Demystifying Fixed $k$-Nearest Neighbor Information Estimators

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Abstract

Estimating mutual information from i.i.d. samples drawn from an unknown joint density function is a basic statistical problem of broad interest with multitudinous applications. The most popular estimator is one proposed by Kraskov and Stögbauer and Grassberger (KSG) in 2004, and is nonparametric and based on the distances of each sample to its $k^{th}$ nearest neighboring sample, where $k$ is a fixed small integer. Despite its widespread use (part of scientific software packages), theoretical properties of this estimator have been largely unexplored. In this paper we demonstrate that the estimator is consistent and also identify an upper bound on the rate of convergence of the bias as a function of number of samples. We argue that the superior performance benefits of the KSG estimator stems from a curious "correlation boosting" effect and build on this intuition to modify the KSG estimator in novel ways to construct a superior estimator. As a byproduct of our investigations, we obtain nearly tight rates of convergence of the $\ell_2$ error of the well known fixed $k$ nearest neighbor estimator of differential entropy by Kozachenko and Leonenko.

1 Introduction

Information theoretic quantities such as mutual information measure "relations" between random variables. A key property of these measures is that they are invariant to one-to-one transformations of the random variables and obey the data processing inequality [10, 20]. These properties combine to make information theoretic quantities attractive in several data science applications involving clustering [34, 54, 9], classification [42] and more generally as a basic feature that can be used in downstream applications [15, 3, 59, 49]. A canonical question in all these applications is to estimate the information theoretic quantities from samples, typically supposed to be drawn i.i.d. from an unknown distribution. This fundamental question has been of longstanding interest in the theoretical statistics community where it is a canonical question of estimating a functional of the (unknown) density [8] but also in the information theory [57, 40, 60, 56], machine learning [16, 25] and theoretical computer science [50, 4, 1] communities, with significant renewed interest of late. The most fundamental information theoretic quantity of interest is the mutual information between a pair of random variables, which is also the primary focus of this paper.

The basic estimation question takes a different hue depending on whether the underlying distribution is discrete or continuous. In the discrete setting, significant understanding of the minimax rate-optimal estimation of functionals, including entropy and mutual information, of an unknown probability mass function is attained via recent works [40, 39, 50, 24, 60]. The continuous setting is significantly different, bringing to fore the interplay of geometry of the Euclidean space as well as the role of dimensionality of the domain in terms of estimating the information theoretic quantities; this setting is the focus of this paper. Among the

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various methods, of great theoretical interest and practical relevance, are the nearest neighbor (NN) methods: the quantities of interest are estimated based on distances (in an appropriate norm) of the samples to their $k$-nearest neighbors ($k$-NN). Of particular practical interest is the situation when $k$ is fixed – typically to 4 or 5 – and the estimators based on fixed $k$-NN statistics typically perform significantly better than alternative approaches (discussed in detail in a later section) both in simulations and when tested in the wild.

The exemplar fixed $k$-NN estimator is that of differential entropy from i.i.d. samples proposed in 1987 by Kozachenko and Leonenko [20] which involved a novel bias correction term, and we refer to as the KL estimator (of differential entropy). Since the mutual information between two random variables is the sum and difference of three differential entropy terms, any estimator of differential entropy naturally lends itself into an estimator of mutual information, which we christen as the 3KL estimator (of mutual information). In an inspired work in 2004, Kraskov and Stögbauer and Grassberger [23], proposed a different fixed $k$-NN estimator of the mutual information, which we name the KSG estimator, that involved subtle (sample dependent) alterations to the 3KL estimator. The authors of [23] empirically demonstrated that their KSG estimator improves over the 3KL estimator and is very simple to implement as well. Indeed, the simplicity of the KSG estimator, combined with its superior performance, has made it a very popular estimator of mutual information in practice.

Despite its widespread use, even basic theoretical properties of the KSG estimator are unknown – it is not even clear if the estimator has vanishing bias (i.e., consistent) as the number of samples grows, much less any understanding of the asymptotic behavior of the bias as a function of the number of samples. As observed elsewhere [17], characterizing the theoretical properties of the KSG estimator is of first order importance – this study could shed light on why the sample-dependent modifications lead to improved performance and perhaps this understanding could lead to the design of even better mutual information estimators. Such are the goals of this paper.

Our main result is to show that the KSG estimator is consistent. We also show upper bounds to the rate of convergence of the bias as a function of the dimensions of the two random variables involved: in the special case when the dimensions of the two random variables are equal and no more than two, the rate of convergence of the bias is $1/\sqrt{N}$, which is the parametric rate of convergence. We show that the improvement of the KSG estimator over the 3KL estimator comes from a “correlation boosting” effect, which can be further amplified by a suitable modification to the KSG estimator. This leads to a novel mutual information estimator, which we call the bias-improved-KSG estimator (BI-KSG). The asymptotic theoretical guarantees we show of the BI-KSG estimator are the same as the KSG estimator, but the improved performance can be seen empirically – especially when $k$ is a small integer and for moderate values of $N$.

In the rest of this section, we formally summarize these main results. A key building block for our results is the asymptotic analysis of the theoretical properties of the KL estimator of differential entropy which we begin with below.

1.1 KL Entropy Estimator and Convergence Rate

Consider a random variable $X \in \mathcal{X} \subseteq \mathbb{R}^d$. Given $N$ i.i.d. samples $X_1, X_2, \ldots, X_N$ from the underlying probability density function $f_X(x)$, we want to estimate the differential entropy $H(X) = -\mathbb{E}[\log f_X(X)]$. As mentioned earlier, a popular approach to estimate the entropy from i.i.d. samples is to use $k$-NN statistics. Precisely, let $\rho_{k,i,p}$ denote the distance from $X_i$ to the $k$th nearest neighbor as measured in $\ell_p$ distance, for some $p \geq 1$. Each $k$-NN distance $\rho_{k,i,p}$ together with the choice of $k$, provides a local view of the underlying distribution around the $i$th sample. Informally, considering the $\ell_p$-ball of radius $\rho_{k,i,p}$ centered at $X_i$ with sufficiently small radius, one can relate the distribution and the number of samples within the ball via

$$\hat{f}_X(X_i)c_{d,p}(\rho_{k,i,p})^d \approx \frac{k}{N}, \quad (1)$$
where \( c_{d,p} \) is the volume of the unit \( \ell_p \) ball in \( d \) dimensions \cite{[48]}: \( (\Gamma(1+\frac{1}{p})^d/\Gamma(1+\frac{d}{p}))2^d \). This simple intuition led Kozachenko and Leonenko to design a powerful and provably consistent differential entropy estimator in \cite{[26]}, which we have called the KL estimator:

\[
\hat{H}(X) = -\frac{1}{N} \sum_{i=1}^{N} \log \hat{f}_X(X_i) \tag{2}
\]

\[
\hat{H}_{KL}(X) = \frac{1}{N} \sum_{i=1}^{N} \left\{ \log \left( \frac{N c_{d,p} (p_{k,i,p})^d}{k} \right) + \frac{\log(k) - \psi(k)}{dx} \right\}, \tag{3}
\]

where \( \psi(x) \) is the digamma function defined as \( \psi(x) = \Gamma^{-1}(x) d\Gamma(x)/dx \), and for large \( x \), it is approximately equal to \( \log(x) \) up to a correction of \( O(1/x) \). Precisely, \( \psi(x) = \log x - 1/2x + o(1/x) \).

The correction term, introduced in \cite{[26]}, is crucial for debiasing the estimator. Note that if we choose \( k \) increasing with \( N \), as commonly done in a significant part of the literature (and summarized in a later section), \( \psi(k) \) converges to \( \log(k) \) and no correction is necessary for consistency. However, in practice, \( k \) is typically a small constant and the correction is crucial. The surprise here is that, not only were Kozachenko and Leonenko able to compute the exact correction term, but it turns out to be a relatively simple digamma function.

This type of an estimate is known as the resubstitution type in the literature, e.g., \cite{[5]}, and refers to a family of estimators that first replaces the expectation by the sample mean, i.e. \( \mathbb{E}[\log f_X(X)] \approx (1/N) \sum_{i=1}^{N} \log \hat{f}_X(X_i) \), and then substitutes \( \log \hat{f}_X \) with an appropriately chosen estimate. Popular choices for resubstituting \( \hat{f}_X \) are based either on \( k \)-NN statistics or kernel density estimators.

Consistency of the KL estimator has been established for \( k = 1 \) by the original authors \cite{[26]} and for general \( k \) by \cite{[45]} and the rate of convergence of the bias and variance has been established (for a certain large class of pdfs) only for one-dimensional random variables \cite{[48]}.

Main Results

We show the following results, which can be viewed as a generalization of the result in \cite{[48]}, under slightly more general conditions for the class of pdfs as considered in \cite{[48]} (precise statement of the assumptions and results are in forthcoming sections). Here \( d \) is the dimension of the random variable whose differential entropy is being estimated.

- We show that the bias is \( \tilde{O}(N^{-\frac{d}{2}}) \) where \( \tilde{O} \)-notation denotes the limiting behavior up to polylogarithmic factors in \( N \) and the variance is \( \tilde{O}(1/N) \). Thus the \( \ell_2 \) error of the KL estimator is \( \tilde{O}(\frac{1}{\sqrt{N}} + N^{-\frac{d}{2}}) \).

- The minimax \( \ell_2 \) error of the KL estimator over the class of functions which has norm-bounded Hessian matrix is lower bounded by \( \tilde{O}(\frac{1}{\sqrt{N}} + N^{-\frac{d-1}{2}}) \).

The optimality gap is characterized by \( \min\{1/2, 8/(d + 8)\} - \min\{0.5, 2/d\} \), which is always non-negative. This characterizes the \( \frac{1}{\sqrt{N}} \) rate of convergence for \( \ell_2 \) error for \( d \leq 4 \) (this is the parametric rate), while there is some gap in the upper and lower bounds for the rates when \( d > 4 \).

