The Nearest Neighbor Information Estimator is Adaptively Near Minimax Rate-Optimal

Jiantao Jiao  
Department of Electrical Engineering and Computer Sciences  
University of California, Berkeley  
jiantao@berkeley.edu

Weihao Gao  
Department of ECE  
Coordinated Science Laboratory  
University of Illinois at Urbana-Champaign  
wgao9@illinois.edu

Yanjun Han  
Department of Electrical Engineering  
Stanford University  
yjhan@stanford.edu

Abstract

We analyze the Kozachenko–Leonenko (KL) fixed $k$-nearest neighbor estimator for the differential entropy. We obtain the first uniform upper bound on its performance for any fixed $k$ over Hölder balls on a torus without assuming any conditions on how close the density could be from zero. Accompanying a recent minimax lower bound over the Hölder ball, we show that the KL estimator for any fixed $k$ is achieving the minimax rates up to logarithmic factors without cognizance of the smoothness parameter $s$ of the Hölder ball for $s \in (0, 2]$ and arbitrary dimension $d$, rendering it the first estimator that provably satisfies this property.

1 Introduction

Information theoretic measures such as entropy, Kullback-Leibler divergence and mutual information quantify the amount of information among random variables. They have many applications in modern machine learning tasks, such as classification [48], clustering [46, 58, 10, 41] and feature selection [1, 17]. Information theoretic measures and their variants can also be applied in several data science domains such as causal inference [18], sociology [49] and computational biology [36]. Estimating information theoretic measures from data is a crucial sub-routine in the aforementioned applications and has attracted much interest in statistics community. In this paper, we study the problem of estimating Shannon differential entropy, which is the basis of estimating other information theoretic measures for continuous random variables.

Suppose we observe $n$ independent identically distributed random vectors $X = \{X_1, \ldots, X_n\}$ drawn from density function $f$ where $X_i \in \mathbb{R}^d$. We consider the problem of estimating the differential entropy

\[ h(f) = -\int f(x) \ln f(x) dx, \quad (1) \]
from the empirical observations \( \mathbf{X} \). The fundamental limit of estimating the differential entropy is given by the minimax risk

\[
\inf_{\hat{h}} \sup_{f \in \mathcal{F}} \left( \mathbb{E}(\hat{h}(\mathbf{X}) - h(f))^2 \right)^{1/2},
\]

where the infimum is taken over all estimators \( \hat{h} \) that is a function of the empirical data \( \mathbf{X} \). Here \( \mathcal{F} \) denotes a (nonparametric) class of density functions.

The problem of differential entropy estimation has been investigated extensively in the literature. As discussed in [2], there exist two main approaches, where one is based on kernel density esti-

\[
\text{mators} \ [30], \text{and the other is based on the nearest neighbor methods} \ [56, 53, 52, 11, 3], \text{which is pioneered by the work of} \ [33].
\]

The problem of differential entropy estimation lies in the general problem of estimating nonparametric functionals. Unlike the parametric counterparts, the problem of estimating nonparametric functionals is challenging even for smooth functionals. Initial efforts have focused on inference of linear, quadratic, and cubic functionals in Gaussian white noise and density models and have laid the foundation for the ensuing research. We do not attempt to survey the extensive literature in this area, but instead refer to the interested reader to, e.g., [24, 5, 12, 16, 6, 32, 37, 8, 9, 54] and the references therein. For non-smooth functionals such as entropy, there is some recent progress [38, 26, 27] on designing theoretically minimax optimal estimators, while these estimators typically require the knowledge of the smoothness parameters, and the practical performances of these estimators are not yet known.

The \( k \)-nearest neighbor differential entropy estimator, or Kozachenko-Leonenko (KL) estimator is computed in the following way. Let \( R_{i,k} \) be the distance between \( X_i \) and its \( k \)-nearest neighbor among \( \{X_1, \ldots, X_{i-1}, X_{i+1}, \ldots, X_n\} \). Precisely, \( R_{i,k} \) equals the \( k \)-th smallest number in the list \( \{\|X_i - X_j\| : j \neq i, j \in [n]\} \), here \( [n] = \{1, 2, \ldots, n\} \). Let \( B(x, \rho) \) denote the closed \( \ell_2 \) ball centered at \( x \) of radius \( \rho \) and \( \lambda \) be the Lebesgue measure on \( \mathbb{R}^d \). The KL differential entropy estimator is defined as

\[
\hat{h}_{n,k}(\mathbf{X}) = \ln k - \psi(k) + \frac{1}{n} \sum_{i=1}^{n} \ln \left( \frac{n \lambda(B(X_i, R_{i,k}))}{k} \right),
\]

where \( \psi(x) \) is the digamma function with \( \psi(1) = -\gamma, \gamma = -\int_{0}^{\infty} e^{-t} \ln t dt = 0.5772156 \ldots \) is the Euler–Mascheroni constant.

There exists an intuitive explanation behind the construction of the KL differential entropy estimator. Writing informally, we have

\[
h(f) = E_f[-\ln f(X)] \approx \frac{1}{n} \sum_{i=1}^{n} -\ln f(X_i) \approx \frac{1}{n} \sum_{i=1}^{n} -\ln \hat{f}(X_i),
\]

where the first approximation is based on the law of large numbers, and in the second approximation we have replaced \( f \) by a nearest neighbor density estimator \( \hat{f} \). The nearest neighbor density estimator \( \hat{f}(X_i) \) follows from the “intuition”\(^1\) that

\[
\hat{f}(X_i) \lambda(B(X_i, R_{i,k})) \approx \frac{k}{n},
\]

Here the final additive bias correction term \( \ln k - \psi(k) \) follows from a detailed analysis of the bias of the KL estimator, which will become apparent later.

We focus on the regime where \( k \) is a fixed: in other words, it does not grow as the number of samples \( n \) increases. The fixed \( k \) version of the KL estimator is widely applied in practice and enjoys smaller computational complexity, see [52].

There exists extensive literature on the analysis of the KL differential entropy estimator, which we refer to [4] for a recent survey. One of the major difficulties in analyzing the KL estimator is that the nearest neighbor density estimator exhibits a huge bias when the density is small. Indeed, it was shown in [32] that the bias of the nearest neighbor density estimator in fact does not vanish even

\(^1\)Precisely, we have \( \int_{B(X_i, R_{i,k})} f(u) du \sim \text{Beta}(k, n - k) \) [4] Chap. 1.2. A Beta\((k, n - k)\) distributed random variable has mean \( \frac{k}{n} \).
when \( n \to \infty \) and deteriorates as \( f(x) \) gets close to zero. In the literature, a large collection of work assume that the density is uniformly bounded away from zero [23, 29, 57, 30, 53], while others put various assumptions quantifying on average how close the density is to zero [25, 40, 56, 14, 20, 52, 11]. In this paper, we focus on removing assumptions on how close the density is to zero.

### 1.1 Main Contribution

Let \( H_d^s(L; [0, 1]^d) \) be the Hölder ball in the unit cube (torus) (formally defined later in Definition 2 in Appendix A) and \( s \in (0, 2) \) is the Hölder smoothness parameter. Then, the worst case risk of the fixed \( k \)-nearest neighbor differential entropy estimator over \( H_d^s(L; [0, 1]^d) \) is controlled by the following theorem.

**Theorem 1** Let \( X = \{X_1, \ldots, X_n\} \) be i.i.d. samples from density function \( f \). Then, for \( 0 < s \leq 2 \), the fixed \( k \)-nearest neighbor KL differential entropy estimator \( \hat{h}_{n,k} \) in (3) satisfies

\[
\left( \sup_{f \in H_d^s(L; [0,1]^d)} \mathbb{E}_f \left( \hat{h}_{n,k}(X) - h(f) \right)^2 \right)^{\frac{1}{2}} \leq C \left( n^{-\frac{1}{2s}} \ln(n+1) + n^{-\frac{s}{2}} \right).
\]

where \( C \) is a constant depends only on \( s, L, k \) and \( d \).

The KL estimator is in fact nearly minimax up to logarithmic factors, as shown in the following result from [26].

**Theorem 2** [26] Let \( X = \{X_1, \ldots, X_n\} \) be i.i.d. samples from density function \( f \). Then, there exists a constant \( L_0 \) depending on \( s, d \) only such that for all \( L \geq L_0 \), \( s > 0 \),

\[
\left( \inf_{h} \sup_{f \in H_d^s(L; [0,1]^d)} \mathbb{E}_f \left( h(X) - h(f) \right)^2 \right)^{\frac{1}{2}} \geq c \left( n^{-\frac{1}{2s}} (\ln(n+1))^{-\frac{1}{2s}} + n^{-\frac{s}{2}} \right),
\]

where \( c \) is a constant depends only on \( s, L \) and \( d \).

