the wavelet bases we use, and define the various norms and spaces used in our analysis.

A.1. Wavelet Bases of \mathbb{R}^d and \mathbb{T}^d

Let $S \in \mathbb{N}$. We begin with an S -regular wavelet basis of $L_2(\mathbb{R})$ generated by scaling function Φ and wavelet function Ψ ,

$$\left\{ \Phi_k = \Phi(\cdot - k), \Psi_{lk} = 2^{l/2} \Psi(2^l(\cdot - k)) : l \geq 0, k \in \mathbb{Z} \right\}.$$

Concretely, we take sufficiently regular Daubechies wavelets: see [12], [18, Chapter 4], [28] for details. Such a wavelet basis has the following properties:

- Φ, Ψ are in $C^S(\mathbb{R})$, $\int_{\mathbb{R}} \Phi = 1$, and Ψ is orthogonal to polynomials of degree $< S$.
- $\|\sum_k |\Phi_k|\|_{\infty} \lesssim 1$, and $\|\sum_k |\Psi_{lk}|\|_{\infty} \lesssim 2^{l/2}$ for a constant depending only on Ψ .
- Letting $V_j = \text{span}(\Phi_k, \Psi_{lk} : l < j)$, for any $f \in V_j$ the following Bernstein estimate holds:

$$\|\nabla f\|_p \lesssim 2^j \|f\|_p,$$

for a constant depending only on the wavelet basis.

- Φ, Ψ are compactly supported.

We then form a tensor product basis of $L_2(\mathbb{R}^d)$ as follows. Let $\mathcal{I} = \{0, 1\}^d \setminus \{0\}$. Define

$$\phi(x) = \Phi(x_1) \cdots \Phi(x_d), \quad x \in \mathbb{R}^d$$

and, writing $\Psi^0 = \Phi, \Psi^1 = \Psi$,

$$\psi^{\iota} = \Psi^{\iota_1}(x_1) \cdots \Psi^{\iota_d}(x_d), \quad \iota \in \mathcal{I}.$$

Then ([18, Section 4.3.6])

$$\left\{ \phi_k = \phi(\cdot - k), \psi_{lk}^{\iota} = 2^{ld/2} \psi^{\iota}(2^l x - k) : l \geq 0, k \in \mathbb{Z}^d, \iota \in \mathcal{I} \right\}$$

defines a wavelet basis of $L_2(\mathbb{R}^d)$. We omit ι from our notation and simply write ψ_{lk} with k now implicitly taking values in $\mathbb{Z}^d \times \mathcal{I}$; any sum over k is to be understood as over all $\iota \in \mathcal{I}$ as well.

- 1) ϕ, ψ are in $C^S(\mathbb{T}^d)$, $\int_{\mathbb{R}^d} \phi = 1$, and ψ is orthogonal to polynomials of degree $< S$.
- 2) $\|\sum_k |\phi_k|\|_{\infty} \lesssim 1$, and $\|\sum_k |\psi_{lk}|\|_{\infty} \lesssim 2^{ld/2}$ for a constant depending only on ψ .
- 3) ϕ, ψ are compactly supported.

These properties follow elementarily from the previously stated properties of Φ and Ψ . Property 3) is used crucially in our analysis on \mathbb{R}^d . Notably, this precludes certain common choices of wavelet basis, such as the Meyer basis.

These properties imply the following relationship between L_p -norms of functions and the ℓ_p -norms of their wavelet coefficients (by an abuse of notation we denote both of these norms by $\|\cdot\|_p$).

Lemma 4. *For any $l \geq 0$, any $p \in [1, \infty]$ and any $c \in \mathbb{R}^{\mathbb{Z}^d}$, we have that*

$$\left\| \sum_{k \in \mathbb{Z}^d} c_k \psi_{lk} \right\|_p \simeq 2^{ld(1/2-1/p)} \|c\|_p,$$

where the constants depend on ψ and p only.

When working on \mathbb{T}^d , we use the tensor product wavelet basis induced by the periodisations of Φ, Ψ ; see [18, Section 4.3.4] for details. This produces a basis of $L_2(\mathbb{T}^d)$ with the following properties:

- 1) $\psi(x) = \prod_{i=1}^d \psi^{(i)}(x_i)$ for some univariate functions $\psi^{(i)}$.
- 2) Setting $\psi_{lk}(\cdot) = 2^{ld/2} \psi(\cdot - 2^{-l}k)$ for $l \geq 0, k \in \mathbb{Z}^d \cap [0, 2^l)^d$, the set

$$\left\{ \phi, \psi_{lk} : l \geq 0, k \in \mathbb{Z}^d \cap [0, 2^l)^d \right\}$$

forms an orthonormal basis of $L_2(\mathbb{T}^d)$. By an abuse of notation, we re-index in k such that $k \in \mathbb{Z}$ varies between $0 \leq k < 2^{ld}$.

- 3) ψ is in $C^S(\mathbb{T}^d)$, and is orthogonal to polynomials of degree $< S$.
- 4) $\|\sum_k |\psi_{lk}|\|_\infty \lesssim 2^{ld/2}$, for a constant depending only on ψ .
- 5) Letting $V_j = \text{span}(\phi, \psi_{lk} : l < j)$, for any $f \in V_j$ the following Bernstein estimate holds:

$$\|\nabla f\|_p \lesssim 2^j \|f\|_p,$$

for a constant depending only on the wavelet basis.

Again, these are basic consequences of properties of Φ, Ψ , and enable the proof of Proposition 1; compare to Appendix C of [41].

A.2. Besov Spaces

In this section, we let (ϕ_k, ψ_{lk}) denote either the S -regular tensor product Daubechies wavelet basis of $L_2(\mathbb{R}^d)$, or the S -regular tensor product periodised Daubechies wavelet basis of $L_2(\mathbb{T}^d)$. It should be understood that any summation is over the full range of indices, for example $\sum_k \psi_{lk}$ denotes $\sum_{k \in \mathbb{Z}^d} \psi_{lk}$ in the \mathbb{R}^d case and $\sum_{k=0}^{2^{ld}-1} \psi_{lk}$ in the \mathbb{T}^d case. We further let \mathcal{D} be either the class of tempered distributions on \mathbb{R}^d , or the class of periodic tempered distributions on \mathbb{T}^d .

Let $1 \leq p \leq \infty$, $1 \leq q \leq \infty$, $s \in \mathbb{R}$, $s < S$. For $f \in \mathcal{D}$, we define the Besov norm

$$\|f\|_{B_{pq}^s} = \|\langle f, \phi \cdot \rangle\|_p + \left(\sum_{l \geq 0} \left[2^{ls} 2^{ld(\frac{1}{2} - \frac{1}{p})} \|\langle f, \psi_l \cdot \rangle\|_p \right]^q \right)^{1/q}, \quad (32)$$

where $\|\cdot\|_p$ is the ℓ_p -norm. When $q = \infty$, the norm is defined as

$$\|f\|_{B_{p\infty}^s} = \|\langle f, \phi \cdot \rangle\|_p + \sup_{l \geq 0} 2^{ls} 2^{ld(\frac{1}{2} - \frac{1}{p})} \|\langle f, \psi_l \cdot \rangle\|_p. \quad (33)$$

We then define the corresponding Besov space B_{pq}^s as

$$B_{pq}^s = \left\{ f \in \mathcal{D} : \|f\|_{B_{pq}^s} < \infty \right\}. \quad (34)$$

We will write $B_{pq}^s(\mathbb{R}^d)$ or $B_{pq}^s(\mathbb{T}^d)$ to remove any ambiguity over the choice of domain, whenever it arises.

The definition of B_{pq}^s is independent of the wavelet basis used, that is, using a different (sufficiently regular) basis in the definition (32) produces an equivalent norm. Moreover, using a C^∞ basis such as the Meyer basis enables us to define B_{pq}^s concurrently for all $s \in \mathbb{R}$.

A.3. The Case of the Unit Cube

We can also define a ‘boundary-corrected’ wavelet basis of $L_2([0, 1]^d)$ based on Φ, Ψ as in [11]; see also [18, Section 4.3.5]. Such a basis possesses completely analogous properties to properties 1)-5) of the periodised basis of $L_2(\mathbb{T}^d)$; moreover, all Besov spaces defined on \mathbb{T}^d are defined on the unit cube $[0, 1]^d$ by replacing the periodised wavelet basis with the boundary-corrected wavelet basis (as used in [40]). Thus all of our results for \mathbb{T}^d hold also for the case of $[0, 1]^d$.