1.2 KSG Mutual Information Estimator, Consistency and Rate

Consider two random variables \( X \) in \( \mathcal{X} \subseteq \mathbb{R}^d \) and \( Y \) in \( \mathcal{Y} \subseteq \mathbb{R}^d \). Given \( N \) i.i.d. samples \( (X_1, Y_1), \ldots, (X_N, Y_N) \) from the underlying joint probability density function \( f_{X,Y}(x,y) \), we want to estimate the mutual information \( I(X;Y) \). Mutual information between two random variables \( X \) and \( Y \) is the sum and difference of differential entropy terms: \( I(X;Y) = H(X) + H(Y) - H(X,Y) \). Thus given KL entropy estimator, there is a straightforward and consistent estimation of the mutual information:

\[
\hat{I}_{KL}(X;Y) = \hat{H}_{KL}(X) + \hat{H}_{KL}(Y) - \hat{H}_{KL}(X,Y). \tag{4}
\]
While this estimator performs fairly well in practice, the authors of [28] introduced a simple, but inspired, modification of the 3KL estimator that does even better. Let \( n_{x,i,p} \equiv \sum_{j \neq i} I\{\|X_j - X_i\|_p \leq \rho_{k,i,p}\} \), which can be interpreted as the number of samples that are within a \(X\)-dimensions-only distance of \(\rho_{k,i,p}\) with respect to sample \(i\). Since \(\rho_{k,i,p}\) is the \(k\)-NN distance (in terms of both the dimensions of \(X\) and \(Y\)) of the sample \(i\) it must be that \(n_{x,i,p} \geq k\). Finally, \(n_{y,i,p}\) is defined analogously. The KSG estimator measures distances using the \(\ell_\infty\) norm, so \(p = \infty\) in the notation above.

The KSG mutual information estimator introduced in [28] is given by:

\[
\hat{I}_{\text{KSG}}(X;Y) \equiv \psi(k) + \log N - \frac{1}{N} \sum_{i=1}^{N} \left( \psi(n_{x,i,\infty} + 1) + \psi(n_{y,i,\infty} + 1) \right),
\]

where \(\psi(x) = \Gamma^{-1}(x)d\Gamma(x)/dx\) is the digamma function. Observe that the estimate of the joint differential entropy \(H(X,Y)\) is done exactly as in the KL estimator using fixed \(k\)-NN distances, but the KL estimates of \(H(X)\) and \(H(Y)\) are done using \(n_{x,\infty}\) and \(n_{y,\infty}\) NN distances, respectively, which are sample dependent. The point is that by this choice, the \(k\)-NN distance terms are canceled away exactly although it is not clear why this would be a good idea. In fact, it is not even clear if the estimator is consistent. On the other hand, the authors of [28] showed empirically that the KSG estimator is uniformly superior to the 3KL estimator in many synthetic experiments. A theoretical understanding of the KSG estimator, including a mathematical justification for the improved performance, has been sorely missing. Our main results fill this gap.

Main Results

- We show that the KSG estimator is consistent and the bias is \(\tilde{O}(N^{-\min(d_x, d_y, 2)})\), without accounting for polylogarithmic terms. When \(d_x = d_y\) and equal to 1 or 2, the bias is \(\tilde{O}(\sqrt{N})\), the parametric rate of \(\ell_2\) error, which cannot be improved upon.

- We show, using an instructive example, that the key idea in the KSG estimator is one of boosting the correlation between \(\hat{H}(X,Y)\) and \(\hat{H}(X)\) (and also between \(\hat{H}(X,Y)\) and \(\hat{H}(Y)\)) and achieving a smaller variance.

- The correlation boosting explanation allows us to propose a new mutual information estimator, that we call the bias-improved KSG (BI-KSG) estimator. The new aspects include using the \(\ell_2\) norm to measure distances and replacing the digamma function of \(n_{x,\cdot,2}, n_{y,\cdot,2}\) by the logarithm – and although the theoretical properties of the BI-KSG estimator we show are the same as that of the KSG estimator we empirically demonstrate its improved performance which is pronounced when \(k\) is small and \(N\) is moderate-valued.

The formal definition of the BI-KSG estimator is the following.

\[
\hat{I}_{\text{BI-KSG}}(X;Y) \equiv \psi(k) + \log N + \log \left( \frac{c_{d_x,2}}{c_{d_x+d_y,2}} \right) - \frac{1}{N} \sum_{i=1}^{N} \left( \log(n_{x,i,2}) + \log(n_{y,i,2}) \right),
\]

where \(c_{d,2} = \pi^d / \Gamma(d/2 + 1)\) be the volume of \(d\)-dimensional unit \(\ell_2\) ball. It remains open to characterize the rate of convergence of the variance of KSG and BI-KSG estimators. Such a study would shed light on any potential tradeoff between bias and variance in these estimators as well as provide a full understanding of the \(\ell_2\) error of these estimators.

1.3 Outline of this paper

In the next two sections we state our main results formally, also providing brief sketches of, and intuitions behind, the corresponding proofs. Detailed proofs are relegated to the appendix. In Section 3 we discuss
the insights behind the KSG estimator: the correlation boosting effect and how this understanding leads to the BI-KSG estimator with improved empirical performance. Finally, Section 5 puts our results in context of the vast literature on entropy (and mutual information) estimators.

2 Convergence Rate of KL Entropy Estimator

Differential entropy estimation is a basic building block towards mutual information estimation. In this section we carefully analyze the performance of the KL estimator of differential entropy in terms of its $\ell_2$ error. We show upper bounds to the rate of convergence of the bias and variance of the KL estimator separately which combine to provide an upper bound on the $\ell_2$ error. A minimax lower bound on the $\ell_2$ error provides a baseline to understand how sharp our upper bound characterization is. We start with the upper bound on the convergence rate of $\ell_2$ error.

2.1 Upper Bounds

The starting point for our exploration is the pioneering work of [48], which established the $\frac{1}{\sqrt{N}}$-consistency of the one-dimensional KL estimator. In particular, [48] proved that the KL estimator (cf. Equation (3)) achieves $\sqrt{N}$-consistency in mean, i.e. $E[H(X)] - H(X) = \tilde{O}(1/\sqrt{N})$, and in variance, i.e. $E[(H(X) - E[H(X)])^2] = \tilde{O}(1/N)$, under the assumption that the $X$ is a one-dimensional random variable and the estimator uses only the nearest neighbor distance with $k = 1$, along with a host of other assumptions on the class of pdfs under consideration. We prove a generalization of this rate of convergence for general dimensions $d$ and for a general $k$, but under some technical assumptions listed below; these mirror the assumptions introduced in [48].

Assumption 1. We make the following assumptions: there exist finite constants $C_a, C_b, C_c, C_d,$ and $C_0$ such that

(a) $f(x) \leq C_a < \infty$ almost everywhere;

(b) There exists $\gamma > 0$ such that $\int f(x) (\log f(x))^{1+\gamma} dx \leq C_b < \infty$;

(c) $\int f(x) \exp\{-bf(x)\} dx \leq C_c e^{-C_0 b}$ for all $b > 1$.

(d) $f(x)$ is twice continuously differentiable and the Hessian matrix $H_f$ satisfy $\|H_f(x)\|_2 < C_d$ almost everywhere.

These assumptions are slightly stronger than those in [48], where assumption (a) was not required (and with some technical finesse can perhaps be eliminated here as well), assumption (b) was mildly weaker requiring only $\int f(x) \log f(x) dx < \infty$, and assumption (c) was weaker requiring only $\int f(x) \exp\{-bf(x)\} \leq O(1/b)$. The assumption (c) is satisfied for pdfs with exponentially decaying tails, for example, the Gaussian pdf and is also immediately met by any distribution with bounded support. It appears that this extra assumption on the tails is essential to handle general dimensions, especially when obtaining a tight upper bound on the bias. The assumption (d) assumes that the pdf is reasonably smooth, and it is essential for NN-based methods. More general families of smoothness conditions have been assumed for other approaches, such as the H"older condition, and we make formal comparisons in Section 5.

We start with a truncated version of the KL estimator, similar to [48]. Consider $\rho_{k,i,p}$ be the distance to the $k^{th}$ nearest neighbor of $X_i$ with respect to $\ell_p$ distance. Fix any $\delta > 0$, define the threshold $a_N$ as:

$$a_N = \left( \frac{(\log N)^{1+\delta}}{N} \right)^{1/d},$$ (7)
for some $\delta > 0$. We define a local estimate $\xi_{k,i,p}(X)$ by:

$$\xi_{k,i,p}(X) = \begin{cases} -\psi(k) + \log N + \log c_{d,p} + d \log \rho_{k,i,p} & , \text{if } \rho_{k,i,p} \leq a_N , \\ 0 & , \text{if } \rho_{k,i,p} > a_N . \end{cases} \tag{8}$$

Then the truncated KL estimator is:

$$\tilde{H}_{tKL}(X) = \frac{1}{N} \sum_{i=1}^{N} \xi_{k,i,p}(X). \tag{9}$$

The following theorems upper bound the bias of the truncated KL entropy estimator. Here $\delta > 0$ is arbitrarily small (and is from the truncation threshold cf. Equation (7)) and $d$ is the dimension of the random variable $X$ and $k$ is any fixed finite integer and for any norm $p$.

The main ideas of the proof are:

1. We use the average pdf of a ball $B(x, r)$ centered at $x$ with small radius $r$ (usually the $k$-NN distance of $x$) to approximation $f(x)$, relying on the smoothness of $f(\cdot)$. The error in this approximation is $O(r^2)$ if the Hessian of $f$ is bounded, and this error dominates the onvergence rate of bias. A similar idea was attempted in [36], but the authors mistakenly claimed that the error introduced by the approximation is $O(r^2 d)$, which is much smaller than $O(r^2)$ for $d > 1$ and leads to an incorrect conclusion.

2. If the density $f(x)$ is extremely small, the $k$-NN distance $r$ of $x$ will be large, which means that the $O(r^2)$ error is large. We truncate the $k$-NN distance by $a_N$ to solve this problem, but at the cost of additional bias. We need to control the total probability of the tail of $f$ to be small enough so that the additional bias introduced by truncation is not too large; this leads to the necessity of Assumption 1(c).