**Remark 1** We emphasize that one cannot remove the condition \( L \geq L_0 \) in Theorem 2. Indeed, if the Hölder ball has a too small width, then the density itself is bounded away from zero, which makes the differential entropy a smooth functional, with minimax rates \( n^{-\frac{1}{2s}} + n^{-1/2} \). [51, 50, 43].

Theorem 1 and 2 imply that for any fixed \( k \), the KL estimator achieves the minimax rates up to logarithmic factors without knowing \( s \) for all \( s \in (0, 2) \), which implies that it is near minimax rate-optimal (within logarithmic factors) when the dimension \( d \leq 2 \). We cannot expect the vanilla version of the KL estimator to adapt to higher order of smoothness since the nearest neighbor density estimator can be viewed as a variable width kernel density estimator with the box kernel, and it is well known in the literature (see, e.g., [55] Chapter 1) that any positive kernel cannot exploit the smoothness \( s > 2 \). We refer to [26] for a more detailed discussion on this difficulty and potential solutions. The Jackknife idea, such as the one presented in [11, 3] might be useful for adapting to \( s > 2 \).

The significance of our work is multi-folded:

- We obtain the first uniform upper bound on the performance of the fixed \( k \)-nearest neighbor KL differential entropy estimator over Hölder balls without assuming how close the density could be from zero. We emphasize that assuming conditions of this type, such as the density is bounded away from zero, could make the problem significantly easier. For example, if the density \( f \) is assumed to satisfy \( f(x) \geq c \) for some constant \( c > 0 \), then the differential entropy becomes a smooth functional and consequently, the general technique for estimating smooth nonparametric functionals [51, 50, 43] can be directly applied here to achieve the minimax rates \( n^{-\frac{1}{2s}} + n^{-1/2} \). The main technical tools that enabled us to remove the conditions on how close the density could be from zero are the Besicovitch covering lemma (Lemma 3) and the generalized Hardy–Littlewood maximal inequality.

- We show that, for any fixed \( k \), the \( k \)-nearest neighbor KL entropy estimator nearly achieves the minimax rates without knowing the smoothness parameter \( s \). In the functional estimation literature, designing estimators that can be theoretically proved to adapt to unknown
levels of smoothness is usually achieved using the Lepski method \cite{39, 22, 45, 44, 27}, which is not known to be performing well in general in practice. On the other hand, a simple plug-in approach can achieve the rate of $n^{-s/(s+d)}$, but only when $s$ is known \cite{26}. The KL estimator is well known to exhibit excellent empirical performance, but existing theory has not yet demonstrated its near-“optimality” when the smoothness parameter $s$ is not known. Recent works \cite{3, 52, 11} analyzed the performance of the KL estimator under various assumptions on how close the density could be to zero, with no matching lower bound up to logarithmic factors in general. Our work makes a step towards closing this gap and provides a theoretical explanation for the wide usage of the KL estimator in practice.

The rest of the paper is organized as follows. Section \ref{sec:proof} is dedicated to the proof of Theorem \ref{thm:main}. We discuss some future directions in Section \ref{sec:future}.

### 1.2 Notations

For positive sequences $a, b, s, L, d, k$, we use the notation $a \lesssim_b b$ to denote that there exists a universal constant $C$ that only depends on $s$ such that $\sup_{t \geq 0} \frac{a(t)}{b(t)} \leq C$, and $a \gtrsim_b b$ is equivalent to $b \lesssim_a a$. Notation $a \ll b$ is equivalent to $a \lesssim_{\log} b$ and $b \gg a$. We write $ab \lesssim_a b$ if the constant is universal and does not depend on any parameters. Notation $a \gg b$ means that $\limsup_{t \to \infty} \frac{a(t)}{b(t)} = \infty$, and $a \ll b$ is equivalent to $b \gg a$. We write $a \wedge b = \min\{a, b\}$ and $a \vee b = \max\{a, b\}$.

### 2 Proof of Theorem \ref{thm:main}

In this section, we will prove that

$$
\left( \mathbb{E} \left( \hat{h}_{n,k}(X) - h(f) \right)^2 \right)^{1/2} \lesssim_{s,L,d,k} n^{-\frac{d}{d+2}} \ln(n+1) + n^{-\frac{d}{d+2}},
$$

for any $f \in \mathcal{H}_2(L; [0, 1]^d)$ and $s \in (0, 2]$. The proof consists two parts: (i) the upper bound of the bias in the form of $O_{s,L,d,k}(n^{-s/(s+d)}\ln(n+1))$; (ii) the upper bound of the variance is $O_{s,L,d,k}(n^{-1})$. Below we show the bias proof and relegate the variance proof to Appendix \ref{sec:appendix}.

First, we introduce the following notation

$$f_t(x) = \frac{\mu(B(x,t))}{\lambda(B(x,t))} = \frac{1}{V_d t^d} \int_{u:|u-x|\leq t} f(u) du.
$$

Here $\mu$ is the probability measure specified by density function $f$ on the torus, $\lambda$ is the Lebesgue measure on $\mathbb{R}^d$, and $V_d = \pi^{d/2} / \Gamma(1+d/2)$ is the Lebesgue measure of the unit ball in $d$-dimensional Euclidean space. Hence $f_t(x)$ is the average density of a neighborhood near $x$. We first state two main lemmas about $f_t(x)$ which will be used later in the proof.

**Lemma 1** If $f \in \mathcal{H}_d^s(L; [0, 1]^d)$ for some $0 < s \leq 2$, then for any $x \in [0, 1]^d$ and $t > 0$, we have

$$|f_t(x) - f(x)| \leq \frac{dLt^s}{s + d},
$$

**Lemma 2** If $f \in \mathcal{H}_d^s(L; [0, 1]^d)$ for some $0 < s \leq 2$ and $f(x) \geq 0$ for all $x \in [0, 1]^d$, then for any $x$ and any $t > 0$, we have

$$f(x) \lesssim_{s,L,d} \max \left\{ f_t(x), \left( f_t(x)V_d t^d \right)^{s/(s+d)} \right\},
$$

Furthermore, $f(x) \lesssim_{s,L,d} 1$.

We relegate the proof of Lemma \ref{lem:lemma1} and Lemma \ref{lem:lemma2} to Appendix \ref{sec:appendix}. Now we investigate the bias of $\hat{h}_{n,k}(X)$. The following argument reduces the bias analysis of $\hat{h}_{n,k}(X)$ to a function analytic problem. For notation simplicity, we introduce a new random variable $X \sim f$ independent of...
\( \{X_1, \ldots, X_n\} \) and study \( \hat{h}_{n+1,k}(\{X_1, \ldots, X_n, X\}) \). For every \( x \in \mathbb{R}^d \), denote \( R_k(x) \) by the \( k \)-nearest neighbor distance from \( x \) to \( \{X_1, X_2, \ldots, X_n\} \) under distance \( d(x, y) = \min_{m \in \mathbb{Z}^d} |m + x - y| \), i.e., the \( k \)-nearest neighbor distance on the torus. Then,

\[
\begin{align*}
E[\hat{h}_{n+1,k}(\{X_1, \ldots, X_n, X\})] - h(f) &= -\psi(k) + E \left[ \ln \left( \frac{f(x)}{\mu(B(X, R_k(X)))} \right) \right] + E \left[ \ln \left((n+1)\mu(B(X, R_k(X)))\right) \right] - \psi(k) \\
&= E \left[ \ln \left( \frac{f(x)\lambda(B(X, R_k(X)))}{\mu(B(X, R_k(X)))} \right) \right] + E \left[ \ln \left((n+1)\mu(B(X, R_k(X)))\right) \right] - \psi(k)
\end{align*}
\]

We first show that the second term \( E \left[ \ln \left((n+1)\mu(B(X, R_k(X)))\right) \right] - \psi(k) \) can be universally controlled regardless of the smoothness of \( f \). Indeed, the random variable \( \mu(B(X, R_k(X))) \) \( \sim \) \( \text{Beta}(k, n+1-k) \) \[4\] Chap. 1.2 and it was shown in \[4\] Theorem 7.2 that there exists a universal constant \( C > 0 \) such that

\[
\left| E \left[ \ln \left((n+1)\mu(B(X, R_k(X)))\right) \right] - \psi(k) \right| \leq \frac{C}{n}.
\]

Hence, it suffices to show that for \( 0 < s \leq 2 \),

\[
E \left[ \ln \left( \frac{f(X)}{f_\ast(R_k(X)} \right) \right] \lesssim_{s,L,d,k} \frac{1}{n} \ln(n+1).
\]

We split our analysis into two parts. Section 2.1 shows that \( E \left[ \ln \left( \frac{f_\ast(R_k(X))}{f(X)} \right) \right] \lesssim_{s,L,d,k} \frac{1}{n} \ln(n+1) \), which completes the proof.