Appendix B: Proofs for Section 3

We first give the definition of our adaptive estimator. The estimator is based on the empirical wavelet coefficients, defined as

$$\hat{f}_{lk} := \frac{1}{n} \sum_{i=1}^n \psi_{lk}(X_i).$$

We also write f_l and \hat{f}_l for the vectors of coefficients $(f_{lk} : 0 \leq k < 2^{ld})$ and $(\hat{f}_{lk} : 0 \leq k < 2^{ld})$ respectively.

Next, define the truncation point l_{\max} such that

$$2^{l_{\max}} \simeq \left(\frac{n}{\log n} \right)^{1/d},$$

and for $0 \leq l \leq l_{\max}$, define the thresholds

$$\tau_l := \tau 2^{\frac{ld}{2}} \left(\frac{\log n}{n} \right)^{1/2},$$

for some $\tau > 0$ to be chosen below, depending only on B, d, M and the wavelet basis. We then define

$$\hat{f}_n := 1 + \sum_{l=0}^{l_{\max}} 1_{\{\|\hat{f}_l\|_2^2 > \tau_l^2\}} \sum_{k=0}^{2^{ld}-1} \hat{f}_{lk} \psi_{lk}. \quad (35)$$

To prove Theorem 3, we must first collect some results on the expectation and concentration of the empirical wavelet coefficients \hat{f}_{lk} .

Lemma 5. *Let $f \in \mathcal{F}(s)$ and let \hat{f}_{lk} be the empirical wavelet coefficients of f based on a sample of n observations. Then for every $t \geq 2$ there exists a constant C_t depending only on t such that for all $l \geq 0$ satisfying $2^{ld} \leq n$,*

$$E \left| \hat{f}_{lk} - f_{lk} \right|^t \leq C_t M \|\psi\|_{\infty}^{t-2} n^{-t/2}.$$

For $t = 2$, the proof is immediate from the i.i.d. assumption on the data, the orthonormality of the wavelets and the bound $\|f\|_{\infty} \leq M$. For $t > 2$, the result follows from the $t = 2$ case and Hoffmann-Jørgensen's inequality ([18, Theorem 3.1.22], [19]). We also require a concentration result for the \hat{f}_{lk} ; for this we use Bernstein's inequality ([18, Theorem 3.1.7]).

Proposition 5. *[Bernstein's Inequality] Let Y_1, \dots, Y_n be independent centred random variables which are almost surely bounded by $c > 0$ in absolute value. Let $\sigma^2 = n^{-1} \sum_{i=1}^n E Y_i^2$ and $S_n = \sum_{i=1}^n Y_i$. Then for all $u \geq 0$,*

$$P(|S_n| > u) \leq 2 \exp \left(- \frac{u^2}{2n\sigma^2 + \frac{2cu}{3}} \right).$$

For fixed l, k and $f \in \mathcal{F}(s)$, the random variables $(\psi_{lk}(X_i) - f_{lk})$ are i.i.d., centred, bounded by $2^{ld/2} \|\psi\|_\infty =: c_l$, and have variance bounded by M . Thus from Bernstein's inequality, we deduce that

$$P_f \left(|\hat{f}_{lk} - f_{lk}| > u \right) \leq 2 \exp \left(-\frac{nu^2}{2M + \frac{2c_l u}{3}} \right). \quad (36)$$

We also need a result on wavelet approximations in the $H^{-1,\delta}$ norm to control bias terms. The following lemma about the error of j -level approximations to Besov functions is standard; see Propositions 4.3.8 and 4.3.14 in [18], for instance.

Lemma 6. *Let $0 \leq s < S$ and $1 \leq q \leq \infty$, $\delta \in \mathbb{R}$. Then for $f \in B_{2q}^s$, we have that*

$$\|K_j(f) - f\|_{H^{-1,\delta}} \leq C \sup_{l \geq j} \left(2^{-l(s+1)} l^\delta \right) \|f\|_{B_{2q}^s}, \quad (37)$$

where the constant C depends only on the wavelet basis. In particular, for $j \geq 1 \vee \frac{\delta}{s+1}$, we have that

$$\|K_j(f) - f\|_{H^{-1,\delta}} \leq C 2^{-j(s+1)} j^\delta \|f\|_{B_{2q}^s}$$

Proof of Theorem 3. Fix $f \in \mathcal{F}(s)$. Define $l_n(s)$ such that

$$2^{l_n(s)} \simeq B^{\frac{1}{s}} \left(\frac{n}{\log n} \right)^{\frac{1}{2s+d}};$$

for all sufficiently large n depending on B , we have that $l_n(s) < l_{\max}$. We then decompose the risk as follows:

$$\begin{aligned} \|f - \hat{f}_n\|_{H^{-1,\delta}}^2 &= \sum_{l=0}^{l_n(s)} 2^{-2l} (l \vee 1)^{2\delta} \|\langle f - \hat{f}_n, \psi_l \rangle\|_2^2 + \sum_{l=l_n(s)+1}^{l_{\max}} 2^{-2l} l^{2\delta} \|\langle f - \hat{f}_n, \psi_l \rangle\|_2^2 \\ &\quad + \sum_{l>l_{\max}} 2^{-2l} l^{2\delta} \|\langle f, \psi_l \rangle\|_2^2 \\ &=: I + II + III. \end{aligned} \quad (38)$$

This is a bias-stochastic decomposition, where we have further divided the stochastic term into terms I and II .

We first deal with the bias term III : a direct application of Lemma 6 gives

$$\begin{aligned} III &= \|K_{l_{\max}}(f) - f\|_{H^{-1,\delta}}^2 \\ &\lesssim l_{\max}^{2\delta} 2^{-2l_{\max}(s+1)} \\ &= o \left((\log n)^{2\delta} \left(\frac{n}{\log n} \right)^{-\frac{2(s+1)}{2s+d}} \right) \end{aligned}$$

for a constant depending on B and the wavelet basis.

Next, we deal with term I . For any $l \geq 0$, by the triangle inequality we have that

$$\|\langle f - \hat{f}_n, \psi_l \cdot \rangle\|_2 \leq \|f_l \cdot - \hat{f}_l \cdot\|_2 + \|\hat{f}_l \cdot\|_2 1_{\{\|\hat{f}_l \cdot\|_2 \leq \tau\}} \leq \|f_l \cdot - \hat{f}_l \cdot\|_2 + \tau 2^{ld/2} \sqrt{\frac{\log n}{n}}.$$

Using Lemma 5 to control the expectation of the square of the first term, we see that

$$\begin{aligned} E_f(I) &\lesssim \sum_{l=0}^{l_n(s)} 2^{-2l} (l \vee 1)^{2\delta} \left[2^{ld} n^{-1} + \tau^2 2^{ld} \frac{\log n}{n} \right] \\ &\lesssim \tau^2 \frac{\log n}{n} (l_n(s))^{2\delta} \sum_{l=0}^{l_n(s)} 2^{l(d-2)}, \end{aligned}$$

for n large enough. Note that $l_n(s) \lesssim \log n$. Thus when $d = 2$, the sum contributes at most some power of $\log n$, and so $E_f(I)$ is clearly sufficiently small. For $d > 2$, the final term dominates the sum and so using the definition of $l_n(s)$,

$$E_f(I) \lesssim \tau^2 (\log n)^{2\delta} \left(\frac{n}{\log n} \right)^{-\frac{2(s+1)}{2s+d}}$$

as required.

Lastly, we must analyse term II . Since we consider resolution levels $l > l_n(s)$, we have that

$$\|f_l \cdot\|_2 \leq B 2^{-ls} < B 2^{-l_n(s)s} \simeq \left(\frac{n}{\log n} \right)^{-\frac{s}{2s+d}},$$

for a constant depending only on B . Moreover,

$$\tau_l = \tau 2^{ld/2} \left(\frac{n}{\log n} \right)^{-1/2} > \tau 2^{l_n(s)d/2} \left(\frac{n}{\log n} \right)^{-1/2} \geq \tau \left(\frac{n}{\log n} \right)^{-\frac{s}{2s+d}},$$

and so for τ chosen sufficiently large depending only on B , we have that $\|f_l \cdot\|_2 \leq \tau_l/2$. Define events

$$A_{l,n} := \left\{ \|\hat{f}_l \cdot\|_2 \leq \tau_l \right\}, \quad l_n(s) < l \leq l_{\max}.$$