**Theorem 1.** Under the Assumption 1 and for finite $k = O(1)$ and $d = O(1)$, the bias of the truncated KL entropy estimator using $N$ i.i.d. samples is bounded by:

$$\mathbb{E} \left[ \tilde{H}_{tKL}(X) \right] - H(X) = O \left( \frac{(\log N)^{(1+\delta)(1+2/d)}}{N^{2/d}} + \frac{(\log N)^{2(1+\delta)}}{N} \right). \tag{10}$$

The following theorem establishes the upper bound for the variance of $\tilde{H}_{tKL}(X)$, cf. (9), which we observe is independent of the dimension $d$ of the random variable $X$. Again $\delta > 0$ is arbitrarily small (and is from the truncation threshold cf. Equation (7)) and $k$ is any fixed integer.

The main step of the proof is the observation that

$$\text{Var} \left[ \tilde{H}_{tKL}(X) \right] \leq \frac{1}{N} \text{Var} \left[ \xi_{k,1,p} \right] + \text{Cov} \left[ \xi_{k,1,p}, \xi_{k,2,p} \right]. \tag{11}$$

The first term is bounded by $O((\log \log N)^2)$ due to the truncation of $k$-NN distances. The second term is actually the covariance of $k$-NN distances of a pair of samples, which we show to be $O(1/N)$ up to a polylogarithmic factor. Putting these two steps together completes the proof.

**Theorem 2.** Under the Assumption 1 and for finite $k = O(1)$ and $d = O(1)$, the variance of the truncated KL entropy estimator using $N$ i.i.d. samples is bounded by:

$$\text{Var} \left[ \tilde{H}_{tKL}(X) \right] = O \left( \frac{(\log \log N)^2 (\log N)^{(2k+2)(1+\delta)}}{N} \right). \tag{12}$$

The Mean Squared Error (MSE) of truncated KL estimator

$$\mathbb{E} \left[ \left( \tilde{H}_{tKL}(X) - H(X) \right)^2 \right] = \mathbb{E} \left[ \tilde{H}_{tKL}(X) - H(X) \right]^2 + \text{Var} \left[ \tilde{H}_{tKL}(X) \right], \tag{13}$$
is the sum of the squared bias and variance. So combining Theorems 1 and 2 we obtain the following upper bound on the MSE of truncated KL estimator. Again \( \delta > 0 \) is arbitrarily small (and is from the truncation threshold cf. Equation 7) and \( k \) is any fixed integer.

**Corollary 1.** Under the Assumption 1 and for finite \( k = O(1) \) and \( d = O(1) \), the MSE of the truncated KL entropy estimator using \( N \) i.i.d. samples is bounded by:

\[
E \left[ \left( \hat{H}_{iKL}(X) - H(X) \right)^2 \right] = O \left( \frac{(\log N)^{(1+\delta)2+4/d}}{N^{4/d}} + \frac{(\log \log N)^2 (\log N)^{(2k+2)(1+\delta)}}{N} \right).
\]

To see how good this bound on rate of convergence is, we derive a worst case lower bound below.

### 2.2 Minimax Lower Bound

We follow the standard techniques to lower bound estimator errors of functionals of a density – Le Cam’s method in general and [8] in particular. Consider the class of smooth distributions:

\[
\mathcal{F}_d = \{ f : \mathbb{R}^d \to \mathbb{R}^+ : \int f(x)dx = 1, \| H_f(x) \| \leq C, \text{a.e.} \},
\]

where \( H_f \) denotes the Hessian matrix of \( f \). We want to estimate the differential entropy of \( f \) from \( n \) i.i.d. samples \( \{X_i\}_{i=1}^n \), where \( X_i \in \mathbb{R}^d \). We summarize a minimax lower bound on the \( \ell_2 \) error rate in the following theorems. Here the \( \Omega(N^{-1}) \) is the parametric minimax lower bound and \( \Omega(N^{-16/(d+8)}) \) follows from the construction in [8].

**Theorem 3.** The minimax error rate for estimating entropy from \( N \) i.i.d. samples is lower bounded by

\[
\inf_{\hat{H}_N} \sup_{f \in \mathcal{F}_d} E \left[ \left( \hat{H}_N(X) - H(X) \right)^2 \right] \geq \Omega(N^{-16/(d+8)} + N^{-1}),
\]

where the infimum is taken over all measurable functions over the \( N \) samples.

### 2.3 Comparing the bounds

The upper and lower bounds of the MSE error of the KL estimator as a function of the number of samples is depicted in Figure 1. We see that the bounds match for \( d \leq 4 \) and in this regime the parametric rate of convergence of \( \tilde{O}(\frac{1}{\sqrt{N}}) \) is achieved. There is a gap when \( d > 4 \) and closing this gap is an interesting future direction of research. To get a feel for whether the upper bound should be improved or the lower bound (or both), it is instructive to plot sample MSE for a specific pdf. In this synthetic experiment, we choose \( N \) i.i.d. samples \( X_1, X_2, \ldots, X_N \) from (Beta(2, 2))\(^d\) and use the KL estimator to estimate entropy. Figure 2 plots the MSE vs the sample size for different dimensions in log scale; we observe that \( \log \text{(MSE)} \) is linear in \( \log N \).

We can use standard linear regression to estimate the slope \( \log \text{(MSE)} / \log N \) – the results are plotted in conjunction with the upper and lower bounds of rate of convergence in Figure 1. We conclude that the simulation results are fairly close to the upper bounds on convergence rate – which suggests that the improvements are to be most expected in the minimax lower bounds.

### 3 KSG Estimator: Consistency and Convergence Rate

A detailed understanding of the KL estimator sets the stage for the main results of this paper: deriving theoretical properties of the KSG estimator of mutual information. Our main result is that the KSG
estimator is consistent, as is our proposed modification, the so-called bias-improved KSG estimator (BI-KSG) – these results are under some (fairly standard) assumptions on the joint pdf of \((X, Y)\). We formally state these results below, delegating the proofs to the appendix.

3.1 Consistency

We make the following assumptions on the joint pdf of \((X, Y)\). The first assumption is essentially needed to define the joint differential entropy of \((X, Y)\), the second assumption makes some regularity conditions on the Radon-Nikodym derivatives of \(X\) and \(Y\), and the third assumption is regarding standard smoothness conditions on the joint pdf. We note that these conditions are readily met by most popular pdfs, including multivariate Gaussians, and no assumption is made on the boundedness of the support.

**Assumption 2.**

(a) \(\int f(x, y) |\log f(x, y)| \, dx \, dy < \infty\).

(b) There exists a finite constant \(C'\) such that the conditional pdf \(f_{Y|X}(y|x) < C'\) and \(f_{X|Y}(x|y) < C'\) almost everywhere.

(c) \(f(x, y)\) is twice continuously differentiable and the Hessian matrix \(H_f\) satisfy \(\|H_f(x, y)\|_2 < C\) almost everywhere.

Under these assumptions, the KSG and the Bi-KSG estimators are both consistent, in probability.

**Theorem 4.** Under the Assumption 2 and for finite \(k > \max\{d_x/d_y, d_y/d_x\}\), \(d_x, d_y = O(1)\), and for all \(\varepsilon > 0\),

\[
\lim_{N \to \infty} \mathbb{P}\left(\left|\hat{I}_{\text{KSG}}(X; Y) - I(X; Y)\right| > \varepsilon\right) = 0, \quad \text{and} \quad (17)
\]
3.2 Convergence rate

To understand the rate of convergence of the bias of the KSG and BI-KSG estimators, we first truncate the k-NN distance $\rho_{k,i}$, similar to the undertaking in Section 2.1. For any $\delta > 0$, let the truncation threshold be:

$$a_N = \left( \frac{\log N}{N} \right)^{1/(d_x + d_y)} / \left( \psi(k) + \log N - \psi(n_{x,i,\infty} + 1) - \psi(n_{y,i,\infty} + 1) \right)$$

where $d_x$ and $d_y$ are the dimensions of the random variables $X$ and $Y$ respectively. We define local information estimates $\iota_{k,i,\infty}$ and $\iota_{k,i,2}$ by:

$$\iota_{k,i,\infty} = \begin{cases} \psi(k) + \log N - \psi(n_{x,i,\infty} + 1) - \psi(n_{y,i,\infty} + 1) & \text{if } \rho_{k,i,\infty} \leq a_N, \\ 0 & \text{if } \rho_{k,i,\infty} > a_N, \end{cases}$$

and

$$\iota_{k,i,2} = \begin{cases} \psi(k) + \log N + \log \left( \frac{c_{d_x,2} c_{d_y,2}}{c_{d_x + d_y,2}} \right) - \log(n_{x,i,2}) - \log(n_{y,i,2}) & \text{if } \rho_{k,i,2} \leq a_N, \\ 0 & \text{if } \rho_{k,i,2} > a_N. \end{cases}$$
The modified (via truncation) KSG and BI-KSG estimators (compare with (5) and (6)) are:

\[
\hat{I}_{KSG}(X;Y) = \frac{1}{N} \sum_{i=1}^{N} \ell_{k,i,\infty}, \quad (22)
\]

\[
\hat{I}_{BI-KSG}(X;Y) = \frac{1}{N} \sum_{i=1}^{N} \ell_{k,i,2}. \quad (23)
\]

The following theorem provides an upper bound on the rate of convergence of the bias, under the conditions in Assumption 3 below, and holds for any \( k \) and \( \delta > 0 \) (parameter in the truncation threshold, cf. (19)).

**Assumption 3.** We make the following assumptions: there exist finite constants \( C_a, C_b, C_c, C_d, C_e \) and \( C_0 \) such that

(a) \( f(x,y) \leq C_a < \infty \) almost everywhere.

(b) There exists \( \gamma > 0 \) such that \( \int f(x,y) (\log f(x,y))^{1+\gamma} \, dx \, dy \leq C_b < \infty \).