### 2.1 Upper bound on \( E \left[ \ln \left( \frac{f_\ast(R_k(X))}{f(X)} \right) \right] \)

By the fact that \( \ln y \leq y - 1 \) for any \( y > 0 \), we have

\[
E \left[ \ln \left( \frac{f_\ast(R_k(X))}{f(X)} \right) \right] \leq E \left[ \frac{f_\ast(R_k(X)) - f(X)}{f(X)} \right] = \int_{[0,1]^d \cap \{x : f(x) \neq 0\}} (E[f_\ast(R_k(x)) - f(x)] - f(x)) \, dx.
\]

Here the expectation is taken with respect to the randomness in \( R_k(x) = \min_{1 \leq i \leq n, m \in \mathbb{Z}^d} \|m + X_i - x\|, x \in \mathbb{R}^d \). Define function \( g(x; f, n) \) as

\[
g(x; f, n) = \sup \left\{ u \geq 0 : V_d u^d f_u(x) \leq \frac{1}{n} \right\},
\]

\( g(x; f, n) \) intuitively means the distance \( R \) such that the probability mass \( \mu(B(x, R)) \) within \( R \) is \( 1/n \). Then for any \( x \in [0,1]^d \), we can split \( E[f_\ast(R_k(x)) - f(x)] \) into three terms as

\[
E[f_\ast(R_k(x)) - f(x)] = E[(f_\ast(R_k(x)) - f(x)] \| (R_k(x) \leq n^{-1/(s+d)}) \]
\[
+ E[(f_\ast(R_k(x)) - f(x)] \| (n^{-1/(s+d)} < R_k(x) \leq g(x; f, n)) \]
\[
+ E[(f_\ast(R_k(x)) - f(x)] \| (R_k(x) > g(x; f, n) \vee n^{-1/(s+d)}) \]
\]

\[
= C_1 + C_2 + C_3.
\]

Now we handle three terms separately. Our goal is to show that for every \( x \in [0,1], C_i \lesssim_{s,L,d} n^{-s/(s+d)} \) for \( i \in \{1, 2, 3\} \). Then, taking the integral with respect to \( x \) leads to the desired bound.

1. Term \( C_1 \): whenever \( R_k(x) \leq n^{-1/(s+d)} \), by Lemma 1 we have

\[
|f_\ast(R_k(x)) - f(x)| \leq \frac{dLR_k(x)^s}{s + d} \lesssim_{s,L,d} n^{-s/(s+d)},
\]

which implies that

\[
C_1 \leq E \left[ |f_\ast(R_k(x)) - f(x)| \| (R_k(x) \leq n^{-1/(s+d)}) \right] \lesssim_{s,L,d} n^{-s/(s+d)}.
\]
2. Term $C_2$: whenever $R_k(x)$ satisfies that $n^{-1/(s+d)} < R_k(x) \leq g(x; f, n)$, by definition of $g(x; f, n)$, we have $V_d R_k(x)^d f_{R_k}(x) \leq \frac{1}{n}$, which implies that

$$f_{R_k}(x) \leq \frac{1}{nV_d R_k(x)^d} \leq \frac{1}{nV_d n^{-d/(s+d)}} \lesssim_{s, L, d} n^{-s/(s+d)}. \quad (27)$$

It follows from Lemma 2 that in this case

$$f(x) \lesssim_{s, L, d} f_{R_k}(x) \lor (f_{R_k}(x) V_d R_k(x)^d)^{s/(s+d)} \quad (28)$$

$$\leq n^{-s/(s+d)} \lor n^{-s/(s+d)} = n^{-s/(s+d)}. \quad (29)$$

Hence, we have

$$C_2 = \mathbb{E} \left[ (f_{R_k}(x) - f(x)) \mathbb{I} \left( n^{-1/(s+d)} < R_k(x) \leq g(x; f, n) \right) \right] \quad (30)$$

$$\leq \mathbb{E} \left[ (f_{R_k}(x) + f(x)) \mathbb{I} \left( n^{-1/(s+d)} < R_k(x) \leq g(x; f, n) \right) \right] \quad (31)$$

$$\lesssim_{s, L, d} n^{-s/(s+d)}. \quad (32)$$

3. Term $C_3$: we have

$$C_3 \leq \mathbb{E} \left[ (f_{R_k}(x) + f(x)) \mathbb{I} \left( R_k(x) > g(x; f, n) \lor n^{-1/(s+d)} \right) \right]. \quad (33)$$

For any $x$ such that $R_k(x) > n^{-1/(s+d)}$, we have

$$f_{R_k}(x) \lesssim_{s, L, d} V_d R_k(x)^d f_{R_k}(x) n^{d/(s+d)}, \quad (34)$$

and by Lemma 2

$$f(x) \lesssim_{s, L, d} f_{R_k}(x) \lor (V_d R_k(x)^d f_{R_k}(x))^{s/(s+d)} \quad (35)$$

$$\leq f_{R_k}(x) + (V_d R_k(x)^d f_{R_k}(x))^{s/(s+d)}. \quad (36)$$

Hence,

$$f(x) + f_{R_k}(x) \lesssim_{s, L, d} 2f_{R_k}(x) + (V_d R_k(x)^d f_{R_k}(x))^{s/(s+d)} \quad (37)$$

$$\lesssim_{s, L, d} V_d R_k(x)^d f_{R_k}(x) n^{d/(s+d)} + (V_d R_k(x)^d f_{R_k}(x))^{s/(s+d)} \quad (38)$$

$$\lesssim_{s, L, d} V_d R_k(x)^d f_{R_k}(x) n^{d/(s+d)}. \quad (39)$$

where in the last step we have used the fact that $V_d R_k(x)^d f_{R_k}(x) > n^{-1}$ since $R_k(x) > g(x; f, n)$. Finally, we have

$$C_3 \lesssim_{s, L, d} V_d^{d/(s+d)} \mathbb{E} \left[ (V_d R_k(x)^d f_{R_k}(x)) \mathbb{I} \left( R_k(x) > g(x; f, n) \right) \right] \quad (40)$$

$$= n^{d/(s+d)} \mathbb{E} \left[ (V_d R_k(x)^d f_{R_k}(x)) \mathbb{I} \left( V_d R_k(x)^d f_{R_k}(x) > 1/n \right) \right]. \quad (41)$$

Note that $V_d R_k(x)^d f_{R_k}(x) \sim \text{Beta}(k, n + 1 - k)$, and if $Y \sim \text{Beta}(k, n + 1 - k)$, we have

$$\mathbb{E}[Y^2] = \left( \frac{k}{n+1} \right)^2 + \frac{k(n+1-k)}{(n+1)^2(n+2)} \lesssim \frac{1}{n^2}. \quad (42)$$

Notice that $\mathbb{E}[Y \mathbb{I} (Y > 1/n)] \leq n \mathbb{E}[Y^2]$. Hence, we have

$$C_3 \lesssim_{s, L, d} n^{d/(s+d)} \frac{n \mathbb{E} \left[ (V_d R_k(x)^d f_{R_k}(x))^2 \right]}{n^2} \quad (43)$$

$$\lesssim_{s, L, d, k} n^{-s/(s+d)}. \quad (44)$$
2.2 Upper bound on $\mathbb{E}\left[ \ln \frac{f(X)}{f_{R_k(X)}(X)} \right]$

By splitting the term into two parts, we have

$$
\mathbb{E}\left[ \ln \frac{f(X)}{f_{R_k(X)}(X)} \right] = \mathbb{E}\left[ \int_{[0,1]^d \cap \{x : f(x) \neq 0\}} f(x) \ln \frac{f(x)}{f_{R_k(x)}} \, dx \right]
$$

$$
= \mathbb{E}\left[ \int_A f(x) \ln \frac{f(x)}{f_{R_k(x)}} 1(f_{R_k(x)}(x) > n^{-s/(s+d)}) \, dx \right] + \mathbb{E}\left[ \int_A f(x) \ln \frac{f(x)}{f_{R_k(x)}} 1(f_{R_k(x)}(x) \leq n^{-s/(s+d)}) \, dx \right]
$$

Here we denote $A = [0, 1]^d \cap \{x : f(x) \neq 0\}$ for simplicity of notation. For the term $C_4$, we have

$$
C_4 \leq \mathbb{E}\left[ \int_A (f(x) - f_{R_k(x)})^2 \, dx \right] + \mathbb{E}\left[ \int_A (f(x) - f_{R_k(x)}) \, dx \right].
$$