Then by the above observations, the triangle inequality, a union bound and the bound (36), we have that

$$\begin{aligned} P_f(A_{l,n}^c) &\leq P_f(\|\hat{f}_l \cdot - f_l \cdot\|_2 > \tau_l/2) \\ &\leq \sum_{k=0}^{2^{ld}-1} P_f \left(|\hat{f}_{lk} - f_{lk}| > \frac{\tau}{2} \sqrt{\frac{\log n}{n}} \right) \\ &\leq 2^{ld} \cdot 2 \exp \left(-\frac{\tau^2 n \log n / 4}{2Mn + \tau c_l \sqrt{n \log n} / 3} \right) \\ &\lesssim \frac{n}{\log n} \exp(-C\tau \log n), \end{aligned} \tag{39}$$

for τ large enough depending on M and the wavelet basis, as $l \leq l_{\max}$ and so $2^l \leq (n/\log n)^{1/d}$. Here, C is an absolute constant. Note that on the event $A_{l,n}^c$, $\langle \hat{f}_n, \psi_{lk} \rangle = \hat{f}_{lk}$, whereas on $A_{l,n}$, $\langle \hat{f}_n, \psi_{lk} \rangle = 0$. Thus for $l_n(s) < l \leq l_{\max}$,

$$E_f \|\langle \hat{f}_n - f, \psi_l \cdot \rangle\|_2^2 1_{A_{l,n}} \leq \|\langle f, \psi_l \cdot \rangle\|_2^2 \lesssim 2^{-2ls} \quad (40)$$

for some constant depending on B , using (3). Next, using Cauchy-Schwarz in conjunction with (39) and Lemma 5,

$$\begin{aligned} E_f \|\langle \hat{f}_n^T - f, \psi_l \cdot \rangle\|_2^2 1_{A_{l,n}^c} &= \sum_{k=0}^{2^{ld}-1} E_f |\hat{f}_{lk} - f_{lk}|^2 1_{A_{l,n}^c} \\ &\leq \sum_{k=0}^{2^{ld}-1} \left(E_f |\hat{f}_{lk} - f_{lk}|^4 \right)^{1/2} \left(P_f(A_{l,n}^c) \right)^{1/2} \\ &\lesssim 2^{ld} (n \log n)^{-1/2} n^{-C\tau/2}. \end{aligned} \quad (41)$$

Combining the estimates (40) and (41), we may bound II as follows:

$$\begin{aligned} E_f(II) &\lesssim \sum_{l=l_n(s)+1}^{l_{\max}} 2^{-2l} l^{2\delta} \left[2^{-2ls} + 2^{ld} (n \log n)^{-1/2} n^{-C\tau/2} \right] \\ &\lesssim (\log n)^{2\delta} \left[2^{-2(s+1)l_n(s)} + (n \log n)^{-1/2} n^{-C\tau/2} \sum_{l \leq l_{\max}} 2^{l(d-2)} \right]. \end{aligned}$$

By the definition of $l_n(s)$, the first term is of the correct order. It remains to consider the second term. When $d = 2$ the sum contributes a logarithmic factor and so the second term is clearly sufficiently small. When $d > 2$, the sum is dominated by its final term and so the second term inside the brackets is of order

$$(n \log n)^{-1/2} n^{-C\tau/2} 2^{l_{\max}(d-2)} \simeq \log n^{-1/2} n^{\frac{1}{2} - \frac{2}{d} - \frac{C\tau}{2}};$$

by choosing τ sufficiently large, we can make this term sufficiently small for all $s \geq 0$. This concludes the proof. \square

We will also later require the following lemma, which gives control of the B_{2q}^s norm of the estimator \hat{f}_n .

Lemma 7. *Under the hypotheses of Theorem 3, given $\alpha \in (0, 1)$ there exists $n_0 = n_0(\alpha)$ such that for all $n \geq n_0$ and any $f \in \mathcal{F}(s)$, with P_f -probability at least $1 - \alpha$,*

$$\|\hat{f}_n\|_{B_{2q}^s} \lesssim B + \tau B^{d/2s},$$

where the constant depends on d, q only.

Proof. Let $l_n(s), A_{l,n}$ be as in the previous proof. Further define events $B_{l,n} = \{\|\hat{f}_{l\cdot} - f_{l\cdot}\|_2 \leq \tau_l\}$, and

$$A_n = \left(\bigcap_{0 \leq l \leq l_n(s)} B_{l,n} \right) \cap \left(\bigcap_{l_n(s) < l \leq l_{\max}} A_{l,n} \right).$$

We have from (39), which holds with $B_{l,n}$ in place of $A_{l,n}$ when $l \leq l_n(s)$, and a union bound that

$$P_f(A_n^c) \lesssim l_{\max} \frac{n}{\log n} \exp(-C\tau \log n) \lesssim n \exp(-C\tau \log n)$$

and so by choosing $\tau > 0$ sufficiently large (independently of α), we can make this smaller than α for all sufficiently large n . Then on the event A_n , using $(a+b)^q \leq 2^{q-1}(a^q + b^q)$,

$$\begin{aligned} \|\hat{f}_n\|_{B_{2q}^s}^q &= 1 + \sum_{l=0}^{l_{\max}} 2^{lqs} 1_{\{\|\hat{f}_{l\cdot}\|_2 > \tau_l\}} \|\hat{f}_{l\cdot}\|_2^q \\ &\lesssim 1 + \sum_{l=0}^{l_n(s)} 2^{lqs} \|f_{l\cdot}\|_2^q + \sum_{l=0}^{l_n(s)} 2^{lqs} \|\hat{f}_{l\cdot} - f_{l\cdot}\|_2^q \\ &\leq \|f\|_{B_{2q}^s}^q + \sum_{l=0}^{l_n(s)} 2^{lqs} \tau_l^q \\ &= B^q + \tau^q \left(\frac{\log n}{n} \right)^{q/2} \sum_{l=0}^{l_n(s)} 2^{lq(\frac{d}{2}+s)} \\ &\lesssim B^q + \tau^q B^{dq/2s}, \end{aligned}$$

by choice of $l_n(s)$, since the sum is dominated by its largest term. □

Proof of Lemma 1. The kernel of the U -statistic is

$$R(x, y) = \sum_{l \leq j-1} 2^{-2l} (l \vee 1)^{2\delta} \sum_{k=0}^{2^l-1} \left[(\psi_{lk}(x) - \langle \psi_{lk}, \tilde{f}_n \rangle) (\psi_{lk}(y) - \langle \psi_{lk}, \tilde{f}_n \rangle) \right]$$

which is symmetric, and so has Hoeffding decomposition (see Section 11.4 of [38])

$$\begin{aligned} U_n(\tilde{f}_n) - E_f^{(2)} U_n(\tilde{f}_n) &= \frac{2}{n} \sum_{i \in \mathcal{S}^2} (\pi_1 R)(X_i) + \frac{2}{n(n-1)} \sum_{i < i', i, i' \in \mathcal{S}^2} (\pi_2 R)(X_i, X_{i'}) \\ &=: L_n + D_n, \end{aligned} \tag{42}$$

with linear kernel

$$(\pi_1 R)(x) = \sum_{l \leq j-1} 2^{-2l} (l \vee 1)^{2\delta} \sum_{k=0}^{2^l-1} \left[(\psi_{lk}(x) - \langle \psi_{lk}, f \rangle) \langle \psi_{lk}, f - \tilde{f}_n \rangle \right]$$

and degenerate kernel

$$(\pi_2 R)(x, y) = \sum_{l \leq j-1} 2^{-2l} (l \vee 1)^{2\delta} \sum_{k=0}^{2^{ld}-1} [(\psi_{lk}(x) - \langle \psi_{lk}, f \rangle)(\psi_{lk}(y) - \langle \psi_{lk}, f \rangle)].$$

One checks that L_n and D_n are uncorrelated. It thus remains to bound their variances separately. For $\text{Var}^{(2)}(L_n)$, we use the uncentred version of the kernel $\pi_1 R$ and orthonormality of the wavelet basis

$$\begin{aligned} \text{Var}^{(2)}(L_n) &\leq \frac{4}{n} \int \left(\sum_{l \leq j-1} 2^{-2l} (l \vee 1)^{2\delta} \sum_{k=0}^{2^{ld}-1} \psi_{lk}(x) \langle \psi_{lk}, f - \tilde{f}_n \rangle \right)^2 f(x) dx \\ &\leq \frac{4\|f\|_\infty}{n} \left(\max_{l \geq -1} 4^{-l} (1 \vee l)^{2\delta} \right) \sum_{l \leq j-1} 2^{-2l} (l \vee 1)^{2\delta} \sum_{k=0}^{2^{ld}-1} \langle \psi_{lk}, f - \tilde{f}_n \rangle^2 \\ &= \frac{4\|f\|_\infty}{n} \left(\max_{l \geq -1} 4^{-l} (1 \vee l)^{2\delta} \right) \|K_j(f - \tilde{f}_n)\|_{H^{-1}, \delta}^2. \end{aligned}$$