(c) \( \int f(x,y) \exp\{-bf(x,y)\} \, dx \, dy \leq C_c e^{-Cb} \) for all \( b > 1 \).

(d) \( f(x,y) \) is twice continuously differentiable and the Hessian matrix \( H_f \) satisfy \( \|H_f(x,y)\|_2 < C_d \) almost everywhere.

(e) The conditional pdf \( f_{Y|X}(y|x) < C_e \) and \( f_{X|Y}(x|y) < C_e \) almost everywhere.

Here Assumption 3(a) – (d) are the same as in Assumption 1 (which were introduced in the context of characterizing the convergence rate of the KL estimator). Assumption 3(e) makes sure that the marginal entropy estimator converges at certain rate. Compared to Assumption 2, we need an upper bound for the joint entropy \( (a) \). The condition \( (b) \) is slightly stronger than Assumption 2 by changing the power from 1 to \( 1 + \gamma \). The condition \( (e) \) is the tail bound which ensures the convergence rate of truncated KL joint entropy estimator.

**Theorem 5.** Under Assumption 3 and for finite \( k > \max\{d_x/d_y, d_y/d_x\} \), \( d_x, d_y = O(1) \),

\[
\mathbb{E} \left[ \hat{I}_{KSG}(X;Y) - I(X;Y) \right] = O \left( \frac{(\log N)^{(1+\delta)(1+\frac{d_y}{d_x+d_y})}}{N^\frac{d_x}{d_x+d_y}} + \frac{(\log N)^{(1+\delta)(1+\frac{d_y}{d_x+d_y})}}{N^\frac{d_y}{d_x+d_y}} + \frac{(\log N)^{(1+\delta)(1+\frac{2}{d_x+d_y})}}{N^\frac{2}{d_x+d_y}} \right). \quad (24)
\]

\[
\mathbb{E} \left[ \hat{I}_{BI-KSG}(X;Y) - I(X;Y) \right] = O \left( \frac{(\log N)^{(1+\delta)(1+\frac{d_y}{d_x+d_y})}}{N^\frac{d_y}{d_x+d_y}} + \frac{(\log N)^{(1+\delta)(1+\frac{d_y}{d_x+d_y})}}{N^\frac{d_y}{d_x+d_y}} + \frac{(\log N)^{(1+\delta)(1+\frac{2}{d_x+d_y})}}{N^\frac{2}{d_x+d_y}} \right). \quad (25)
\]

It is instructive to compare these upper bounds on the rate of convergence of the bias to that of the 3KL estimator, which can be derived directly from Corollary 1

\[
\mathbb{E} \left[ \hat{I}_{KSG}(X;Y) - I(X;Y) \right] = \tilde{O} \left( N^-\frac{2}{d_x+d_y} \right), \quad (26)
\]

where \( \tilde{O} \)-notation denotes that we are neglecting polylogarithmic terms. We see that the rate of convergence of the bias terms (at least viewed through their upper bounds) is only worse for the KSG (and BI-KSG) estimator as compared to the 3KL estimator, and equal in the important special case below.
Corollary 2. If \( d_x = d_y = 1 \) or \( d_x = d_y = 2 \), we obtain:

\[
\mathbb{E} \left[ \hat{I}_{KSG}(X;Y) \right] - I(X;Y) = O \left( \sqrt{\frac{(\log N)^{4(1+\delta)}}{N}} \right) .
\] (27)

\[
\mathbb{E} \left[ \hat{I}_{BI-KSG}(X;Y) \right] - I(X;Y) = O \left( \sqrt{\frac{(\log N)^{4(1+\delta)}}{N}} \right) .
\] (28)

This establishes the \( 1/\sqrt{N} \) convergence rate of the bias of the KSG and BI-KSG and 3KL estimators up to a poly-logarithmic factor; this (parametric) convergence rate cannot be improved upon.

We note that these results only provide an understanding of the bias of the estimators. Clearly the MSE improvement of the KSG estimator over the 3KL estimator must come from reduced variance, and most important and interesting direction of future research is to have a theoretical understanding of the variance of the 3KL, KSG and BI-KSG estimators.

4 Discussion

Perhaps to build an intuition towards a deeper theoretical understanding of the KSG estimator, we ask for the key features that make it perform better than the 3KL one. This is the focus of the present section, where we see a curious correlation boosting effect.

4.1 Correlation Boosting Effect

We begin by rewriting the KSG estimator, cf. [5], as:

\[
\hat{I}_{KSG}(X;Y) = \frac{1}{N} \sum_{i=1}^{N} \epsilon_{k,i,\infty} = \frac{1}{N} \sum_{i=1}^{N} (\xi_{k,i,\infty}(X) + \xi_{k,i,\infty}(Y) - \xi_{k,i,\infty}(X,Y))
\] (29)

where

\[
\xi_{k,i,\infty}(X, Y) \equiv -\psi(k) + \log N + \log cd_{x,\infty}cd_{y,\infty} + (d_x + d_y) \log \rho_{k,i,\infty}
\]

\[
\xi_{k,i,\infty}(X) \equiv -\psi(n_{x,i,\infty} + 1) + \log N + \log cd_{x,\infty} + d_x \log \rho_{k,i,\infty}
\]

\[
\xi_{k,i,\infty}(Y) \equiv -\psi(n_{y,i,\infty} + 1) + \log N + \log cd_{y,\infty} + d_y \log \rho_{k,i,\infty}.
\] (30)

Here \( \xi_{k,i,\infty}(X,Y), \xi_{k,i,\infty}(X) \) and \( \xi_{k,i,\infty}(Y) \) are local estimates of the differential entropies \( H(X,Y), H(X) \) and \( H(Y) \), respectively, at the \( i \)th sample. We will show that the bias of joint entropy estimate

\[
b_{k,i,\infty}(X,Y) = \xi_{k,i,\infty}(X,Y) - H(X,Y)
\] (31)

is positively correlated to the bias of marginal entropy estimates

\[
b_{k,i,\infty}(X) = \xi_{k,i,\infty}(X) - H(X)
\] (32)

and

\[
b_{k,i,\infty}(Y) = \xi_{k,i,\infty}(Y) - H(Y).
\] (33)

Since the bias of the KSG estimator is simply equal to \( \frac{1}{N} \sum_{i=1}^{N} b_{k,i,\infty}(X,Y) - b_{k,i,\infty}(X) - b_{k,i,\infty}(Y) \) the bias is reduced if \( b_{k,i,\infty}(X,Y) \) is positively correlated with \( b_{k,i,\infty}(X) \) and \( b_{k,i,\infty}(Y) \). The same effect is true for the 3KL estimator, which is already based on estimating the three differential entropy terms separately.
We tabulate the Pearson correlation coefficients of the biases in Table 1 for two exemplar pdfs (independent uniforms and Gaussians). The main empirical observation is that the correlation is positive even for the 3KL estimator but is significantly higher for the KSG estimator.

|         | \( (X,Y) \sim \text{Unif}([0,1]^2) \) | \( (X,Y) \sim \mathcal{N}(0,I_2) \) |
|---------|-------------------------------|-------------------------------|
| \( N \) | 1024 2048 4096 | 1024 2048 4096 |
| 3KL     | 0.1276 0.1259 0.0930 | 0.4602 0.4471 0.3717 |
| KSG     | 0.9312 0.9328 0.9085 | 0.6750 0.7151 0.6687 |
| BI-KSG  | 0.9253 0.9251 0.8880 | \textbf{0.6823} \textbf{0.7330} \textbf{0.6939} |

Table 1: Pearson Correlation Coefficient \( \rho(b(X,Y), b(X)) \) for different mutual information estimators.

We hypothesize that this correlation boosting effect is the main reason for the KSG estimator having smaller mean-square error than the 3KL one. We simulate 100 i.i.d. samples uniformly from \([0,1]^2\) and map the scatter-plot of the biases \( b(X,Y) \) and \( b(X) \) in Figure 3, where the boosted correlation for the KSG estimator is visibly significant.

![Figure 3](image-url)

Figure 3: Scatter plot of the biases \( b(X,Y) \) and \( b(X) \) to illustrate the correlation boosting effect. Left: 3KL. Right: KSG.

4.2 Choice of \( \ell_2 \) distance

Given the understanding of the correlation boosting effect, it is natural to ask if this can lead to a new estimator that furthers the improvement in MSE. This goal is achieved below, where we discuss potential areas of improvement of the KSG estimator and conclude with our proposal: Bias Improved KSG (BI-KSG) estimator of mutual information. One of the key differences comes from using \( \ell_2 \) norm to measure \( k \)-NN distances, while KSG uses \( \ell_\infty \) distance. Next, BI-KSG uses \( \log(n_{x,i,2}) \) and \( \log(n_{y,i,2}) \) instead of \( \psi(n_{x,1,\infty} + 1) \)
and \( \psi(n_{y,i,\infty} + 1) \), respectively. We briefly discuss the intuitions behind these changes below. We begin by noting that the KSG estimator can be written as:

\[
\hat{I}_{\text{KSG}}(X;Y) = \hat{H}_{\text{KSG}}(X) + \hat{H}_{\text{KSG}}(Y) - \hat{H}_{\text{KL}}(X,Y),
\]

where \( \hat{H}_{\text{KL}}(X;Y) \) is the KL entropy estimator (and already known to be consistent). The marginal entropy estimator is

\[
\hat{H}_{\text{KSG}}(X) = \frac{1}{N} \sum_{i=1}^{N} \left( -\psi(n_{x,i,\infty} + 1) + \psi(N) + \log c_{d_x,\infty} + d_x \log \rho_{k,i,\infty} \right),
\]