In the proof of upper bound of $\mathbb{E}\left[ \ln \frac{f_{R_k(x)}(X)}{f(x)} \right]$, we have shown that $\mathbb{E}[f_{R_k(x)}(x) - f(x)] \lesssim_{s,L,d,k} n^{-s/(s+d)}$ for any $x \in A$. Similarly as in the proof of upper bound of $\mathbb{E}\left[ \ln \frac{f_{R_k(x)}(X)}{f(x)} \right]$, we have $\mathbb{E}[|f_{R_k(x)}(x) - f(x)|^2] \lesssim_{s,L,d,k} n^{-2s/(s+d)}$ for every $x \in A$. Therefore, we have

$$
C_4 \lesssim_{s,L,d,k} n^{s/(s+d)}n^{-2s/(s+d)} + n^{-s/(s+d)} \lesssim_{s,L,d,k} n^{-s/(s+d)}.
$$

Now we consider $C_5$. We conjecture that $C_5 \lesssim_{s,L,d,k} n^{-s/(s+d)}$ in this case, but we were not able to prove it. Below we prove that $C_5 \lesssim_{s,L,d,k} n^{-s/(s+d)} \ln(n + 1)$. Define the function

$$
M(x) = \sup_{t>0} \frac{1}{f_t(x)}.
$$

Since $f_{R_k(x)}(x) \leq n^{-s/(s+d)}$, we have $M(x) = \sup_{t>0} (1/f_t(x)) \geq 1/f_{R_k(x)}(x) \geq n^{s/(s+d)}$. Denote $\ln^+ (y) = \max{\{\ln(y), 0\}}$ for any $y > 0$, therefore, we have that

$$
C_5 \leq \mathbb{E}\left[ \int_A f(x) \ln^+ \left( \frac{f(x)}{f_{R_k(x)}} \right) 1(f_{R_k(x)}(x) \leq n^{-s/(s+d)}) \, dx \right] + \mathbb{E}\left[ \int_A f(x) \ln^+ \left( \frac{f(x)}{f_{R_k(x)}} \right) 1(M(x) \geq n^{s/(s+d)}) \, dx \right]
$$

$$
\leq \mathbb{E}\left[ \int_A f(x) \ln^+ \left( \frac{1}{(n + 1)V_d R_k(x)^d f_{R_k(x)}} \right) 1(M(x) \geq n^{s/(s+d)}) \, dx \right] + \mathbb{E}\left[ \int_A f(x) \ln^+ \left( (n + 1)V_d R_k(x)^d f(x) \right) 1(M(x) \geq n^{s/(s+d)}) \, dx \right]
$$

$$
= C_{51} + C_{52}.
$$
where the last inequality uses the fact \( \ln^+(xy) \leq \ln^+ x + \ln^+ y \) for all \( x, y \geq 0 \). As for \( C_{51} \), since
\[
V_d R_k(x) f R_k(x)(x) \sim \text{Beta}(k, n+1-k),
\]
and for \( Y \sim \text{Beta}(k, n+1-k) \), we have
\[
\mathbb{E} \left[ \ln^+ \left( \frac{1}{(n+1)Y} \right) \right] = \int_0^{\infty} \ln \left( \frac{1}{(n+1)x} \right) p_Y(x) \, dx
\]
\[
= \mathbb{E} \left[ \ln \left( \frac{1}{(n+1)Y} \right) \right] + \int_1^{\infty} \ln \left( (n+1)x \right) p_Y(x) \, dx
\]
\[
\leq \mathbb{E} \left[ \ln \left( \frac{1}{(n+1)Y} \right) \right] + \ln(n+1) \int_1^{\infty} p_Y(x) \, dx
\]
\[
\leq \mathbb{E} \left[ \ln \left( \frac{1}{(n+1)Y} \right) \right] + \ln(n+1)
\]
\[
\leq \ln(n+1)
\]
where in the last inequality we used the fact that \( \mathbb{E} \left[ \ln \left( \frac{1}{(n+1)Y} \right) \right] = \psi(n+1) - \psi(k) - \ln(n+1) \leq 0 \) for any \( k \geq 1 \). Hence,
\[
C_{51} \lesssim_s, L, d \ln(n+1) \int_A f(x) \mathbbm{1}(M(x) \geq n^{s/(s+d)}) \, dx.
\]  \hspace{1cm} (65)

Now we introduce the following lemma, which is proved in Appendix C.

**Lemma 3** Let \( \mu_1, \mu_2 \) be two Borel measures that are finite on the bounded Borel sets of \( \mathbb{R}^d \). Then, for all \( t > 0 \) and any Borel set \( A \subset \mathbb{R}^d \),
\[
\mu_1 \left( \left\{ x \in A : \sup_{0 < \rho \leq D} \frac{\mu_2(B(x, \rho))}{\mu_1(B(x, \rho))} > t \right\} \right) \leq \frac{C_d}{t} \mu_2(A_D).
\]  \hspace{1cm} (66)

Here \( C_d > 0 \) is a constant that depends only on the dimension \( d \) and
\[
A_D = \{ x : \exists y \in A, |y - x| \leq D \}.
\]  \hspace{1cm} (67)

Applying the second part of Lemma 3 with \( \mu_2 \) being the Lebesgue measure and \( \mu_1 \) being the measure specified by \( f(x) \) on the torus, we can view the function \( M(x) \) as
\[
M(x) = \sup_{0 < \rho \leq 1/2} \frac{\mu_2(B(x, \rho))}{\mu_1(B(x, \rho))}.
\]  \hspace{1cm} (68)

Taking \( A = [0, 1]^d \cap \{ x : f(x) \neq 0 \} \), \( t = n^{s/(s+d)} \), then \( \mu_2(A_{1/2}) \leq 2^d \), so we know that
\[
C_{51} \lesssim_s, L, d \ln(n+1) \cdot \int_A f(x) \mathbbm{1}(M(x) \geq n^{s/(s+d)}) \, dx
\]
\[
= \ln(n+1) \cdot \mu_1 \left( \left\{ x \in [0, 1]^d : f(x) \neq 0, M(x) \geq n^{s/(s+d)} \right\} \right)
\]
\[
\leq \ln(n+1) \cdot C_d n^{-s/(s+d)} \mu_2(A_{1/2}) \lesssim_s, L, d n^{-s/(s+d)} \ln(n+1).
\]  \hspace{1cm} (71)

Now we deal with \( C_{52} \). Recall that in Lemma 2 we know that \( f(x) \lesssim_s, L, d 1 \) for any \( x \), and \( R_k(x) \leq 1 \), so \( \ln^+ ((n+1)V_d R_k(x) f(x)) \lesssim_s, L, d \ln(n+1) \). Therefore,
\[
C_{52} \lesssim_s, L, d \ln(n+1) \cdot \int_A f(x) \mathbbm{1}(M(x) \geq n^{s/(s+d)}) \, dx
\]
\[
\lesssim_s, L, d n^{-s/(s+d)} \ln(n+1).
\]  \hspace{1cm} (73)

Therefore, we have proved that \( C_5 \leq C_{51} + C_{52} \lesssim_s, L, d n^{-s/(s+d)} \ln(n+1) \), which completes the proof of the upper bound on \( \mathbb{E} \left[ \ln \frac{f(X)}{\hat{R}_s(x) M(x)} \right] \).
3 Future directions

It is an tempting question to ask whether one can close the logarithmic gap between Theorem 1 and 2. We believe that neither the upper bound nor the lower bound are tight. In fact, we conjecture that the upper bound in Theorem 1 could be improved to $n^{-s} + n^{-1/2}$ due to a more careful analysis of the bias, since Hardy–Littlewood maximal inequalities apply to arbitrary measurable functions but we have assumed regularity properties of the underlying density. We conjecture that the minimax lower bound could be improved to $(\ln n)^{-s} + n^{-1/2}$, since a kernel density estimator based differential entropy estimator was constructed in [26] which achieves upper bound $(\ln n)^{-s} + n^{-1/2}$ over $\mathcal{H}_d^s(L; [0, 1]^d)$ with the knowledge of $s$.

It would be interesting to extend our analysis to that of the $k$-nearest neighbor based Kullback–Leibler divergence estimator [59]. The discrete case has been studied recently [28, 7].

It is also interesting to analyze $k$-nearest neighbor based mutual information estimators, such as the KSG estimator [34], and show that they are “near”-optimal and adaptive to both the smoothness and the dimension of the distributions. There exists some analysis of the KSG estimator [21] but we suspect the upper bound is not tight. Moreover, a slightly revised version of KSG estimator is proved to be consistent even if the underlying distribution is not purely continuous nor purely discrete [19], but the optimality properties are not yet well understood.
References

[1] R. Battiti. Using mutual information for selecting features in supervised neural net learning. Neural Networks, IEEE Transactions on, 5(4):537–550, 1994.