We next bound $\text{Var}^{(2)}(D_n)$. By the degeneracy of the kernel, the summands are uncorrelated. So

$$\begin{aligned} \text{Var}^{(2)}(D_n) &\leq E^{(2)} \left(\frac{2}{n(n-1)} \sum_{i < i', i, i' \in \mathcal{S}^2} (\pi_2 R)(X_i, X_{i'}) \right)^2 \\ &\leq \frac{2}{n(n-1)} E_f^{(2)} \left(\sum_{l \leq j-1} 2^{-2l} (l \vee 1)^{2\delta} \sum_{k=0}^{2^{ld}-1} [\psi_{lk}(X_i) \psi_{lk}(X_{i'})] \right)^2 \\ &\leq \frac{2\|f\|_\infty^2}{n(n-1)} \sum_{l \leq j-1} 2^{-4l} (l \vee 1)^{4\delta} \sum_{k=0}^{2^{ld}-1} \left(\int \psi_{lk}(x)^2 dx \right)^2 \\ &= \frac{2\|f\|_\infty^2}{n(n-1)} \sum_{l \leq j-1} 2^{l(d-4)} (l \vee 1)^{4\delta}, \end{aligned}$$

using the orthonormality of the wavelet basis. Combining these two estimates concludes the proof. \square

Proof of Theorem 4. We first establish the coverage condition (7). By Lemma 7, for all n sufficiently large we have with P_f -probability at least $1 - \alpha/2$ that \hat{f}_n is in a B_{2q}^s -norm ball of constant radius. Thus for any $f \in \mathcal{F}(r)$, with P_f -probability at least $1 - \alpha/2$, for $n \geq n_0(B, \alpha)$ we have from (37) that

$$\|K_{j_n}(f - \hat{f}_n) - (f - \hat{f}_n)\|_{H^{-1}, \delta}^2 \leq G(j_n).$$

By conditioning on this event, we have that

$$\begin{aligned} P_f(f \in C_n) &= P_f \left(U_{n,j}(\hat{f}_n) - \|f - \hat{f}_n\|_{H^{-1}, \delta}^2 \geq -G(j) - z_\alpha \kappa_{n,j,\delta}(f) \right) \\ &\geq \left(1 - \frac{\alpha}{2} \right) P_f^{(2)} \left(U_{n,j}(\hat{f}_n) - \|K_j(f - \hat{f}_n)\|_{H^{-1}, \delta}^2 \geq -z_\alpha \kappa_{n,j,\delta}(f) \right) \end{aligned}$$

$$\begin{aligned}
&\geq \left(1 - \frac{\alpha}{2}\right) \left(1 - \frac{\text{Var}_f^{(2)}(U_{n,j}(\hat{f}_n))}{(z_\alpha \kappa_{n,j,\delta}(f))^2}\right) \\
&\geq \left(1 - \frac{\alpha}{2}\right)^2 \\
&\geq 1 - \alpha
\end{aligned}$$

by Chebyshev's inequality and Lemma 1.

We now move on to checking the diameter shrinkage conditions (8) and (9). Writing $S_j := \sum_{l < j} 2^{l(d-4)}(l \vee 1)^{4\delta}$ and using the fact that for positive numbers a, b , $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$, for $g \in \mathcal{F}(r)$ we have that $\kappa_{n,j_n,\delta}(g) \leq 2\sqrt{M}n^{-1/2}\|g - \hat{f}_n\|_{H^{-1,\delta}} + 2M\sqrt{S_{j_n}}n^{-1}$ and so $g \in C_n$ if and only if

$$\|g - \hat{f}_n\|_{H^{-1,\delta}} \leq \sqrt{z_\alpha \frac{2M}{n} \sqrt{S_{j_n}} + U_{j_n} + G(j_n)} + n^{-1/4} \sqrt{2z_\alpha \sqrt{M}} \sqrt{\|g - \hat{f}_n\|_{H^{-1,\delta}}}.$$

For positive numbers x, a, b , the inequality $x \leq b + a\sqrt{x}$ implies that $x \leq 2b + 2a^2$. Applying this inequality with the values $x = \|g - \hat{f}_n\|_{H^{-1,\delta}}$, $a = n^{-1/4} \sqrt{2z_\alpha \sqrt{M}}$, $b = \sqrt{z_\alpha \frac{2M}{n} \sqrt{S_{j_n}} + U_{j_n} + G(j_n)}$, and further using that for any positive numbers x, y we have that $\sqrt{x+y} \leq \sqrt{x} + \sqrt{y}$, one sees that the diameter of C_n is bounded by a multiple of

$$n^{-1/2} S_{j_n}^{1/4} + \sqrt{U_{j_n}} + \sqrt{G_{j_n}} + n^{-1/2}.$$

We consider each of these terms separately; note that the final term is always sufficiently small.

First, consider $G(j_n)$: this is deterministic, of order

$$G(j_n) \lesssim (\log n)^{1+2\delta} \left(\frac{n}{\log n} \right)^{-\frac{2(r+1)}{2r+d/2}} = o(R_n(s)^2) = o(R_n(r)^2).$$

(When $d \leq 4$ this is trivial; for $d > 4$, it necessitates the assumption on s .)

Next, $n^{-2} S_{j_n}$ is of order

$$n^{-2} \sum_{l \leq j_n-1} 2^{l(d-4)}(l \vee 1)^{4\delta}.$$

When $d \leq 4$, this contributes at most a logarithmic factor in n times n^{-2} , so this is clearly $o(R_n(s)^4)$ and $o(R_n(r)^4)$. When $d > 4$, the final term dominates the sum and so the contribution is of order

$$(\log n)^{4\delta - \frac{d-4}{2r+d/2}} n^{-\frac{4(r+1)}{2r+d/2}} = O(R_n(s)^4) = o(R_n(r)^4),$$

again by the assumption on s .

Finally, since $\text{Var}(U_{j_n}) \rightarrow 0$ as $n \rightarrow \infty$, we know that

$$U_{j_n} = O_P(E_f U_{j_n}) = O_P(E_f \|K_j(f - \hat{f}_n)\|_{H^{-1,\delta}}^2) = O_P(E_f \|f - \hat{f}_n\|_{H^{-1,\delta}}^2).$$

As \hat{f}_n converges at the rates $R_n(s)$ and $R_n(r)$ uniformly over $\mathcal{F}(s)$ and $\mathcal{F}(r)$ respectively, U_{j_n} is of the correct order in probability in both cases. This concludes the proof. \square

Proof of Theorem 5. For some sequence $L_n \rightarrow \infty$, to be defined below, and any $\omega \in \{-1; 1\}^{\mathbb{Z}^d \cap [0, 2^{L_n})^d}$, we define for some $\epsilon > 0$,

$$f_{n,\omega} := 1 + \epsilon 2^{-L_n(r+d/2)} \sum_{k \in \mathbb{Z} \cap [0, 2^{L_n})^d} \omega_k \psi_{L_n,k}.$$

Provided that $B > 1$,

$$\begin{aligned} \|f_{n,\omega}\|_{B_{2q}^r} &= 1 + 2^{L_n r} \left(\sum_{k \in \mathbb{Z} \cap [0, 2^{L_n})^d} |\langle f_{n,\omega}, \psi_{L_n,k} \rangle|^2 \right)^{1/2} \\ &= 1 + \epsilon 2^{L_n r} 2^{-L_n(r+d/2)} 2^{dL_n/2} \\ &= 1 + \epsilon, \end{aligned}$$

ensuring that $f_{n,\omega}$ is in the $\|\cdot\|_{B_{2q}^r}$ -Besov ball of radius B for ϵ small enough. Also, $\int_{\mathbb{T}^d} f_{n,\omega}(t) dt = 1$ and, as the tensor product wavelet basis is assumed to be S -regular (cf. Appendix A),

$$\left\| \sum_k |\psi_{L_n,k}| \right\|_{\infty} \lesssim 2^{dL_n/2},$$

for some constant depending on the basis only. Therefore,

$$\|f_{n,\omega} - 1\|_{\infty} \leq \epsilon c 2^{-rL_n},$$

so that, for any $M > 1 \geq m > 0$, $f_{n,\omega} \in \mathcal{F}(r)$ for n large enough (or ϵ small enough if $r = 0$). Finally, for any $\rho_n = o\left(n^{-\frac{1+r}{2r+d/2}}\right)$, $f_{n,\omega} \in \tilde{\mathcal{F}}(r, \rho_n)$ if, for any $g \in \mathcal{F}(s)$, $W_2(f_{n,\omega}, g) \geq \rho_n$. By definition of $\mathcal{F}(r)$, $\mathcal{F}(s)$ and Proposition 1, we have, for n large enough

$$\begin{aligned} W_2(f_{n,\omega}, g)^2 &\gtrsim \|f_{n,\omega} - g\|_{B_{2\infty}^{-1}}^2 \\ &\geq 2^{-2L_n} \|\langle f_{n,\omega} - g, \psi_{L_n,\cdot} \rangle\|_2^2 \\ &\geq 2^{-2L_n} \left[\left(\sum_{k=0}^{2^{L_n d}-1} |\langle f_{n,\omega}, \psi_{L_n,k} \rangle|^2 \right)^{1/2} - \left(\sum_{k=0}^{2^{L_n d}-1} |\langle g, \psi_{L_n,k} \rangle|^2 \right)^{1/2} \right]^2 \\ &\geq 2^{-2L_n} \left[\epsilon 2^{-L_n r} - B 2^{-L_n s} \right]^2 \\ &\geq \frac{\epsilon^2}{2} 2^{-2L_n(1+r)}. \end{aligned}$$