and we note that this has a form similar to that of the KL entropy estimator, except that \( k \) is replaced by \( n_{x,i,\infty} + 1 \), which is sample dependent. Suppose \( (X_i^{(k)}, Y_i^{(k)}) \) be the \( k \)-NN of \( (X_i, Y_i) \) with distance \( \rho_{k,i,\infty} \), then the “KSG entropy estimator” in (35) implicitly assumes that \( \rho_{k,i,\infty} \) is both the \( (n_{x,i,\infty} + 1) \)-NN distance of \( X_i \) on \( X \)-space and the \( (n_{y,i,\infty} + 1) \)-NN of \( Y_i \) on \( Y \)-space. But since \( \ell_{\infty} \)-distance is used, \( (X_i^{(k)}, Y_i^{(k)}) \) either lies on the \( X \)-boundary of the hypercube \( S(X,Y,\rho_{k,i,\infty}) = \{ (x,y) : \max \{ \| x - X_i \|_{\infty}, \| y - Y_i \|_{\infty} \} \leq \rho_{k,i,\infty} \} \), or on the \( Y \)-boundary of \( S(X,Y,\rho_{k,i,\infty}) \) (the chance of lying on a corner, and thus on both the boundaries, has zero probability). If the \( k \)-NN lies on the \( X \)-boundary, i.e. \( \| X_i^{(k)} - X_i \| = \rho_{k,i,\infty} \) and \( \| Y_i^{(k)} - Y_i \| < \rho_{k,i,\infty} \), then \( \rho_{k,i,\infty} \) is the \( (n_{x,i,\infty} + 1) \)-NN distance of \( X_i \), but not the \( (n_{y,i,\infty} + 1) \)-NN distance of \( Y_i \). Thus, while the estimate of entropy of \( X \) is correct, the entropy of \( Y \) is over-estimated. Since \( \rho_{k,i,\infty} \) is between the \( n_{y,i,\infty} \)-th and \( (n_{y,i,\infty} + 1) \)-th NN distance, the “KSG entropy estimator” in (35) introduces a bias of order \( 1/n_{y,i,\infty} \). Similarly, a \( 1/n_{x,i,\infty} \)-bias if \( (X_i^{(k)}, Y_i^{(k)}) \) is introduced if the \( k \)-NN sample lies on the \( Y \)-boundary.

![Figure 4: Illustration of choice of \( \rho_{k,i} \) for \( k = 3 \). Left: use \( \ell_{\infty} \)-distance. Right: use \( \ell_2 \)-distance](image)

This discussion suggests that we use an \( \ell_2 \) ball, instead of an \( \ell_{\infty} \) ball to find the \( k \)-NN (See Figure 4). This would ensure that \( \rho_{k,i,2} \) is neither the \( (n_{x,i,2} + 1) \)-NN distance of \( X_i \) on \( X \)-space nor the \( (n_{y,i,2} + 1) \)-NN distance of \( Y_i \) on \( Y \)-space. But then, we are unable to directly use the KL estimator for \( H(X) \) and \( H(Y) \) with this distance. The following theorem sheds some light on this conundrum, with the proof relegated to the appendix.

**Theorem 6.** Under the Assumption 1(c), and given \( (X_i, Y_i) = (x,y) \) and \( \rho_{k,i,2} = r < r_N \) for some deterministic sequence of \( r_N \) such that \( \lim_{N \to \infty} r_N = 0 \), the number of neighbors \( n_{x,i,2} - k \) is distributed as \( \sum_{l=k+1}^{N-1} U_l \), where \( U_l \) are i.i.d. Bernoulli random variables with mean \( p \), and there exists a positive constant
such that
\[ r^{-d_x} | p - f_X(x)c_{d_x,2} \rho^{d_x} | \leq C_1 \left( r^2 + r^{d_y} \right), \] (36)
for sufficiently large \( N \).

Intuitively, the theorem says that \( E[n_{x,i,2}] \approx N f_X(x)c_{d_x,2} \rho^{d_x} \). This suggests that we estimate the log of the density (log \( \int f_X(x) \)) by \( \log(n_{x,i,2}) - \log N - \log c_{d_x,2} - d_x \log \rho_{k,i,2} \). The resubstitution estimate of the marginal entropy \( H(X) \) is now:
\[ \hat{H}_{\text{BI-KSG}}(X) = \frac{1}{N} \sum_{i=1}^{N} (- \log(n_{x,i,2}) + \log N + \log c_{d_x,2} + d_x \log \rho_{k,i,2}) \] (37)
which is different from the KL estimate only via replacing the digamma function by the logarithm. This technique kills the \( O(1/n_{x,i,2} + 1/n_{y,i,2}) \) bias of the “KSG entropy estimator”.

Notice that as \( N \) gets large, so do \( n_{x,i,2} \) and \( n_{y,i,2} \), and hence the KSG estimator is consistent. But when \( k \) is small and \( N \) is moderate and \( X \) and \( Y \) are not independent, then \( n_{x,i,2} \) and \( n_{y,i,2} \) are expected to be small. In such cases, BI-KSG should outperform KSG. We demonstrate this empirically in Table 2 where we choose \( k = 1 \) and \( X \) and \( Y \) are joint Gaussian with mean 0 and covariance \( \Sigma = \begin{pmatrix} 1 & 0.9 \\ 0.9 & 1 \end{pmatrix} \). We can see that all the estimators converges to the ground truth as \( N \) goes to infinity, but BI-KSG has the best sample complexity for moderate values of \( N \).

| \( N \)  | 100  | 200  | 400  | 800  | 1600 | 3200 |
|-------|------|------|------|------|------|------|
| 3-KL  | 0.0590 | 0.1025 | 0.0313 | 0.0053 | 0.0097 | 0.0079 |
| KSG   | 0.0240 | 0.0100 | 0.0217 | 0.0024 | 0.0087 | 0.0046 |
| BI-KSG | 0.0096 | -0.0035 | 0.0133 | -0.0012 | 0.0071 | 0.0032 |

Table 2: Comparison of bias for different mutual information estimators.

5 Related Work

A conceptually straightforward way to estimate the differential entropy and mutual information is to use a kernel density estimator (KDE) \([44, 22, 2, 13, 41, 18]\): the densities \( f_{X,Y}, f_X, f_Y \) are separately estimated from samples and the estimated densities are then used to calculate the entropy and mutual information via the resubstitution estimator. A typical approach to avoid overfitting is to conduct data splitting (DS): split the samples and use one part for KDE and the other for the resubstitution.

In some cases, the parametric rate of convergence of \( \sqrt{N} \) of \( \ell_2 \) error is achieved: of particular interest is the result of \([22]\) where the parametric rate is achieved for differential entropy estimation via KDE of density followed by the resubstitution estimator when the dimension is no more than 4 – curiously, this exactly matches the result obtained in this paper for the fixed \( k \)-NN KL estimator. This “coincidence” of matching upper bounds for two different estimator approaches as well as numerical evidence (cf. Figure 1 and Section 2.3) suggesting that the upper bounds are tight for all dimensions, lends further evidence to the hypothesis that the lower bounds derived in Theorem 3 could perhaps be improved when the dimension is more than 4. Under certain very strong conditions on the density class (that are relevant in certain applications on graphical model selection \([30]\)), exponential rate of convergence can be demonstrated \([46, 47]\). Recent works \([29, 23]\) have studied the performance of the leave-one-out (LOO) approach where all but the sample of resubstitution are used for KDE, involving techniques such as von Mises expansion methods.

Alternative methods involve estimation of the entropies using spacings \([53, 51]\), the Edgeworth expansion \([52]\), and convex optimization \([35]\). Among the \( k \)-NN methods, there are two variants: either \( k \) is chosen to...
grow with the sample size $N$ or $k$ is fixed. There is a large literature on the former, where the classical result is the possibility of consistent estimation of the density from $k$-NN distances [32, 14], including recent sharper consistency characterizations [6, 27]. Several works have applied this basic insight towards the estimation of the specific case of information theoretic quantities [11, 55] and extensions to generalized NN graphs [32]. For fixed $k$-NN methods, apart from the works referred to in the main text, detailed experimental comparisons are in [15] and local Gaussian approaches studied in [16, 17, 33] bringing together local likelihood density estimation methods [31, 19] with $k$-NN driven choices of kernel bandwidth.

In this paper we have considered the smoothness of the class of pdfs studied via bounded Hessians. In nonparametric estimation, a standard feature is to consider whole families of smooth pdfs as defined by how the differences of derivatives relate to the differences of the samples [17]. Of specific interest is the Hölder family: $\Sigma(s, C)$, i.e., for any tuple $r = (r_1, \ldots, r_d)$, define $D^r = \sum_{j=1}^d \frac{\partial^{r_j}}{\partial x_1^{r_1}\ldots\partial x_d^{r_d}}$. Then for any $r$ such that $\sum_j r_j = [s]$, where $[s]$ is the largest integer smaller than $s$, we have:

$$\|D^r f(x) - D^r f(y)\| \leq C\|x - y\|^s - \sum_j r_j,$$

for any $x, y$. The rate of convergence of various nonparametric estimators depends on the parameter $s$ of the Hölder family under consideration, cf. [29, 23] for recent work on convergence rate characterization of information theoretic quantities via KDE and resubstitution estimators as a function of the smoothness parameter $s$. It is natural to ask if such smoothness considerations could lead to a refined understanding of the rates of convergence of the fixed $k$-NN KL and KSG estimators studied here.

In the context of the KL estimator, the only place where smoothness plays a critical role is in the statement (and proof) of Lemma 4. For small enough $r$, defining $P(x, r)(u) = \mathbb{P}\{\|X - x\| < r\}$, we seek to understand how this probability can be approximated by the density at $x$. With bounded Hessian norms, Lemma 4 asserts the following:

$$\left| P(x, r) - f(x)c_d r^d \right| \leq C d^d r^{d+2},$$

which is crucial in deriving the rate of convergence upper bounds on the KL estimator. A fairly straightforward calculation shows that this condition does not change even if we allow for smoother class of families of pdfs, as defined via the Hölder class – we conclude that refined rates of convergence for fixed $k$-NN estimators do not materialize by standard approaches such as the Hölder class.