[2] Jan Beirlant, Edward J Dudewicz, László Györfi, and Edward C Van der Meulen. Nonparametric entropy estimation: An overview. International Journal of Mathematical and Statistical Sciences, 6(1):17–39, 1997.

[3] Thomas B Berrett, Richard J Samworth, and Ming Yuan. Efficient multivariate entropy estimation via k-nearest neighbour distances. arXiv preprint arXiv:1606.00304, 2016.

[4] Gérard Biau and Luc Devroye. Lectures on the nearest neighbor method. Springer, 2015.

[5] Peter J Bickel and Yaacov Ritov. Estimating integrated squared density derivatives: sharp best order of convergence estimates. Sankhyä: The Indian Journal of Statistics, Series A, pages 381–393, 1988.

[6] Lucien Birgé and Pascal Massart. Estimation of integral functionals of a density. The Annals of Statistics, pages 11–29, 1995.

[7] Yuheng Bu, Shaofeng Zou, Yingbin Liang, and Venugopal V Veeravalli. Estimation of KL divergence between large-alphabet distributions. In 2016 IEEE International Symposium on Information Theory (ISIT), pages 1118–1122. IEEE, 2016.

[8] T Tony Cai and Mark G Low. A note on nonparametric estimation of linear functionals. Annals of statistics, pages 1140–1153, 2003.

[9] T Tony Cai and Mark G Low. Nonquadratic estimators of a quadratic functional. The Annals of Statistics, pages 2930–2956, 2005.

[10] C. Chan, A. Al-Bashabsheh, J. B. Ebrahimi, T. Kaced, and T. Liu. Multivariate mutual information inspired by secret-key agreement. Proceedings of the IEEE, 103(10):1883–1913, 2015.

[11] Sylvain Delattre and Nicolas Fournier. On the kozachenko–leonenko entropy estimator. Journal of Statistical Planning and Inference, 185:69–93, 2017.

[12] David L Donoho and Michael Nussbaum. Minimax quadratic estimation of a quadratic functional. Journal of Complexity, 6(3):290–323, 1990.

[13] Bradley Efron and Charles Stein. The jackknife estimate of variance. The Annals of Statistics, pages 586–596, 1981.

[14] Fidah El Haje Hussein and Yu Golubev. On entropy estimation by m-spacing method. Journal of Mathematical Sciences, 163(3):290–309, 2009.

[15] Lawrence Craig Evans and Ronald F Gariepy. Measure theory and fine properties of functions. CRC press, 2015.

[16] Jianqing Fan. On the estimation of quadratic functionals. The Annals of Statistics, pages 1273–1294, 1991.

[17] F. Fleuret. Fast binary feature selection with conditional mutual information. The Journal of Machine Learning Research, 5:1531–1555, 2004.

[18] Weihao Gao, Sreeram Kannan, Sewoong Oh, and Pramod Viswanath. Conditional dependence via Shannon capacity: Axioms, estimators and applications. In International Conference on Machine Learning, pages 2780–2789, 2016.

[19] Weihao Gao, Sreeram Kannan, Sewoong Oh, and Pramod Viswanath. Estimating mutual information for discrete-continuous mixtures. In Advances in Neural Information Processing Systems, pages 5988–5999, 2017.

[20] Weihao Gao, Sewoong Oh, and Pramod Viswanath. Breaking the bandwidth barrier: Geometrical adaptive entropy estimation. In Advances in Neural Information Processing Systems, pages 2460–2468, 2016.

[21] Weihao Gao, Sewoong Oh, and Pramod Viswanath. Demystifying fixed k-nearest neighbor information estimators. In Information Theory (ISIT), 2017 IEEE International Symposium on, pages 1267–1271. IEEE, 2017.
[22] Evarist Giné and Richard Nickl. A simple adaptive estimator of the integrated square of a density. Bernoulli, pages 47–61, 2008.

[23] Peter Hall. Limit theorems for sums of general functions of m-spacings. In Mathematical Proceedings of the Cambridge Philosophical Society, volume 96, pages 517–532. Cambridge University Press, 1984.

[24] Peter Hall and James Stephen Marron. Estimation of integrated squared density derivatives. Statistics & Probability Letters, 6(2):109–115, 1987.

[25] Peter Hall and Sally C Morton. On the estimation of entropy. Annals of the Institute of Statistical Mathematics, 45(1):69–88, 1993.

[26] Yanjun Han, Jiantao Jiao, Tsachy Weissman, and Yihong Wu. Optimal rates of entropy estimation over lipschitz balls. arXiv preprint arXiv:1711.02141, 2017.

[27] Yanjun Han, Jiantao Jiao, Rajarshi Mukherjee, and Tsachy Weissman. On estimation of $l_r$-norms in gaussian white noise models. arXiv preprint arXiv:1710.03863, 2017.

[28] Yanjun Han, Jiantao Jiao, and Tsachy Weissman. Minimax rate-optimal estimation of divergences between discrete distributions. arXiv preprint arXiv:1605.09124, 2016.

[29] Harry Joe. Estimation of entropy and other functionals of a multivariate density. Annals of the Institute of Mathematical Statistics, 41(4):683–697, 1989.

[30] Kirthevasan Kandasamy, Akshay Krishnamurthy, Barnabas Poczos, Larry Wasserman, et al. Nonparametric von Mises estimators for entropies, divergences and mutual informations. In Advances in Neural Information Processing Systems, pages 397–405, 2015.

[31] Rhoana J Karunamuni and Tom Alberts. On boundary correction in kernel density estimation. Statistical Methodology, 2(3):191–212, 2005.

[32] Gérad Kerkyacharian and Dominique Picard. Estimating nonquadratic functionals of a density using haar wavelets. The Annals of Statistics, 24(2):485–507, 1996.

[33] LF Kozachenko and Nikolai N Leonenko. Sample estimate of the entropy of a random vector. Problemy Peredachi Informatsii, 23(2):9–16, 1987.

[34] Alexander Kraskov, Harald Stögbauer, and Peter Grassberger. Estimating mutual information. Physical Review E, 69(6):066138, 2004.

[35] Akshay Krishnamurthy, Kirthevasan Kandasamy, Barnabas Poczos, and Larry Wasserman. Nonparametric estimation of Rényi divergence and friends. In International Conference on Machine Learning, pages 919–927, 2014.

[36] Smita Krishnaswamy, Matthew H Spitzer, Michael Mingueneau, Sean C Bendall, Oren Litvin, Erica Stone, Dana Pe’er, and Garry P Nolan. Conditional density-based analysis of t cell signaling in single-cell data. Science, 346(6213):1250689, 2014.

[37] Béatrice Laurent. Efficient estimation of integral functionals of a density. The Annals of Statistics, 24(2):659–681, 1996.

[38] Oleg Lepski, Arkady Nemirovski, and Vladimir Spokoiny. On estimation of the $L_r$ norm of a regression function. Probability theory and related fields, 113(2):221–253, 1999.

[39] Oleg V Lepski. On problems of adaptive estimation in white gaussian noise. Topics in nonparametric estimation, 12:87–106, 1992.

[40] Boris Ya Levit. Asymptotically efficient estimation of nonlinear functionals. Problemy Peredachi Informatsii, 14(3):65–72, 1978.

[41] Pan Li and Olgica Milenkovic. Inhomogenous hypergraph clustering with applications. arXiv preprint arXiv:1709.01249, 2017.

[42] YP Mack and Murray Rosenblatt. Multivariate $k$-nearest neighbor density estimates. Journal of Multivariate Analysis, 9(1):1–15, 1979.

[43] Rajarshi Mukherjee, Whitney K Newey, and James M Robins. Semiparametric efficient empirical higher order influence function estimators. arXiv preprint arXiv:1705.07577, 2017.

[44] Rajarshi Mukherjee, Eric Tchetgen Tchetgen, and James Robins. On adaptive estimation of nonparametric functionals. arXiv preprint arXiv:1608.01364, 2016.
[45] Rajarshi Mukherjee, Eric Tchetgen Tchetgen, and James Robins. Lepski’s method and adaptive estimation of nonlinear integral functionals of density. *arXiv preprint arXiv:1508.00249*, 2015.

[46] A. C. Müller, S. Nowozin, and C. H. Lampert. *Information theoretic clustering using minimum spanning trees*. Springer, 2012.

[47] Arkadi Nemirovski. *Topics in non-parametric*. *Ecole d'Eté de Probabilités de Saint-Flour*, 28:85, 2000.