Therefore, if L_n^* is such that $2^{-2L_n^*(1+r)} \asymp n^{-\frac{1+r}{2r+d/2}}$, it is possible to find $L_n > L_n^*$ such that $\rho_n^2 \leq \frac{\epsilon^2}{2} 2^{-2L_n(1+r)} = o\left(n^{-\frac{1+r}{2r+d/2}}\right)$. This choice ensures that, for any ω , $f_{n,\omega} \in \tilde{\mathcal{F}}(r, \rho_n)$. Note also that the density $f_0 := 1$ naturally belongs to $\mathcal{F}(s)$.

Re-index $\{-1; 1\}^{\mathbb{Z}^d \cap [0, 2^{L_n})^d}$ as $\{\omega^{(i)} : i = 1, \dots, 2^{2^{L_n}}\}$ and denote by P_i the distribution with Lebesgue density $f_i := f_{n, \omega^{(i)}}$, $Q := 2^{-2^{L_n}} \sum_{i=1}^{2^{2^{L_n}}} P_i$ and P_0 the distribution with density f_0 . Then, with μ the Lebesgue measure and for any test Ψ_n ,

$$\begin{aligned}
\sup_{f \in \Sigma_0} \mathbb{E}_f[\Psi_n] + \sup_{f \in \Sigma(\rho_n)} \mathbb{E}_f[1 - \Psi_n] &\geq \mathbb{E}_{f_0}[\Psi_n] + 2^{-2^{L_n}} \sum_{i=1}^{2^{2^{L_n}}} \mathbb{E}_{f_i}[1 - \Psi_n] \\
&\geq \int (\Psi_n(x_1, \dots, x_n) + 1 - \Psi_n(x_1, \dots, x_n)) \\
&\quad \left(\prod_{j=1}^n f_0(x_j) \wedge 2^{-2^{L_n}} \sum_{i=1}^{2^{2^{L_n}}} \prod_{j=1}^n f_i(x_j) \right) d\mu^{\otimes n}(x_1, \dots, x_n) \\
&= 1 - \frac{1}{2} \|P_0^{\otimes n} - Q^{\otimes n}\|_1 \\
&\geq 1 - \frac{1}{2} \sqrt{\chi^2(Q^{\otimes n}, P_0^{\otimes n})}.
\end{aligned}$$

where $\chi^2(Q, P) = \int (dP/dQ - 1)^2 dQ$ if $P \ll Q$, $\chi^2(Q, P) = +\infty$ otherwise. Also, for any $1 \leq \gamma, \kappa \leq 2^{2^{L_n}}$, the orthonormality of the wavelet basis gives

$$\begin{aligned}
&\int \frac{dP_\gamma^{\otimes n}}{dP_0^{\otimes n}} \frac{dP_\kappa^{\otimes n}}{dP_0^{\otimes n}} dP_0^{\otimes n} \\
&= \prod_{i=1}^n \int_{\mathbb{T}^d} \left[1 + \epsilon 2^{-L_n(r+d/2)} \sum_k \omega_k^{(\gamma)} \psi_{L_n, k}(x_i) \right] \left[1 + \epsilon 2^{-L_n(r+d/2)} \sum_k \omega_k^{(\kappa)} \psi_{L_n, k}(x_i) \right] dx_i \\
&= \left(1 + \epsilon^2 2^{-L_n(2r+d)} \sum_k \omega_k^{(\gamma)} \omega_k^{(\kappa)} \right)^n.
\end{aligned}$$

Then, for $\gamma_n = n\epsilon^2 2^{-L_n(2r+d)} \rightarrow 0$ and R_k, R'_k i.i.d. Rademacher random variables,

$$\begin{aligned}
\chi^2(Q^{\otimes n}, P_0^{\otimes n}) &= 2^{-2^{L_n}} \sum_{\gamma, \kappa} \left(1 + \epsilon^2 2^{-L_n(2r+d)} \langle \omega^{(\gamma)}, \omega^{(\kappa)} \rangle \right)^n - 1 \\
&\leq \mathbb{E} \left[\exp \left(n\epsilon^2 2^{-L_n(2r+d)} \sum_k R_k R'_k \right) \right] - 1 \\
&= \mathbb{E} \left[\exp \left(n\epsilon^2 2^{-L_n(2r+d)} \sum_k R_k \right) \right] - 1 \\
&= \cosh(\gamma_n)^{2^{L_n d}} - 1,
\end{aligned}$$

where we used that $1 + x \leq e^x$ for $x \in \mathbb{R}$ in the second line and that $R_k R'_k$ is distributed as R_k in the third. Using that $\cosh(z) = 1 + z^2/2 + o_{|z| \rightarrow 0}(z^2)$ and $1 + x \leq e^x$ once again, for any $\delta > 0$,

$$(\cosh(\gamma_n))^{2^{dL_n}} - 1 = \left(1 + \frac{\gamma_n^2}{2}(1 + o(1))\right)^{2^{dL_n}} - 1 \leq \exp\left(\gamma_n^2 2^{dL_n-1}(1 + o(1))\right) - 1 \leq \delta^2$$

for n large enough, since $\gamma_n^2 2^{dL_n} = o(1)$. We have proven that, for any $\beta < 1$ and $\rho_n = o(\rho_n^*)$,

$$\liminf_n \inf_{\Psi_n} \left[\sup_{f \in \mathcal{F}(s)} \mathbb{E}_f[\Psi_n] + \sup_{f \in \tilde{\mathcal{F}}(r, \rho_n)} \mathbb{E}_f[1 - \Psi_n] \right] \geq \beta,$$

which concludes the proof. \square

Appendix C: Proofs for Section 4

Proof of Proposition 4. As f and \tilde{f}_n have the same total mass, we may without loss of generality take the supremum over functions $h \in \text{Lip}_1(\mathbb{R}^d)$ for which $h(0) = 0$; observe that $x \mapsto \|x\|$ is an envelope for this function class. Since both f and \tilde{f}_n have finite first moments (almost surely), the wavelet expansion of any h in this class converges in $L_1(f)$ and $L_1(\tilde{f}_n)$ and so

$$\int_{\mathbb{R}^d} h(f - \tilde{f}_n) = \sum_{k \in \mathbb{Z}^d} \langle h, \phi_k \rangle \langle f - \tilde{f}_n, \phi_k \rangle + \sum_{l \geq 0} \sum_{k \in \mathbb{Z}^d} \langle h, \psi_{lk} \rangle \langle f - \tilde{f}_n, \psi_{lk} \rangle.$$

As the father wavelets ϕ_k are compactly supported in some interval about k ,

$$|\langle h, \phi_k \rangle| \lesssim |h(k)| \leq \|k\|$$

for some constant depending on the wavelet basis. Moreover, $h - K(h) = \sum_{l \geq 0} \sum_{k \in \mathbb{Z}^d} \langle h, \psi_{lk} \rangle \psi_{lk}$ is in a $B_{\infty\infty}^1$ -ball of radius depending only on the wavelet basis, and so by (3),

$$\sup_{k \in \mathbb{Z}^d} |\langle h, \psi_{lk} \rangle| \lesssim 2^{-l(\frac{d}{2}+1)}.$$

Plugging these uniform estimates for the wavelet coefficients of h into the first equation gives the result. \square

Proof of Theorem 6. When $d = 1$, the empirical measure achieves the stated rate ([16]). Thus we assume $d \geq 2$.