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Appendix

A Proof of Theorem 1

We follow closely the proof from [48] of the $\sqrt{N}$-consistency of the one-dimensional entropy estimator introduced in [26]. It was proved in [48] that the entropy estimator in Equation (3) achieves $\sqrt{N}$-consistency in mean, i.e. $E[\hat{H}(X) - H(X)] = O(1/\sqrt{N})$, and in variance, i.e. $E[(\hat{H}(X) - E[\hat{H}(X)])^2] = O(1/N)$, under the assumption that the $X$ is a one-dimensional random variable and the estimator uses only the nearest neighbor distance with $k = 1$. In the process of proving our main result, we prove a generalization of this rate of convergence of the KL entropy estimator for general $d$-dimensional space and for a general $k$. Also notice that our proof works for any choice of $\ell_p$ distance for $1 \leq p \leq \infty$, so we will drop the subscribe $p$ in the proof of Theorem 1 and Theorem 2.

Firstly, we notice that $\xi_{k,i}(X)$ are identically distributed and $\xi_{k,i} = 0$ if $\rho_{k,i} > a_N$, so we have:

$$
\mathbb{E} \left[ \hat{H}_{KL}(X) \right] = \frac{1}{N} \sum_{i=1}^{N} \mathbb{E} \left[ \xi_{k,i}(X) \right] = \mathbb{E} \left[ \xi_{k,1}(X) \right] = \mathbb{E} \left[ \xi_{k,1}(X) \cdot I\{\rho_{k,1} \leq a_N\} \right].
$$

(40)

We introduce the following notations. Let $b_N = e^{-\psi(k)}NcdN = e^{-\psi(k)}c_d(\log N)^{1+\delta}$ and for every $u > 0$ define

$$
r_N(u) = \left( \frac{ue^{\psi(k)}}{c_dN} \right)^{1/d}.
$$

(41)

such that $r_N(e^{\xi_{k,1}(X)}) = \rho_{k,1}$ for $\rho_{k,1} \leq a_N$ and $r_N(b_N) = a_N$. It is easy to check that $\frac{dr_N(u)}{du} = \frac{r_N(u)}{ud}$. These definitions provide a new representation of the expectation in (40) using a change of variables $u = r_N^{-1}(\rho_{k,1})$:

$$
\mathbb{E} \left[ \xi_{k,1}(X) \cdot I\{\rho_{k,1} \leq a_N\} \right] = \mathbb{E} \left[ \log u \cdot I\{u \leq b_N\} \right] = \int \left( \int_{0}^{b_N} \log u \cdot dF_{N,x}(u) \right) f(x)dx,
$$

(42)

where we define the following distribution:

$$
F_{N,x}(u) = \mathbb{P} \left( e^{\xi_{k,1}(X)} < u \mid X_1 = x \right) = \mathbb{P} \left( \rho_{k,1} < r_N(u) \mid X_1 = x \right).
$$

(43)

Similar change of variables holds for the actual entropy as follows.

Lemma 1.

$$
H(X) = \int \left( \int_{0}^{\infty} \log u \cdot dF_{x}(u) \right) f(x)dx,
$$

(44)

where

$$
F_{x}(u) = 1 - \exp\{-ue^{\psi(k)}f(x)\} \sum_{j=0}^{k-1} \frac{(ue^{\psi(k)}f(x))^j}{j!}.
$$

(45)

This allows us to decompose the bias into three terms, each of which can be bounded separately.

$$
\left| \mathbb{E} \left[ \hat{H}_{KL}(X) \right] - H(X) \right| = \left| \mathbb{E} \left[ \xi_{k,1}(X) \cdot I\{\rho_{k,1} \leq a_N\} - H(X) \right] \right| \leq \int (I_1(x) + I_2(x) + I_3(x)) f(x)dx,
$$

(46)

(47)
where

\[
I_1(x) = \left| \int_{b_N}^{\infty} \log u dF_x(u) \right|,
\]

\[
I_2(x) = \left| \int_{0}^{1} \log u dF_{N,x}(u) - \int_{0}^{b_N} \log u dF_x(u) \right|,
\]

\[
I_3(x) = \left| \int_{1}^{b_N} \log u dF_{N,x}(u) - \int_{1}^{b_N} \log u dF_x(u) \right|. \tag{48}
\]

We will bound the three terms separately. The main idea is that \( I_1(x) \) is small when \( b_N \) is sufficiently large, and \( I_2(x) \) and \( I_3(x) \) are small when \( f_2(u) \) and \( f_{N,x}(u) \) are close.

\( I_1(x) \): We upper bound the tail probability that the \( k \)-NN distance is truncated. By plugging in the cdf \([45]\) of \( F_x(u) \), we get:

\[
I_1(x) = \left| \int_{b_N}^{\infty} \log u dF_x(u) \right| = \left| \int_{b_N}^{\infty} \log u \frac{dF_x(u)}{du} du \right| = \left| \frac{1}{(k-1)!} \int_{b_N}^{\infty} (\log u) e^{\psi(k)} f(x) \exp\{-ue^{\psi(k)} f(x)\}(ue^{\psi(k)} f(x))^{k-1} du \right|
\]

\[
= \left| \frac{1}{(k-1)!} \int_{b_N}^{\infty} (\log t - \psi(k) - \log f(x)) e^{-t k^{-1}} dt \right|, \tag{49}
\]

where the third equality is from Equation \([61]\) and the last equality comes from changing of variable \( t = ue^{\psi(k)} f(x) \). Now we consider two cases:

1. \( b_N e^{\psi(k)} f(x) < 1 \). Then \([49]\) is upper bounded by:

\[
\frac{1}{(k-1)!} \left| \int_{b_N e^{\psi(k)} f(x)}^{\infty} (\log t - \psi(k) - \log f(x)) e^{-t k^{-1}} dt \right|
\]

\[
\leq \left| \frac{1}{(k-1)!} \left( \int_{b_N e^{\psi(k)} f(x)}^{\infty} \log t e^{-t k^{-1}} dt + |\psi(k) + \log f(x)| \int_{b_N e^{\psi(k)} f(x)}^{\infty} e^{-t k^{-1}} dt \right) \right|
\]

\[
\leq \frac{1}{(k-1)!} \left( \int_{0}^{\infty} |\log t| e^{-t k^{-1}} dt + |\psi(k) + \log f(x)| \int_{0}^{\infty} e^{-t k^{-1}} dt \right)
\]

\[
\leq C_1(1 + |\psi(k) + \log f(x)|). \tag{50}
\]

where \( C_1 = \max \left\{ \frac{1}{(k-1)!} \int_{0}^{\infty} |\log t| e^{-t k^{-1}} dt, \frac{1}{(k-1)!} \int_{0}^{\infty} e^{-t k^{-1}} dt \right\} \).

2. \( b_N e^{\psi(k)} f(x) \geq 1 \). Then \([49]\) is upper bounded by:

\[
\frac{1}{(k-1)!} \left| \int_{b_N e^{\psi(k)} f(x)}^{\infty} (\log t - \psi(k) - \log f(x)) e^{-t k^{-1}} dt \right|
\]

\[
\leq \left| \frac{1}{(k-1)!} \left( \int_{b_N e^{\psi(k)} f(x)}^{\infty} \log t e^{-t k^{-1}} dt + |\psi(k) + \log f(x)| \int_{b_N e^{\psi(k)} f(x)}^{\infty} e^{-t k^{-1}} dt \right) \right|
\]

\[
\leq C_2(1 + |\psi(k) + \log f(x)|) \int_{b_N e^{\psi(k)} f(x)}^{\infty} e^{-t/2} dt
\]

\[
\leq 2C_2(1 + |\psi(k) + \log f(x)|) \exp\{-b_N e^{\psi(k)} f(x)\}, \tag{51}
\]
where $C_2$ is a constant satisfying $\log t \cdot t^{b-1}/(k-1)! < C_2e^{t/2}$ and $t^{b-1}/(k-1)! < C_2e^{t/2}$ for all $t > 1$.

Now combining the two cases, $I_1(x)$ is bounded by:

$$I_1(x) \leq (1 + |\psi(k) + \log f(x)|) \left(C_1 \mathbb{I}\{b_N e^{\psi(k)} f(x) < 1\} + 2C_2 \exp\{-b_N e^{\psi(k)} f(x)\}\right)$$

$$\leq C_3(1 + |\log f(x)|) \exp\{-b_N e^{\psi(k)} f(x)\},$$

where we use the fact that $\mathbb{I}\{b_N e^{\psi(k)} f(x) < 1\} \leq \exp\{1 - b_N e^{\psi(k)} f(x)\}$. Here $C_3 = (C_1 e + 2C_2)(1 + |\psi(k)|)$.

$I_2(x)$ can be bounded by:

$$I_2(x) = \left|\int_0^1 \log u \, dF_{N,x}(u) - \int_0^1 \log u \, dF_x(u)\right| \leq \int_0^1 |\log u| \, |f_{N,x}(u) - f_x(u)| \, du$$

where $f_{N,x}(u)$ and $f_x(u)$ are the corresponding pdfs of $F_{N,x}(u)$ and $F_x(u)$, respectively. In the following lemma we give an upper bound for the difference of $f_{N,x}(u)$ and $f_x(u)$.

**Lemma 2.** Under the Assumption I

$$|f_{N,x}(u) - f_x(u)| \leq C_4 \left(N^{-2/d} + N^{-1}\right),$$

for $u \leq 1$.

Using Lemma 2 and the fact that $\int_0^1 |\log u| \, du = 1$, $I_2(x)$ is upper bounded by:

$$I_2(x) \leq C_4(N^{-2/d} + N^{-1}) \int_0^1 |\log u| \, du \leq C_4(N^{-2/d} + N^{-1}).$$

$I_3(x)$ can be bounded by:

$$I_3(x) = \left|\int_1^{b_N} \log u \, dF_{N,x}(u) - \int_1^{b_N} \log u \, dF_x(u)\right|$$

$$= \left|\int_1^{b_N} \frac{1}{u}(1 - F_{N,x}(u)) \, du - \int_1^{b_N} \frac{1}{u}(1 - F_x(u)) \, du\right|$$

$$\leq \int_1^{b_N} \frac{1}{u}|F_{N,x}(u) - F_x(u)| \, du.$$

In the following lemma we give an upper bound for the difference of $F_{N,x}(u)$ and $F_x(u)$.