[48] H. Peng, F. Long, and C. Ding. Feature selection based on mutual information criteria of max-dependency, max-relevance, and min-redundancy. *Pattern Analysis and Machine Intelligence, IEEE Transactions on*, 27(8):1226–1238, 2005.

[49] David N Reshef, Yakir A Reshef, Hilary K Finucane, Sharon R Grossman, Gilean McVean, Peter J Turnbaugh, Eric S Lander, Michael Mitzenmacher, and Pardis C Sabeti. Detecting novel associations in large data sets. *science*, 334(6062):1518–1524, 2011.

[50] James Robins, Lingling Li, Rajarshi Mukherjee, Eric Tchetgen Tchetgen, and Aad van der Vaart. Higher order estimating equations for high-dimensional models. *The Annals of Statistics (To Appear)*, 2016.

[51] James Robins, Lingling Li, Eric Tchetgen, and Aad van der Vaart. Higher order influence functions and minimax estimation of nonlinear functionals. In *Probability and Statistics: Essays in Honor of David A. Freedman*, pages 335–421. Institute of Mathematical Statistics, 2008.

[52] Shashank Singh and Barnabás Póczos. Finite-sample analysis of fixed-k nearest neighbor density functional estimators. In *Advances in Neural Information Processing Systems*, pages 1217–1225, 2016.

[53] Kumar Sricharan, Raviv Raich, and Alfred O Hero. Estimation of nonlinear functionals of densities with confidence. *IEEE Transactions on Information Theory*, 58(7):4135–4159, 2012.

[54] Eric Tchetgen, Lingling Li, James Robins, and Aad van der Vaart. Minimax estimation of the integral of a power of a density. *Statistics & Probability Letters*, 78(18):3307–3311, 2008.

[55] A. Tsybakov. *Introduction to Nonparametric Estimation*. Springer-Verlag, 2008.

[56] Alexandre B Tsybakov and EC van der Meulen. Root-n consistent estimators of entropy for densities with unbounded support. *Scandinavian Journal of Statistics*, pages 75–83, 1996.

[57] Bert Van Es. Estimating functionals related to a density by a class of statistics based on spacings. *Scandinavian Journal of Statistics*, pages 61–72, 1992.

[58] G. Ver Steeg and A. Galstyan. Maximally informative hierarchical representations of high-dimensional data. *stat*, 1050:27, 2014.

[59] Qing Wang, Sanjeev R Kulkarni, and Sergio Verdú. Divergence estimation for multidimensional densities via k-nearest-neighbor distances. *Information Theory, IEEE Transactions on*, 55(5):2392–2405, 2009.
A Definition of Hölder Ball

In order to define the Hölder ball in the unit cube $[0,1]^d$, we first review the definition of Hölder ball in $\mathbb{R}^d$.

Definition 1 (Hölder ball in $\mathbb{R}^d$) The Hölder ball $\mathcal{H}_s^d(L;\mathbb{R}^d)$ is specified by the parameters $s > 0$ (order of smoothness), $d \in \mathbb{Z}_+$ (dimension of the argument) and $L > 0$ (smoothness constant) and is as follows. A positive real $s$ can be uniquely represented as

$$s = m + \alpha,$$  \hspace{1cm} (74)

where $m$ is a nonnegative integer and $0 < \alpha \leq 1$. By definition, $\mathcal{H}_s^d(L;\mathbb{R}^d)$ is comprised of all $m$ times continuously differentiable functions

$$f : \mathbb{R}^d \mapsto \mathbb{R},$$  \hspace{1cm} (75)

with Hölder continuous, with exponent $\alpha$ and constant $L$, derivatives of order $m$:

$$\|D^m f(x)[\delta_1, \ldots, \delta_m] - D^m f(x')[\delta_1, \ldots, \delta_m]\| \leq L \|x - x'\|^{\alpha}, \quad \forall x, x' \in \mathbb{R}^d, \delta \in \mathbb{R}^d. \hspace{1cm} (76)$$

Here $\| \cdot \|$ is the Euclidean norm on $\mathbb{R}^d$, and $D^m f(x)[\delta_1, \ldots, \delta_m]$ is the $m$-th differential of $f$ taken as a point $x$ along the directions $\delta_1, \ldots, \delta_m$:

$$D^m f(x)[\delta_1, \ldots, \delta_m] = \left. \frac{\partial^m f}{\partial t_1 \cdots \partial t_m} \right|_{t_1 = t_2 = \ldots = t_m = 0} f(x + t_1 \delta_1 + \ldots + t_m \delta_m). \hspace{1cm} (77)$$

In this paper, we consider functions that lie in Hölder balls in $[0,1]^d$. The Hölder ball in the compact set $[0,1]^d$ is defined as follows.

Definition 2 (Hölder ball in the unit cube) A function $f : [0,1]^d \mapsto \mathbb{R}$ is said to belong to the Hölder ball $\mathcal{H}_s^d(L;[0,1]^d)$ if and only if there exists another function $f_1 \in \mathcal{H}_s^d(L;\mathbb{R}^d)$ such that

$$f(x) = f_1(x), \quad x \in [0,1], \hspace{1cm} (78)$$

and $f_1(x)$ is a 1-periodic function in each variable. Here $\mathcal{H}_s^d(L;[0,1]^d)$ is introduced in Definition 7.

In other words,

$$f_1(x + e_j) = f_1(x), \quad \forall x \in \mathbb{R}^d, 1 \leq j \leq d, \hspace{1cm} (79)$$

where $\{e_j : 1 \leq j \leq d\}$ is the standard basis in $\mathbb{R}^d$.

Definition 2 has appeared in the literature [33]. It is motivated by the observations that sliding window kernel methods usually can not deal with the boundary effects without additional assumptions [31]. Indeed, near the boundary the sliding window kernel density estimator may have a significantly larger bias than that of the interior points. In the nonparametric statistics literature, it is usually assumed that the density has its value and all the derivatives vanishing at the boundary, which is stronger than our assumptions.

B Variance upper bound in Theorem 1

Our goal is to prove

$$\text{Var} \left( \hat{h}_{n,k}(X) \right) \lesssim_{d,k} \frac{1}{n}. \hspace{1cm} (80)$$

The proof is based on the analysis in [4, Section 7.2] which utilizes the Efron–Stein inequality. Let $X^{(i)} = \{X_1, \ldots, X_{i-1}, X'_i, X_{i+1}, \ldots, X_n\}$ be a set of sample where only $X_i$ is replaced by $X'_i$. Then Efron–Stein inequality [13] states

$$\text{Var} \left( \hat{h}_{n,k}(X) \right) \leq \frac{1}{2} \sum_{i=1}^n \mathbb{E} \left[ \left( \hat{h}_{n,k}(X) - \hat{h}_{n,k}(X^{(i)}) \right)^2 \right] \hspace{1cm} (81)$$
Note that KL estimator is symmetric of sample indices, so \( \hat{h}_{n,k}(X) - \hat{h}_{n,k}(X^{(i)}) \) has the same distribution for any \( i \). Furthermore, we bridge \( \hat{h}_{n,k}(X) \) and \( \hat{h}_{n,k}(X^{(i)}) \) by introducing an estimator from \( n - 1 \) samples. Precisely, for any \( i = 2, \ldots, n \) define \( R'_{i,k} \) be the \( k \)-nearest neighbor distance from \( X_i \) to \( \{ X_2, \ldots, X_n \} \) (note that \( X_1 \) is removed), under the distance \( d(x, y) = \min_{m \in \mathbb{Z}^d} ||x - y - m|| \). Define

\[
\hat{h}_{n-1,k}(X) = -\psi(k) + \frac{1}{n} \sum_{i=2}^{n} \ln(n\lambda(B(X_i, R'_{i,k}))) . \tag{82}
\]

Notice that \( \hat{h}_{n,k}(X) - \hat{h}_{n-1,k}(X) \) has the same distribution as \( \hat{h}_{n,k}(X^{(1)}) - \hat{h}_{n-1,k}(X) \). Therefore, the variance is bounded by

\[
\text{Var} \left( \hat{h}_{n,k}(X) \right) \leq \frac{n}{2} \mathbb{E} \left[ \left( \hat{h}_{n,k}(X) - \hat{h}_{n,k}(X^{(1)}) \right)^2 \right] = 2n \mathbb{E} \left[ \left( \hat{h}_{n,k}(X) - \hat{h}_{n-1,k}(X) \right)^2 \right] . \tag{83}
\]