The estimator we use is

$$\hat{f}_n := \sum_{\|k\|_\infty \leq \kappa_{-1n}} \hat{f}_{-1k} \phi_k + \sum_{l \leq l_n(s)} \sum_{\|k\|_\infty \leq \kappa_{ln}} \hat{f}_{lk} \psi_{lk},$$

where \hat{f}_{lk} are empirical wavelet coefficients and the cutoffs $\kappa_{ln}, l_n(s)$ are chosen such that

$$2^{l_n(s)} \simeq n^{\frac{1}{2s+d}}, \kappa_{-1n} = \kappa_{0n} \simeq (\log n)^\gamma, \kappa_{ln} = 2^l \kappa_{0n},$$

where γ is to be chosen below. We then use the decomposition in Proposition 4, which we further split to obtain six terms:

$$\begin{aligned}
W_1(f, \hat{f}_n) &\lesssim \sum_{\|k\|_\infty \leq \kappa_{-1n}} \|k\| |\hat{f}_{-1k} - f_{-1k}| + \sum_{\|k\|_\infty > \kappa_{-1n}} \|k\| |f_{-1k}| \\
&\dots + \sum_{l < l_n(s)} 2^{-l(\frac{d}{2}+1)} \sum_{\|k\|_\infty \leq \kappa_{ln}} |\hat{f}_{lk} - f_{lk}| + \sum_{l < l_n(s)} 2^{-l(\frac{d}{2}+1)} \sum_{\|k\|_\infty > \kappa_{ln}} |f_{lk}| \\
&\dots + \sum_{l \geq l_n(s)} 2^{-l(\frac{d}{2}+1)} \sum_{\|k\|_\infty \leq \kappa_{ln}} |f_{lk}| + \sum_{l \geq l_n(s)} 2^{-l(\frac{d}{2}+1)} \sum_{\|k\|_\infty > \kappa_{ln}} |f_{lk}| \\
&=: I + II + III + IV + V + VI.
\end{aligned}$$

We first consider the bias terms II, IV, VI . For term II , we have that

$$\sum_{\|k\|_\infty > \kappa_{-1n}} \|k\| |f_{-1k}| \leq \int_{\mathbb{R}^d} \sum_{\|k\|_\infty > \kappa_{-1n}} \|k\| |\phi_k(x)| f(x) \, dx.$$

Since each ϕ_k is compactly supported in some interval about k , and $\sum_{k \in \mathbb{Z}^d} |\phi_k|$ is uniformly bounded on \mathbb{R}^d , we have that

$$\sum_{\|k\|_\infty > \kappa_{-1n}} \|k\| |\phi_k(x)| \lesssim \|x\|$$

for some constant depending on the wavelet basis. Moreover, the integrand is supported for all large enough n in $([-\kappa_{-1n}/2, \kappa_{-1n}/2]^d)^c =: D_n$. Thus, for n large enough,

$$II \lesssim \int_{D_n} \|x\| f(x) \, dx \leq \mathcal{E}_{\alpha, \beta}(f) \kappa_{-1n} \exp\left(-\beta \left(\frac{\kappa_{-1n}}{2}\right)^\alpha\right). \quad (43)$$

Since $\sum_{k \in \mathbb{Z}^d} |\psi_{lk}|$ is uniformly bounded by a constant depending on the wavelet basis times $2^{ld/2}$, we analogously have

$$\sum_{\|k\|_\infty > \kappa_{ln}} |f_{lk}| \lesssim 2^{ld/2} \mathcal{E}_{\alpha, \beta}(f) \exp\left(-\beta \left(\frac{\kappa_{0n}}{2}\right)^\alpha\right). \quad (44)$$

Thus

$$IV + VI \lesssim \mathcal{E}_{\alpha, \beta}(f) \exp\left(-\beta \left(\frac{\kappa_{0n}}{2}\right)^\alpha\right).$$

Choosing $\gamma > 0$ sufficiently large depending on α, β , these terms converge faster than $n^{-1/2}$.

Next, we deal with the final bias term V . By Cauchy-Schwarz and the fact that $\|f\|_{B_{2q}^s} \leq B$,

$$\sum_{\|k\|_\infty \leq \kappa_{ln}} |f_{lk}| \leq \sqrt{\kappa_{ln}^d} \|f_l\|_2 \lesssim (\log n)^{\gamma d/2} 2^{l(\frac{d}{2}-s)},$$

and so

$$V \lesssim \sum_{l \geq l_n(s)} 2^{-l(s+1)} (\log n)^{\gamma d/2} \simeq (\log n)^{\gamma d/2} 2^{-l_n(s)(s+1)}$$

which is of the correct order by the definition of $l_n(s)$.

To bound the stochastic terms I and III , we use the expectation bound Lemma 5, whose proof generalises naturally to the case of \mathbb{R}^d . We have for all $l \geq -1$ such that $2^{ld} \leq n$ and $k \in \mathbb{Z}^d$ that

$$E_f |\hat{f}_{lk} - f_{lk}| \lesssim n^{-1/2},$$

for some constant depending on M and the wavelet basis. So

$$E_f(I) \lesssim (\kappa_{-1n})^{d+1} n^{-1/2}$$

and

$$E_f(III) \lesssim (\log n)^{\gamma d} n^{-1/2} \sum_{l < l_n(s)} 2^{l(\frac{d}{2}-1)}.$$

When $d = 2$, the sum contributes an extra $\log n$ factor as in the statement. For $d \geq 3$, the final term of the sum dominates, and so

$$E_f(III) \lesssim (\log n)^{\gamma d/2} n^{-\frac{s+1}{2s+d}}$$

as stated. \square

Proof of Theorem 7. Define the thresholds $\kappa_{-1n} = \kappa_{0n} \simeq (\log n)^\gamma$, $\kappa_{ln} = 2^l \kappa_{0n}$ for γ chosen as in Theorem 6. As before, let l_{\max} be such that $2^{l_{\max}} \simeq (n/\log n)^{1/d}$, for $0 \leq l \leq l_{\max}$, define the thresholds τ_l via

$$\tau_l^2 = \tau^2 \kappa_{ln}^d \frac{\log n}{n},$$

where $\tau > 0$ is to be chosen below. For any sequence $(a_k)_{k \in \mathbb{Z}^d}$, set $\|a\|_{2, \kappa_{ln}} := \left(\sum_{\|k\|_\infty \leq \kappa_{ln}} a_k^2 \right)^{1/2}$. The thresholded estimator is then defined as

$$\hat{f}_n = \sum_{\|k\|_\infty \leq \kappa_{-1n}} \hat{f}_{-1k} \phi_k + \sum_{l=0}^{l_{\max}} 1_{\{\|\hat{f}_l\|_{2, \kappa_{ln}} > \tau_l\}} \sum_{\|k\|_\infty \leq \kappa_{ln}} \hat{f}_{lk} \psi_{lk}. \quad (45)$$

We perform a decomposition of the risk similar to that in the previous proof:

$$\begin{aligned} W_1(f, \hat{f}_n) &\lesssim \sum_{\|k\|_\infty \leq \kappa_{-1n}} \|k\| |\hat{f}_{-1k} - f_{-1k}| + \sum_{\|k\|_\infty > \kappa_{-1n}} \|k\| |f_{-1k}| \\ &\quad + \sum_{l \leq l_{\max}} 2^{-l(\frac{d}{2}+1)} \sum_{\|k\|_\infty \leq \kappa_{ln}} \left| 1_{\{\|\hat{f}_l\|_{2, \kappa_{ln}} > \tau_l\}} \hat{f}_{lk} - f_{lk} \right| \\ &\quad + \sum_{l \leq l_{\max}} 2^{-l(\frac{d}{2}+1)} \sum_{\|k\|_\infty > \kappa_{ln}} |f_{lk}| \\ &\quad + \sum_{l > l_{\max}} 2^{-l(\frac{d}{2}+1)} \sum_{\|k\|_\infty \leq \kappa_{ln}} |f_{lk}| + \sum_{l > l_{\max}} 2^{-l(\frac{d}{2}+1)} \sum_{\|k\|_\infty > \kappa_{ln}} |f_{lk}| \\ &=: I + II + III + IV + V + VI. \end{aligned}$$