**Lemma 3.** Under the Assumption I

$$|F_{N,x}(u) - F_x(u)| \leq C_5 \left(u^{1+2/d}N^{-2/d} + u^2/N\right)$$

Using Lemma 3, $I_3(x)$ is upper bounded by:

$$I_3(x) \leq C_5 \int_1^{b_N} \left((u/N)^{2/d} + u/N\right) \, du$$

$$\leq C_5 \left(b_N^{1+2/d}N^{-2/d} + b_N^2N^{-1}\right),$$

Combining the upper bounds of $I_1(x)$, $I_2(x)$ and $I_3(x)$ and defining $C_6 = \max\{C_3, C_4, C_5\}$, the bias is
bounded by:

\[ \mathbb{E} \left[ \tilde{H}_{\text{KL}}(X) \right] - H(X) \]

\[ \leq \int (I_1(x) + I_2(x) + I_3(x)) f(x)dx \]

\[ \leq C_0 \int \left( |1 + \log f(x)| \exp\{-b_N e^{\psi(k)} f(x)\} \right) N^{-2/d} + N^{-1} + b_N^{1+2/d} N^{-2/d} + b_N^2 N^{-1} f(x)dx \]

\[ \leq C_0 \left( \int f(x) \exp\{-b_N e^{\psi(k)} f(x)\} + \int f(x) |\log f(x)| \exp\{-b_N e^{\psi(k)} f(x)\} + b_N^{1+2/d} N^{-2/d} + b_N^2 N^{-1} \right) \]

By Assumption 1(c), the first term is bounded by: \( \int f(x) \exp\{-b_N e^{\psi(k)} f(x)\} \leq C_d e^{-b_N C_0} \). The second term is bounded by Hölder inequality as:

\[ \int f(x) |\log f(x)| \exp\{-b_N e^{\psi(k)} f(x)\} \]

\[ \leq \left( \int f(x) (|\log f(x)|)^{1+\gamma} dx \right)^{1/(1+\gamma)} \left( \int f(x) \exp\{-\frac{1}{\gamma} b_N e^{\psi(k)} f(x)\} dx \right)^{\gamma/(1+\gamma)} \]

\[ \leq C_b^{1/(1+\gamma)} \left( C_d e^{-\frac{1}{\gamma} b_N C_0} \right)^{\gamma/(1+\gamma)}. \] (60)

By choosing \( b_N = e^{-\psi(k)} c_d (\log N)^{1+\delta} \) for some \( \delta > 0 \), we know that \( e^{-C_0 b_N} \) decays faster than \( N^{-\alpha} \) for any \( \alpha \). This completes the proof.

### A.1 Proof of Lemma 1

Since \( F_x(u) \) is a continuous CDF, the corresponding pdf is given by:

\[ f_x(u) = \frac{dF_x(u)}{du} = -\exp\{-ue^{\psi(k)} f(x)\} \sum_{j=1}^{k-1} \frac{(ue^{\psi(k)} f(x))^{j-1}}{(j-1)!} e^{\psi(k)} f(x) \]

\[ + e^{\psi(k)} f(x) \exp\{-ue^{\psi(k)} f(x)\} \sum_{j=0}^{k-1} \frac{(ue^{\psi(k)} f(x))^j}{j!} \]

\[ = \frac{1}{(k-1)!} e^{\psi(k)} f(x) \exp\{-ue^{\psi(k)} f(x)\} (ue^{\psi(k)} f(x))^{k-1}. \] (61)

Therefore,

\[ \int_0^\infty \log udF_x(u) = \frac{1}{(k-1)!} \int_0^\infty \log u e^{\psi(k)} f(x) \exp\{-ue^{\psi(k)} f(x)\} (ue^{\psi(k)} f(x))^{k-1} du \]

\[ = \frac{1}{(k-1)!} \int_0^\infty (\log t - \psi(k) - \log f(x)) e^{-t} t^{k-1} dt \]

\[ = \psi(k) - \psi(k) - \log f(x) \]

\[ = -\log f(x), \] (62)

where the third to last equation comes from change of variable \( t = ue^{\psi(k)} f(x) \). The penultimate equation comes from the fact that \( \psi(k) = \frac{1}{(k-1)!} \int_0^\infty (\log t) t^{k-1} e^{-t} dt \) and \( 1 = \frac{1}{(k-1)!} \int_0^\infty t^{k-1} e^{-t} dt \). Therefore,

\[ \int \left( \int_0^\infty \log udF_x(u) \right) f(x)dx = \int (-\log f(x)) f(x)dx = H(X). \] (63)
A.2 Proof of Lemma 2

Recall that

\[ f_x(u) = \frac{1}{(k-1)!} e^{\psi(k)} f(x) \exp\{-ue^{\psi(k)} f(x)\} (ue^{\psi(k)} f(x))^{k-1}. \]  

(64)

Notice that \( r_N(u) \) is the \( k^{th} \) order statistic of \( \{ \|X_1 - x\|, \|X_2 - x\|, \ldots, \|X_{N-1} - x\| \} \). Therefore the density \( f_{N,x}(u) \) is given by:

\[
\begin{align*}
  f_{N,x}(u) &= f_{r_N(u)} \frac{dr_N(u)}{du} \\
  &= \frac{(N-1)!}{(k-1)!N^{k-1}} \left( P(x,r_N(u)) \right)^{k-1} \left( 1 - P(x,r_N(u)) \right)^{N-k-1} \frac{dP(x,r_N(u))}{dr_N(u)} \frac{dr_N(u)}{du} \\
  &= \frac{(N-1)!}{(k-1)!N^{k-1}} \left( P(x,r_N(u)) \right)^{k-1} \left( 1 - P(x,r_N(u)) \right)^{N-k-1} \frac{dP(x,r_N(u))}{du}. \n\end{align*}
\]

(65)

Here \( P(x,r(u)) = \mathbb{P}\{\|X - x\| < r\} = \int_{t \in B(x,r)} f(t) dt \). Since \( f \) is twice differentiable and \( r_N(u) \) goes to 0 as \( N \) goes to infinity, we can use \( f(z) \text{Vol}(B(z,r_N(u))) \) to estimate \( P(z,r_N(u)) \). The following lemma bounds the error of this estimation:

**Lemma 4.** Under Assumption 1 there exists a constant \( C \) such that for sufficiently small \( r \), we have

\[
\left| P(x,r) - f(x)c_dr^d \right| \leq Cr^{d+2},
\]

(66)

and

\[
\left| \frac{dP(x,r)}{dr} - f(x)dc_dr^{d-1} \right| \leq Cr^{d+1}.
\]

(67)

Using Lemma 3 and substituting \( r = r_N(u) = \left(ue^{\psi(k)}/(c_dN)^{1/d}\right) \), we have:

\[
\left| P(x,r_N(u)) - \frac{ue^{\psi(k)} f(x)}{N} \right| = \left| P(x,r_N(u)) - f(x)c_dr_N(u)^d \right| \leq C_1(r_N(u))^{d+2}.
\]

(68)

Similarly, \( \left| \frac{d}{du} P(x,r_N(u)) - \frac{e^{\psi(k)} f(x)}{N} \right| \) can be bounded by:

\[
\begin{align*}
  \left| \frac{d}{du} P(x,r_N(u)) - \frac{e^{\psi(k)} f(x)}{N} \right| &= \left| \frac{dr_N(u)}{du} \frac{d}{dr_N(u)} P(x,r_N(u)) - \left( \frac{dr_N(u)}{du} \right)^{-1} e^{\psi(k)} f(x) \right| \\
  &= \frac{r_N(u)}{u} \left| \frac{d}{dr_N(u)} P(x,r_N(u)) - f(x)dc_d(r_N(u))^{d-1} \right| \\
  &\leq C_1(r_N(u))^{d+2}.
\end{align*}
\]

(69)

Now we can write the difference of \( f_{N,x}(u) \) and \( f_x(u) \) via two terms:

\[
\left| f_{N,x}(u) - f_x(u) \right| \leq \left| f_{N,x}(u) - f_{N,x}^{(1)}(u) \right| + \left| f_{N,x}^{(1)}(u) - f_x(u) \right|,
\]

(70)
where \( f_{N,x}^{(1)}(u) \) defined as:

\[
    f_{N,x}^{(1)}(u) = \frac{(N-1)!}{(k-1)!(N-k-1)!} \left( \frac{u e^{\psi(k)} f(x)}{N} \right)^{k-1} \left( 1 - \frac{u e^{\psi(k)} f(x)}{N} \right)^{N-k-1} \frac{e^{\psi(k)} f(x)}{N}.
\]

(71)

Consider the function \( g(p) = \frac{(N-1)!}{(k-1)!(N-k-1)!} p^{k-1}(1-p)^{N-k-1} \) for \( p \in (0,1) \). By basic calculus, we can see that \( g(p) \leq C_2 N \) and \( |g'(p)| \leq C_3 N^2 \) for \( p \in (0,1) \). Therefore, the first term in (70) can be bounded as:

\[
    |f_{N,x}(u) - f_{N,x}^{(1)}(u)|
    \leq C_{1}C_{2}N(r_N(u))^{d+2}/u + C_{1}C_{3}N^2(r_N(u))^{d+2+2} \frac{e^{\psi(k)} f(x)}{N}
    \leq C_{4}u^{1+2/d}N^{-2/d} (1 + \frac{1}{u})
    \leq C_{4}N^{-2/d},
\]

(72)

for \( u \leq 1 \). Here \( C_4 = \max \{C_1C_2 (e^{\psi(k)} C_a)^{1+2/d}, C_1C_3 (e^{\psi(k)} C_a)^{2+2/d} \} \), where \( C_a = \sup_x f(x) \) by Assumption 1(a). For the second term, we denote \( q = u e^{\psi(k)} f(x) \) for short. Then the second term in (70) can be bounded as:

\[
    |f_{N,x}^{(1)}(u) - f_x(u)|
    = \frac{1}{u} \left| \frac{(N-1)!}{(k-1)!(N-k-1)!} \left( \frac{q}{N} \right)^k \left( 1 - \frac{q}{N} \right)^{N-k-1} \frac{1}{(k-1)!} q^k e^{-q} \right|
    = \frac{k}{u} \left| \frac{(N-1)!}{(N-1)!} \left( \frac{q}{N} \right)^k \left( 1 - \frac{q}{N} \right)^{N-k-1} \frac{q^k e^{-q} k!}{k!} \right|.
\]

(73)

Notice that the difference inside the absolute value is just the difference of \( P(X = k) \) under \( \text{Bino}(N-1,q/N) \) and \( \text{Poisson}(q) \). The difference is bounded by:

**Lemma 5.** For \( q < C \sqrt{N} \), we have:

\[
    \left| \left( \frac{N-1}{k} \right) \left( \frac{q}{N} \right)^k \left( 1 - \frac{q}{N} \right)^{N-k-1} - \frac{q^k e^{-q} k!}{k!} \right| \leq C_5 q^{k+2} e^{-q} N^{-1},
\]

(74)

for some \( C_5 > 0 \).