Now we deal with the term \( \mathbb{E} \left[ \left( \hat{h}_{n,k}(X) - \hat{h}_{n-1,k}(X) \right)^2 \right] \). Define the indicator function

\[
E_{i}^{(k)} = \mathbb{I}\{ X_1 \text{ is in the } k \text{-nearest neighbor of } X_i \} . \tag{84}
\]

for \( i \neq 1 \). Note that \( R'_{1,k} = R_{i,k} \) if \( E_{i}^{(k)} \neq 1 \) and \( i \neq 1 \). As shown in [19] Lemma B.1, the set \( S = \{ i : E_{i}^{(k)} = 1 \} \) has cardinality at most \( k\beta_d \) for a constant \( \beta_d \) only depends on \( d \). Therefore, we have

\[
\text{Var} \left( \hat{h}_{n,k}(X) \right) \leq 2n \mathbb{E} \left[ \left( \hat{h}_{n,k}(X) - \hat{h}_{n-1,k}(X) \right)^2 \right] . \tag{85}
\]

\[
\leq 2n \mathbb{E} \left[ \frac{1}{n^2} \left( \sum_{i \in S \cup \{1\}} \ln(n\lambda(B(X_i, R_{i,k}))) - \sum_{i \in S} \ln(n\lambda(B(X_i, R_{i,k}))) \right)^2 \right] . \tag{86}
\]

\[
\leq \frac{2}{n} \mathbb{E} \left[ (1 + 2|S|) \left( \sum_{i \in S \cup \{1\}} \ln^2(n\lambda(B(X_i, R_{i,k}))) + \sum_{i \in S} \ln^2(n\lambda(B(X_i, R_{i,k}))) \right) \right] . \tag{87}
\]

\[
\lesssim_{d,k} \frac{1}{n} \mathbb{E} \left[ \ln^2(n\lambda(B(X_1, R_{1,k}))) \right] + \mathbb{E} \left[ \ln^2(n\lambda(B(X_1, R'_{1,k}))) \right] . \tag{88}
\]

Now we prove that \( \mathbb{E} \left[ \ln^2(n\lambda(B(X_1, R_{1,k}))) \right] \lesssim_{d,k} 1 \) and \( \mathbb{E} \left[ \ln^2(n\lambda(B(X_1, R'_{1,k}))) \right] \lesssim_{d,k} 1 \). Using Cauchy-Schwarz inequality, we have

\[
\mathbb{E} \left[ \ln^2(n\lambda(B(X_1, R_{1,k}))) \right] \leq 2 \left( \mathbb{E} \left[ \ln^2(\frac{\lambda(B(X_1, R_{1,k}))}{\mu(B(X_1, R_{1,k}))}) \right] + \mathbb{E} \left[ \ln^2(n\mu(B(X_1, R_{1,k}))) \right] \right) , \tag{89}
\]

\[
\mathbb{E} \left[ \ln^2(n\lambda(B(X_1, R'_{1,k}))) \right] \leq 3 \left( \mathbb{E} \left[ \ln^2(\frac{\lambda(B(X_1, R'_{1,k}))}{\mu(B(X_1, R'_{1,k}))}) \right] + \mathbb{E} \left[ \ln^2((n-1)\mu(B(X_1, R'_{1,k}))) \right] + \ln^2(\frac{n}{n-1}) \right) . \tag{90}
\]

Since \( \mu(B(X_1, R_{1,k})) \sim \text{Beta}(k, n + 1 - k) \) and \( \mu(B(X_1, R'_{1,k})) \sim \text{Beta}(k, n - k) \), therefore we know that both \( \mathbb{E} \left[ \ln^2(n\mu(B(X_1, R_{1,k}))) \right] \) and \( \mathbb{E} \left[ \ln^2((n-1)\mu(B(X_1, R'_{1,k}))) \right] \) equal to certain constants that only depends on \( k \). \( \ln^2(n/(n-1)) \) is smaller than \( \ln^2 2 \) for \( n \geq 2 \). So we only need
to prove that $\mathbb{E} \left[ \ln^2 \left( \frac{\lambda(B(X_1, R_{1,k}))}{\mu(B(X_1, R_{1,k}))} \right) \right] \leq d, k \leq 1$ and $\mathbb{E} \left[ \ln^2 \left( \frac{\lambda(B(X_1, R'_{1,k}))}{\mu(B(X_1, R'_{1,k}))} \right) \right] \leq d, k \leq 1$. Recall that we have defined the maximal function as follows,

$$M(x) = \sup_{0 \leq r \leq 1/2} \frac{\lambda(B(x, r))}{\mu(B(x, r))}.$$ (91)

Similarly, we define

$$m(x) = \sup_{0 \leq r \leq 1/2} \frac{\mu(B(x, r))}{\lambda(B(x, r))}.$$ (92)

Therefore,

$$\mathbb{E} \left[ \ln^2 \left( \frac{\lambda(B(X_1, R_{1,k}))}{\mu(B(X_1, R_{1,k}))} \right) \right] \leq \mathbb{E} \left[ \max \{ \ln^2(M(x)), \ln^2(m(x)) \} \right] \leq \mathbb{E} \left[ \ln^2(M(x) + 1) + \ln^2(m(x) + 1) \right] = \mathbb{E} \left[ \ln^2(M(x) + 1) \right] + \mathbb{E} \left[ \ln^2(m(x) + 1) \right].$$ (93)

Similarly this inequality holds if we replace $R_{1,k}$ by $R'_{1,k}$. By Lemma[3] we have

$$\mathbb{E} \left[ \ln^2(M(x) + 1) \right] = \int_{[0,1]^d} \ln^2(M(x) + 1) d\mu(x)$$ (96)

$$= \int_{t=0}^{\infty} \mu \left( \{ x \in [0,1]^d : \ln^2(M(x) + 1) > t \} \right) dt$$ (97)

$$= \int_{t=0}^{\infty} \mu \left( \{ x \in [0,1]^d : M(x) > e^{\sqrt{t} - 1} \} \right) dt$$ (98)

$$\leq_d \int_{t=0}^{\infty} \frac{1}{e^{\sqrt{t} - 1} - 1} dt \leq_d 1.$$ (99)

For $\mathbb{E}[\ln^2(m(x) + 1)]$, we rewrite the term as

$$\mathbb{E} \left[ \ln^2(m(x) + 1) \right] = \int_{[0,1]^d} f(x) \ln^2(m(x) + 1) d\lambda(x)$$ (100)

$$= \int_{t=0}^{\infty} \lambda \left( \{ x \in [0,1]^d : f(x) \ln^2(m(x) + 1) > t \} \right) dt.$$ (101)

For $t \leq 100$, simply we use $\lambda \left( \{ x \in [0,1]^d : f(x) \ln^2(m(x) + 1) > t \} \right) \leq 1$. For $t > 100$, $f(x) \ln^2(m(x) + 1) > t$ implies either $m(x) > t^2$ or $f(x) > t / \ln^2(t^2 + 1)$. Moreover, if $f(x) > t / \ln^2(t^2 + 1)$ then

$$f(x) \ln^2 f(x) > \frac{(\ln t - 2 \ln \ln(t^2 + 1))^2}{\ln^2(t^2 + 1)} > \frac{t}{10000}$$ (102)

since $(\ln t - 2 \ln \ln(t^2 + 1))^2 / \ln^2(t^2 + 1) > 1 / 10000$ for any $t > 100$. So for $t > 100$,

$$\lambda \left( \{ x \in [0,1]^d : f(x) \ln^2(m(x) + 1) > t \} \right) \leq \lambda \left( \{ x \in [0,1]^d : m(x) > t^2 \} \right) + \lambda \left( \{ x \in [0,1]^d : f(x) \ln^2 f(x) > t / 10000 \} \right).$$ (103)

Therefore,

$$\int_{t=0}^{\infty} \lambda \left( \{ x \in [0,1]^d : f(x) \ln^2(m(x) + 1) > t \} \right) dt = 100 + \int_{t=0}^{\infty} \lambda \left( \{ x \in [0,1]^d : m(x) > t^2 \} \right) dt$$ (104)

$$+ \int_{t=100}^{\infty} \lambda \left( \{ x \in [0,1]^d : f(x) \ln^2 f(x) > t / 10000 \} \right) dt$$ (105)

$$\leq_d 100 + \int_{t=100}^{\infty} \frac{1}{t^2} dt + 10000 \int_{[0,1]^d} f(x) \ln^2 f(x) dx$$ (106)

$$\leq 1.$$ (107)

Hence, the proof is completed.
C Proof of lemmas

In this section we provide proofs of lemmas used in the paper.