We treat terms I, II, IV and VI identically to before. Term V is also dealt with as in the previous proof, noting that for all n sufficiently large, $2^{l_{\max}} > n^{1/(2s+d)}$. It remains to deal with term III ; by Cauchy-Schwarz and the definition of κ_{ln} , we have that

$$III \lesssim (\log n)^{\frac{\gamma d}{2}} \sum_{l=0}^{l_{\max}} 2^{-l} \left\| 1_{\{\|\hat{f}_l\|_{2, \kappa_{ln}} > \tau_l\}} \hat{f}_l - f_l \right\|_{2, \kappa_{ln}},$$

where the constant depends on d . By splitting this sum into two parts at $l_n(s)$,

$$2^{l_n(s)} \simeq B^{1/s} (n/\log n)^{1/(2s+d)},$$

one can bound it exactly as in the proof of Theorem 3 □

Proof of Theorem 8. We first establish coverage. Define the thresholds κ_{ln} as in the previous proof. Given $f \in \mathcal{G}(s)$, as in the proof of Theorems 3 and 7, on an event of probability tending to 1, for all l such that $l_n(r) \leq l \leq l_{\max}$, $\langle \hat{f}_n, \psi_l \rangle \equiv 0$. Note that $l_{\max} > j_n > l_n(s) > l_n(r)$. So on this event, by Cauchy-Schwarz,

$$\begin{aligned} \left(\sum_{l \geq j_n} 2^{-l(\frac{d}{2}+1)} \sum_{\|k\|_{\infty} \leq \kappa_{ln}} |\langle f - \hat{f}_n, \psi_{lk} \rangle| \right)^2 &\lesssim (\log n)^{\gamma d} \left(\sum_{l \geq j_n} 2^{-l} \|\langle f, \psi_l \rangle\|_2 \right)^2 \\ &\lesssim (\log n)^{\gamma d} B 2^{-2j_n(r+1)} \\ &\leq G_{j_n} \end{aligned}$$

for all n sufficiently large, i.e. this quantity is $O_P(G_{j_n})$. The other term in $\tilde{W}^{(n)}(f, \hat{f}_n)^2$ is precisely $E_f^{(2)} V_{j_n}$; by Chebyshev's inequality we obtain condition (23).

It remains to confirm the diameter conditions (24) and (25) with the rates $R_n(r), R_n(s)$ as given in the statement of the result. As the remainder term $\sqrt{r_n}$ converges up to a logarithmic factor at the rate $n^{-1/2}$, it is dominated by $\tilde{W}^{(n)}$ for diameter considerations. As observed previously, we may instead prove the diameter conditions for the $\tilde{W}^{(n)}$ distance with the augmented rates

$$\bar{R}_n(r) = (\log n)^{\gamma d/2} \left(\frac{n}{\log n} \right)^{-\frac{r+1}{2r+d}}, \quad \bar{R}_n(s) = (\log n)^{\gamma d/2} \left(\frac{n}{\log n} \right)^{-\frac{s+1}{2s+d}}.$$

By the same argument as in the proof of Theorem 4, the $\tilde{W}^{(n)}$ -diameter of C_n is bounded by a constant multiple of

$$(\log n)^{\gamma d/4 + 1/2} n^{-1/2} \left(\sum_{l < j} 2^{l(d-4)} \right)^{1/4} + \sqrt{V_{j_n}} + \sqrt{G_{j_n}} + n^{-1/2}.$$

The final term is dominated by the first, and (using the condition on s when $d > 4$) $\sqrt{G_{j_n}} = O(\bar{R}_n(s)) = o(\bar{R}_n(r))$. One checks the first term is of the correct order as in Theorem 4. Finally, since $\text{Var}_f^{(2)}(V_{j_n}) \rightarrow 0$ (one shows that $\tilde{W}^{(n, j_n)}(f, \hat{f}_n) \rightarrow 0$ analogously to the proof of Theorem 3), we have that

$$V_{j_n} = O_{P_f}(E_f V_{j_n});$$

as in the proof of Theorem 7, this expectation is of order $\bar{R}_n(r)$ or $\bar{R}_n(s)$ when f belongs to $\mathcal{G}(r)$ or $\mathcal{G}(s)$ respectively. \square

Proof of Theorem 9. For some $\alpha' > \alpha$, $D > 0$ and $\alpha(x) = \alpha' e^{-1/(\|x\|_2 - D)} \mathbf{1}_{B(0,D)^c}(x)$, the density f defined by

$$f(x) \propto e^{-\beta \|x\|_2^{\alpha(x)}}$$

is such that $\mathbb{E}_f[e^{\beta \|X\|^\alpha}] < +\infty$. Then, for $\sigma > 0$, if $X \sim P_f$, σX has density $g : x \mapsto \sigma^{-d} f(\sigma^{-1}x)$ satisfying

$$\mathbb{E}_g[e^{\beta \|X\|^\alpha}] = \mathbb{E}_f[e^{\sigma^\alpha \beta \|X\|^\alpha}] < +\infty.$$

Then, we verify that $f \in H_2^m(\mathbb{R}^d) \subset B_{2\infty}^m(\mathbb{R}^d) \subset B_{2q}^s(\mathbb{R}^d)$, for any $m \in \mathbb{N}$ and $s < m$. Also, $\|g\|_p = \sigma^{-d(1-1/p)} \|f\|_p$ and, the moduli of continuity of g satisfies, for $t > 0$ and an integer $r > s$,

$$\begin{aligned} \omega_r(g, t, 2) &:= \sup_{0 \leq \|h\| \leq t} \left\| \sum_{k=0}^r \binom{r}{k} (-1)^{r-k} \sigma^{-d} f(\sigma^{-1} \cdot + k \sigma^{-1} h) \right\|_2 \\ &= \sigma^{-d} \sup_{0 \leq \|h\| \leq \sigma^{-1} t} \left\| \sum_{k=0}^r \binom{r}{k} (-1)^{r-k} \sigma^d f(\sigma^{-1} \cdot + k h) \right\|_2 \\ &= \sigma^{-d/2} \omega_r(f, \sigma^{-1} t, 2). \end{aligned}$$

Therefore, with $|f|_{B_{pq}^s} := \left[\int_0^\infty \left| \frac{\omega_r(f, t, p)}{t^s} \right|^q \frac{dt}{t} \right]^{1/q}$, we have

$$\|g\|_{B_{pq}^s} = \|g\|_p + |g|_{B_{pq}^s} = \sigma^{-d(1-1/p)} \|f\|_p + \sigma^{-d(1-1/p)-s} |f|_{B_{pq}^s}, \quad (46)$$

so that $\|g\|_{B_{2q}^s} \leq B$ for σ large enough. Also, since $f \in L_\infty(\mathbb{R}^d)$, $g \leq M$ for σ large enough. So, for some large L , $g \in \mathcal{G}(s)$.

For some sequence $L_n \rightarrow \infty$, and any $\omega \in \{-1; 1\}^{\mathbb{Z} \cap [0, 2^{L_n}]^d \times \mathcal{I}}$, we define for some $\epsilon > 0$,

$$f_\omega^n = g + \epsilon 2^{-L_n(r+d/2)} \sum_{k \in \mathbb{Z} \cap [0, 2^{L_n}]^d, \iota \in \mathcal{I}} \omega_{k, \iota} \Psi_{L_n k}^\iota.$$

Assuming that the scaling and mother wavelets functions are compactly supported (as assumed in Appendix A), the $\Psi_{L_n k}^\iota$, for $k \in \mathbb{Z} \cap [0, 2^{L_n}]^d$, $\iota \in \mathcal{I}$, are supported on a compact set K independent of n . Then, since

$$\begin{aligned} \|f_\omega^n\|_{B_{2q}^r} &\leq \|g\|_{B_{2q}^r} + \epsilon 2^{-L_n(r+d/2)} \left\| \sum_{k \in \mathbb{Z} \cap [0, 2^{L_n}]^d, \iota \in \mathcal{I}} \omega_{k, \iota} \Psi_{L_n k}^\iota \right\|_{B_{2q}^r} \\ &\leq \|g\|_{B_{2q}^r} + C\epsilon, \end{aligned}$$

for some $C > 0$ depending on d only, reasoning as for (46), and since $B_{2q}^s \subset B_{2q}^r$, f_ω^n is the $\|\cdot\|_{B_{2q}^r}$ -Besov ball of radius B for ϵ small enough and σ large enough. Then, by assumption, $\int_{\mathbb{R}^d} f_\omega^n(t) dt = 1$ and, since

$$\left\| 2^{-L_n(r+d/2)} \sum_{k \in \mathbb{R}^d, \ell \in \mathcal{I}} |\Psi_{L_n k}^\ell| \right\|_\infty \lesssim 2^{-rL_n},$$

$0 < f_\omega^n \leq M$ for n, σ large enough (or ϵ small enough if $r = 0$). Indeed, g is lower bounded by a some positive constant on K . So, f_ω^n actually is a density function.

For these to belong to the alternative hypothesis, it remains to check that these are well separated from the null hypothesis. For any $h \in \mathcal{G}(s)$, the reversed triangular inequality gives

$$\begin{aligned} W_1(f_\omega^n, h) &\gtrsim \|f_\omega^n - h\|_{B_{1\infty}^{-1}} \\ &\gtrsim 2^{-L_n(d/2+1)} \sum_{k \in \mathbb{Z} \cap [0, 2^{L_n})^d, \ell \in \mathcal{I}} |\langle f_\omega^n - h, \Psi_{L_n k}^\ell \rangle| \\ &\geq 2^{-L_n(d/2+1)} \left| \sum_{k, \ell} |\langle f_\omega^n - g, \Psi_{L_n k}^\ell \rangle| - \sum_{k, \ell} |\langle h - g, \Psi_{L_n k}^\ell \rangle| \right| \\ &= 2^{-L_n(d/2+1)} \left[C 2^{-L_n(r-d/2)} - C' 2^{-L_n(s-d/2)} \right] \\ &\gtrsim 2^{-L_n(1+r)}, \end{aligned}$$

for constants independent of n . Above, we used that $s > r$ and that, for any $s > 0$, $\mathcal{G}(s) \subset \{f : \|f\|_{B_{1q}^s} \leq B'\}$ for some $B' > 0$ according to Lemma 20.

The last inequality holds for n large enough. Therefore, if L_n^* is such that $2^{-L_n^*(1+r)} \asymp \xi_n$, it is possible to take $L_n > L_n^*$ such that $\rho_n \leq C' 2^{-L_n(1+r)} = o(\xi_n)$, so that, for any ω , $f_\omega^n \in \tilde{\mathcal{G}}(s, \rho_n)$.

For $N_n = 2^{2^{dL_n}(2^d-1)}$, let's index $\omega \in \{-1; 1\}^{\mathbb{Z} \cap [0, 2^{L_n})^d \times \mathcal{I}} = \{w^{(m)} : m = 1, \dots, N_n\}$ and denote $P_m = P_{f_{\omega^{(m)}}}$. Then,

$$\liminf_n \inf_{\Psi_n} \left[\sup_{f \in H_0} \mathbb{E}_f[\Psi_n] + \sup_{f \in H_1(r_n)} \mathbb{E}_f[1 - \Psi_n] \right] \geq 1 - \frac{1}{2} \sqrt{\chi^2(Q^{\otimes n}, P_0^{\otimes n})},$$

where $Q = N_n^{-1} \sum_{m=1}^{N_n} P_m$ and P_0 has density $g \in H_0$. Then, for any $1 \leq m, q \leq N_n$, one has by properties of the wavelet basis, denoting $\nu_m = f_{\omega^{(m)}} - g$,

$$\begin{aligned} &\int \frac{dP_m^{\otimes n}}{dP_0^{\otimes n}} \frac{dP_q^{\otimes n}}{dP_0^{\otimes n}} dP_0^{\otimes n} \\ &= \prod_{i=1}^n \int_{[0,1]^d} \left[g(x_i) + \epsilon 2^{-L_n(r+d/2)} \sum_{k, \ell} \omega_{k, \ell}^{(m)} \Psi_{L_n k}^\ell(x_i) \right] \end{aligned}$$

$$\begin{aligned} & \left[g(x_i) + \epsilon 2^{-L_n(r+d/2)} \sum_{k,l} \omega_{k,l}^{(q)} \Psi_{L_n k}^l(x_i) \right] g^{-1}(x_i) dx_i \\ &= \left(1 + \int_{\mathbb{R}^d} \frac{\nu_m(x) \nu_q(x)}{g(x)} dx \right)^n. \end{aligned}$$

For σ large enough, g is constant on the compact support of ν_m and ν_q , equal to $g(0)$. Hence, following the same arguments as above,

$$\chi^2(Q^{\otimes n}, P_0^{\otimes n}) = (\cosh \gamma_n)^{2^{dL_n}(2^d-1)} - 1,$$

where $\gamma_n = n\epsilon^2 g(0)^{-1} 2^{-L_n(2r+d)}$, and for any $\delta > 0$, $\chi^2(Q^{\otimes n}, P_0^{\otimes n}) \leq \delta^2$ for n large enough. This concludes the proof. \square

Lemma 8. *Let $B \geq 1, M > 0, \alpha > 0, \beta > 0, L > 0, 1 \leq q \leq \infty$, and $s \geq 0$. Then, there exists a constant B' , depending on the class parameters, the wavelet basis and the dimension d , such that*

$$\mathcal{G}_{s,2,q}(B, M; \alpha, \beta, L) \subset \mathcal{G}_{s,1,q}(B', M; \alpha, \beta, L).$$

Proof. Let $f \in \mathcal{G}_{s,2,q}(B, M; \alpha, \beta, L)$. All we have to prove is that

$$\|f\|_{B'_{1,q}} = \|\langle f, \phi \cdot \rangle\|_1 + \left(\sum_{l \geq 0} [2^{l(s-d/2)} \|\langle f, \psi_l \cdot \rangle\|_1]^q \right)^{1/q} \leq B',$$

for some B' as in the lemma. Let $\kappa > 0$. Then,

$$\|\langle f, \phi \cdot \rangle\|_1 = \sum_{\|k\|_\infty \leq \kappa} |\langle f, \phi_k \rangle| + \sum_{\|k\|_\infty > \kappa} |\langle f, \phi_k \rangle|.$$

For the second term, the same arguments as the one used to obtain (43) give that it is bounded by $\mathcal{E}_{\alpha,\beta}(f) \exp(-\beta(\frac{\kappa}{2})^\alpha)$, up to a constant depending on the wavelet basis. The first term is controlled via the Cauchy-Schwarz inequality

$$\sum_{\|k\|_\infty \leq \kappa} |\langle f, \phi_k \rangle| \lesssim (2\kappa + 1)^d \left(\sum_{\|k\|_\infty \leq \kappa} |\langle f, \phi_k \rangle|^2 \right)^{1/2} \leq (2\kappa + 1)^d \|\langle f, \phi \cdot \rangle\|_2,$$

for a constant depending on d only.

Next consider, for $l \geq 0$, $\|\langle f, \psi_l \cdot \rangle\|_1$. As before, letting $\kappa_l = 2^{l/2}$, we have

$$\|\langle f, \psi_l \cdot \rangle\|_1 = \sum_{\|k\|_\infty \leq \kappa_l} |\langle f, \psi_{lk} \rangle| + \sum_{\|k\|_\infty > \kappa_l} |\langle f, \psi_{lk} \rangle|.$$

Arguing as with (44), the second term is bounded by $2^{ld/2} \mathcal{E}_{\alpha,\beta}(f) \exp(-\beta(\frac{\kappa_l}{2})^\alpha)$, up to a constant depending on the wavelet basis. The first term is controlled as above. Then, using the l^q triangular

inequality,

$$\begin{aligned}
& \left(\sum_{l \geq 0} [2^{l(s-d/2)} \|\langle f, \psi_l \cdot \rangle\|_1]^q \right)^{1/q} \\
& \lesssim \left(\sum_{l \geq 0} 2^{ql(s-d/2)} \left[2^{ld/2} \mathcal{E}_{\alpha, \beta}(f) \exp \left(-\beta \left(\frac{\kappa_l}{2} \right)^\alpha \right) + (2\kappa_l + 1)^d \|\langle f, \psi_l \cdot \rangle\|_2 \right]^q \right)^{1/q} \\
& \lesssim \left(\sum_{l \geq 0} [2^{ls} \mathcal{E}_{\alpha, \beta}(f) \exp \left(-2^{-\alpha} \beta 2^{l\alpha/2} \right)]^q \right)^{1/q} + \left(\sum_{l \geq 0} [2^{ls} \|\langle f, \psi_l \cdot \rangle\|_2]^q \right)^{1/q},
\end{aligned}$$

for constants depending on the wavelet basis and d . The first term is upper bounded by

$$\mathcal{E}_{\alpha, \beta}(f) \left(\sum_{l \geq 0} 2^{qls} \exp \left(-q 2^{-\alpha} \beta 2^{l\alpha/2} \right) \right)^{1/q} \lesssim \mathcal{E}_{\alpha, \beta}(f),$$

as the series converges.

In the end, following our assumptions on $\|f\|_{B_{2q}^s}$,

$$\begin{aligned}
\|f\|_{B_{1q}^s} & \lesssim (2\kappa + 1)^d \|\langle f, \phi \cdot \rangle\|_2 + \left(\sum_{l \geq 0} [2^{ls} \|\langle f, \psi_l \cdot \rangle\|_2]^q \right)^{1/q} + \mathcal{E}_{\alpha, \beta}(f) \exp \left(-\beta \left(\frac{\kappa}{2} \right)^\alpha \right) \\
& \quad + \mathcal{E}_{\alpha, \beta}(f) \\
& \lesssim B + \mathcal{E}_{\alpha, \beta}(f) \leq B + L,
\end{aligned}$$

where the constants depend on the wavelet basis, d , the arbitrary $\kappa > 0$ we took, s , α , β and q . □

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