C.1 Proof of Lemma 1

We consider the cases \( s \in (0, 1] \) and \( s \in (1, 2] \) separately. For \( s \in (0, 1] \), following the definition of Hölder smoothness, we have,

\[
| f_t(x) - f(x) | = \left| \frac{1}{V_d t^d} \int_{|u-x| \leq t} f(u)du - f(x) \right| \tag{108}
\]

\[
\leq \frac{1}{V_d t^d} \int_{|u-x| \leq t} |f(u) - f(x)|du \tag{109}
\]

\[
\leq \frac{1}{V_d t^d} \int_{|u-x| \leq t} L\|u-x\|^s du. \tag{110}
\]

By denoting \( \rho = \|u - x\| \) and considering \( \theta \in S^{d-1} \) on the unit \( d \)-dimensional sphere, we rewrite the above integral using polar coordinate system and obtain,

\[
| f_t(x) - f(x) | \leq \frac{1}{V_d t^d} \int_{\rho=0}^1 \int_{\theta \in S^{d-1}} L\rho^s \rho^{d-1} d\rho d\theta \tag{111}
\]

\[
= \frac{1}{V_d t^d} \int_{\rho=0}^1 dV_d L\rho^{s+d-1} d\rho \tag{112}
\]

\[
= \frac{dV_d L\rho^{s+d}}{(s+d)V_d t^d} = \frac{dLt^s}{s+d}. \tag{113}
\]

Now we consider the case \( s \in (1, 2] \). Now we rewrite the difference as

\[
| f_t(x) - f(x) | = \left| \frac{1}{V_d t^d} \int_{|u-x| \leq t} f(u)du - f(x) \right| \tag{114}
\]

\[
= \left| \frac{1}{2V_d t^d} \int_{|u-v| \leq t} (f(x+v) + f(x-v)) dv - f(x) \right| \tag{115}
\]

\[
\leq \frac{1}{2V_d t^d} \int_{|v| \leq t} \left| f(x+v) + f(x-v) - 2f(x) \right| dv. \tag{116}
\]

For fixed \( v \), we bound \( |f(x+v) + f(x-v) - 2f(x)| \) using the Gradient Theorem and the definition of Hölder smoothness as follows,

\[
|f(x+v) + f(x-v) - 2f(x)| \tag{117}
\]

\[
= \left| (f(x+v) - f(x)) + (f(x-v) - f(x)) \right| \tag{118}
\]

\[
= \left| \int_{\alpha=0}^{1} \nabla f(x + \alpha v) \cdot d(x + \alpha v) + \int_{\alpha=0}^{1} \nabla f(x + \alpha v) \cdot d(x + \alpha v) \right| \tag{119}
\]

\[
= \left| \int_{\alpha=0}^{1} \nabla f(x + \alpha v) \cdot v d\alpha - \int_{\alpha=0}^{1} \nabla f(x - \alpha v) \cdot v d\alpha \right| \tag{120}
\]

\[
= \left| \int_{\alpha=0}^{1} (\nabla f(x + \alpha v) - \nabla f(x - \alpha v)) \cdot v d\alpha \right| \tag{121}
\]

\[
\leq \int_{\alpha=0}^{1} \| \nabla f(x + \alpha v) - \nabla f(x - \alpha v) \| v d\alpha \tag{122}
\]

\[
\leq \int_{\alpha=0}^{1} L\|2\alpha v\|^s \|v\| d\alpha \tag{123}
\]

\[
= \int_{\alpha=0}^{1} L\|v\|^s \left( 2\alpha \right)^{s-1} d\alpha = \frac{L\|v\|^s 2^{s-1}}{s}. \tag{124}
\]
Plug it into (116) and using the similar method in the \( s \in (0, 1] \) case, we have

\[
|f_t(x) - f(x)| \leq \frac{1}{2V_d t^d} \int_{v:|v| \leq t} L\|v\|^{s-1} \frac{d\nu}{s} \leq \frac{1}{2V_d t^d} \int_{\rho=0}^{t} \int_{0 \leq \theta < t} \frac{L\rho^{s-1}}{s} \rho^{d-1} d\rho d\theta
\]

(125)

\[
= \frac{1}{2V_d t^d} \int_{\rho=0}^{t} \int_{S^{d-1}} \frac{L\rho^{s-1}}{s} dV_{d-1} \rho^{d-1} d\rho d\theta
\]

(126)

\[
= \frac{1}{2V_d t^d} \int_{\rho=0}^{t} \frac{dV_{d}L\rho^{s+d-1}2^{s-1}}{s} \rho^{d-1} d\rho
\]

(127)

\[
= \frac{1}{2V_d t^d} \frac{dV_{d}L2^{-s}}{s+d} \leq \frac{dLd}{s+d},
\]

(128)

where the last inequality uses the fact that \( s \in (1, 2] \).

### C.2 Proof of Lemma 2

We consider the following two cases. If \( f(x) \geq 2dLt^s/(s+d) \), then by Lemma 1, we have

\[
f(x) \leq f_t(x) + \frac{dLt^s}{s+d} \leq f_t(x) + \frac{f(x)}{2},
\]

(129)

Hence, \( f(x) \leq 2f_t(x) \) in this case. If \( f(x) < 2dLt^s/(s+d) \), then define \( t_0 = (f(x)(s+d)/2dL)^{1/s} \). By the nonnegativity of \( f \), we have

\[
f_t(x) = \int_{B(x, t)} \frac{f(x)dx}{d}\geq \int_{B(x, t_0)} \frac{f(x)dx}{d} = f_t_0(x)V_d t_{0}^d
\]

(130)

\[
\geq \left( f(x) - \frac{dLt_0^s}{s+d} \right) V_d t_0^d
\]

(131)

\[
= f(x) V_d \left( \frac{f(x)(s+d)}{2dL} \right)^{d/s} - \frac{dL}{s+d} V_d \left( \frac{f(x)(s+d)}{2dL} \right)^{(s+d)/s}
\]

(132)

\[
= f(x) V_d \left( \frac{s+d}{2dL} \right)^{d/s} \left( 2^{-d/s} - 2^{-(s+d)/s} \right).
\]

(133)

Therefore, we have \( f(x) \lesssim_{s, L, d} \left( f_t(x) V_d t^d \right) s/(s+d) \) in this case. We obtain the desired statement by combining the two cases. Furthermore, by taking \( t = 1/2 \), we have \( V_d t^d f_t(x) < 1 \), so \( f_t(x) \lesssim_{s, L, d} 1 \). By applying this lemma immediately we obtain \( f(x) \lesssim_{s, L, d} 1 \).

### C.3 Proof of Lemma 3

We first introduce the Besicovitch covering lemma, which plays a crucial role in the analysis of nearest neighbor methods.

**Lemma 4** [15] **Theorem 1.27** [Besicovitch covering lemma] Let \( A \subset \mathbb{R}^d \), and suppose that \( \{B_x\}_{x \in A} \) is a collection of balls such that \( B_x = B(x, r_x), r_x > 0 \). Assume that \( A \) is bounded or that \( \text{sup}_{x \in A} r_x < \infty \). Then there exist an at most countable collection of balls \( \{B_j\} \) and a constant \( C_d \) depending only on the dimension \( d \) such that

\[
A \subset \bigcup_j B_j, \quad \text{and} \quad \sum_j \chi_{B_j}(x) \leq C_d.
\]

(135)

Here \( \chi_{B}(x) = \mathbb{1}(x \in B) \).

Now we are ready to prove the lemma. Let

\[
M(x) = \sup_{0 < \rho \leq D} \left( \frac{\mu_2(B(x, \rho))}{\mu_1(B(x, \rho))} \right).
\]

(136)
Let \( O_t = \{ x \in A : M(x) > t \} \). Hence, for all \( x \in O_t \), there exists \( B_x = B(x, r_x) \) such that \( \mu_2(B_x) > \frac{t}{\mu_1(B_x)}, 0 < r_x \leq D \). It follows from the Besicovitch lemma applying to the set \( O_t \) that there exists a set \( E \subset O_t \), which has at most countable cardinality, such that

\[
O_t \subset \bigcup_{j \in E} B_j, \quad \text{and} \quad \sum_{j \in E} \chi_{B_j}(x) \leq C_d. \tag{137}
\]

Let \( A_D = \{ x : \exists y \in A, |y - x| \leq D \} \), therefore \( B_j \subset A_D \) for every \( j \). Then,

\[
\mu_1(O_t) \leq \sum_{j \in E} \mu_1(B_j) < \frac{1}{t} \sum_{j \in E} \mu_2(B_j) = \frac{1}{t} \int_{A_D} \sum_{j \in E} \chi_{B_j} d\mu_2 = \frac{1}{t} \int_{A_D} \chi_{B_j} d\mu_2 \leq \frac{C_d}{t} \mu_2(A_D). \tag{138}
\]