Therefore, by lemma 5 we have:

\[
    |f_{N,x}^{(1)}(u) - f_x(u)| \leq C_5 \frac{kq^{k+2} e^{-q}}{uN} \leq C_5 \frac{k(e^{\psi(k)} f(x))^{k+2} u^{k+1}}{N} \leq C_6 N^{-1},
\]

(75)

for \( u \leq 1 \), here \( C_6 = C_5 k(e^{\psi(k)} C_a)^{k+1} \). Therefore, combining (72) and (75), we have the desired statement.
A.3 Proof of Lemma 3

Recall that

\[ F_x(u) = 1 - \exp\{-ue^{\psi(k)}f(x)\} \sum_{j=0}^{k-1} \frac{ue^{\psi(k)}f(x)^j}{j!}. \]  

(76)

The cdf \( F_{N,x}(u) = P(\rho_{k,i} < r_N(u)|X_i = x) \) is just the probability that at least \( k \) samples are inside the ball \( B(x, r_N(u)) \) and hence

\[ F_{N,x}(u) = 1 - \sum_{j=0}^{k-1} \frac{(N-1)!}{j!(N-j-1)!} (P(x, r_N(u)))^j (1 - P(x, r_N(u)))^{N-j-1}. \]

(77)

So we have:

\[
|F_{N,x}(u) - F_x(u)| = \left| \sum_{j=0}^{k-1} \frac{(N-1)!}{j!(N-j-1)!} (P(x, r_N(u)))^j (1 - P(x, r_N(u)))^{N-j-1} - \exp\{-ue^{\psi(k)}f(x)\} \sum_{j=0}^{k-1} \frac{ue^{\psi(k)}f(x)^j}{j!} \right| 
\leq \sum_{j=0}^{k-1} \frac{1}{j!} \left| \frac{(N-1)!}{j!(N-j-1)!} (P(x, r_N(u)))^j (1 - P(x, r_N(u)))^{N-j-1} - \exp\{-ue^{\psi(k)}f(x)\} \right| \exp\{ue^{\psi(k)}f(x)\}. 
\]

(78)

Let

\[ h_{N,x,j}(u) = \frac{(N-1)!}{j!(N-j-1)!} (P(x, r_N(u)))^j (1 - P(x, r_N(u)))^{N-j-1}, \]

(79)

and

\[ h_{x,j}(u) = \frac{1}{j!} \exp\{-ue^{\psi(k)}f(x)\} \exp\{ue^{\psi(k)}f(x)\}. \]

(80)

Consider

\[ h_{N,x,j}^{(1)}(u) = \frac{(N-1)!}{j!(N-j-1)!} \left( \frac{ue^{\psi(k)}f(x)}{N} \right)^j \left( 1 - \frac{ue^{\psi(k)}f(x)}{N} \right)^{N-j-1}. \]

(81)

We will bound \( |h_{N,x,j}(u) - h_{x,j}(u)| \) by \( |h_{N,x,j}(u) - h_{N,x,j}^{(1)}(u)| + |h_{N,x,j}^{(1)}(u) - h_{x,j}(u)| \). For the first term, consider function \( g_j(p) = \frac{(N-1)!}{j!(N-j-1)!} p^j (1 - p)^{N-j-1} \). It is easy to see that \( |g_j'(p)| \leq C_1 N \) for any \( p \in (0, 1) \). Therefore, by Lemma 4, we obtain:

\[
|h_{N,x,j}(u) - h_{N,x,j}^{(1)}(u)| = \left| g(P(x, r_N(u))) - g\left( \frac{ue^{\psi(k)}f(x)}{N} \right) \right| 
\leq \max_{p \in (0,1)} |g'(p)| \left| P(x, r_N(u)) - \frac{ue^{\psi(k)}f(x)}{N} \right| 
\leq C_1 N (r_N(u))^{d+2} 
\leq C_2 u^{1+2/d} N^{-2/d},
\]

(82)
where \( C_2 = C_1(e^{\psi(k)}C_\alpha)^{1+2/d} \). For the second term, let \( q = ue^{\psi(k)}f(x) \), and using a similar analysis as (85), we obtain:

\[
|h_N^{(1)}(u) - h_{x,j}(u)| = \left| \binom{N-1}{j} \left( q \right)_{j} (1 - \frac{q}{N})^{N-j-1} - \frac{q^je^{-q}}{j!} \right| 
\leq C_3 \frac{q^{j+2}e^{-q}}{N}. \tag{83}
\]

Combine (82) and (83), and we obtain:

\[
|F_{N,x}(u) - F_x(u)| \leq \sum_{j=0}^{k-1} |h_{N,x,j}(u) - h_{x,j}(u)| 
\leq \sum_{j=0}^{k-1} \left( |h_{N,x,j}(u) - h_{N,x,j}^{(1)}(u)| + |h_{N,x,j}^{(1)}(u) - h_{x,j}(u)| \right) 
\leq kC_2u^{1+2/d}N^{-2/d} + C_3 \sum_{j=0}^{k-1} \frac{q^je^{-q}}{N} 
\leq kC_2u^{1+2/d}(N)^{-2/d} + (k-1)!C_3q^2/N 
\leq kC_2u^{1+2/d}(N)^{-2/d} + (k-1)!C_3(e^{\psi(k)}C_\alpha)^2u^2/N, \tag{84}
\]

where we used the fact that \( \sum_{j=1}^{k-1} q^je^{-q} \leq (k-1)! \sum_{j=1}^{k-1} \frac{q^je^{-q}}{(k-1)!} \leq (k-1)! \). Therefore, we have the desired statement by \( C_5 = \max\{kC_2, (k-1)!C_3(e^{\psi(k)}C_\alpha)^2\} \).

### A.4 Proof of Lemma 4

Under Assumption (4)\((d)\), we have \( \|H_f(x)\| \leq C_d \) almost everywhere, and hence, there exists a \( y = at + (1-a)x \) for some \( a \in [0, 1] \) such that

\[
\left| P(x,r) - f(x) \right| d^{d-1} = \left| \int_{t \in B(x,r)} (f(t) - f(x)) \, dt \right| 
\leq \int_{t \in B(x,r)} \left( f(x) + (\nabla f(x))^T (t - x) + (t - x)^T H_f(y)(t-x) - f(x) \right) \, dt 
\leq \int_{t \in B(x,r)} \|t-x\|^2 dt 
\leq C_d \Vol(B(x,r)) \cdot d \cdot r^2 \leq C_1 r^{d+2}, \tag{85}
\]

where \( \Vol(B(x,r)) \) is the volume of \( B(x,r) \). \( \|t-x\|^2 \leq d \cdot r^2 \) for all \( t \in B(z,r) \) (here \( B(z,r) \) can be any \( p \)-norm ball with \( 1 \leq p \leq \infty \)). For the second part, let \( S(B(x,r)) \) be the surface of \( B(x,r) \). Consider \( m^{d-1} \) be the Lebesgue measure on \( \mathbb{R}^{d-1} \), so \( m^{d-1}(S(B(x,r))) = d_c x^{d-1} \). Similarly we have:

\[
\left| \frac{dP(x,r)}{dr} - f(x) \right| d^{d-1} = \left| \int_{t \in S(B(x,r))} (f(t) - f(x)) \, dm^{d-1}(t) \right| 
\leq C_d \int_{t \in S(B(x,r))} \|t-x\|^2 dm^{d-1}(t) 
\leq C_2 r^{d+1}. \tag{86}
\]
A.5 Proof of Lemma 5

We will prove that:
\[
|\log \left( \binom{N}{k} \frac{q}{N}^k \left(1 - \frac{q - C}{N}\right)^{N-k} \right) - \log \left( \frac{q^k e^{-q}}{k!} \right)| \leq Cq^2/N. \tag{87}
\]

Then for sufficiently small \( q \) such that \( \exp\{Cq^2/N\} \leq 2Cq^2/N \), we obtain our desired statement by the fact that \( |x - y| \leq |\log x - \log y| \cdot \frac{1}{2} \) for small enough \( |\log x - \log y| \). Using Stirling’s formula: \( \log(N!) = N \log N - N + \frac{1}{2} \log(2\pi N) + O(1/N) \), the difference (87) is given by:
\[
|\log \left( \binom{N}{k} \frac{q}{N}^k \left(1 - \frac{q - C}{N}\right)^{N-k} \right) - \log \left( \frac{q^k e^{-q}}{k!} \right)|
= |\log N! - \log(N - k)! - k \log q + (N - k) \log(N - q) - N \log N - k \log q + q + \log(k!)|
\leq N \log N - N + \frac{1}{2} \log(2\pi N) - (N - k) \log(N - k) + (N - k)
- \frac{1}{2} \log(2\pi(N - k)) + (N - k) \log(N - q) - N \log N + q + C/N
\leq \frac{(k - q)^2}{2(N - k)} + Cq^3/N^2 + C/N
\leq Cq^2/N, \tag{88}
\]

where we used the assumption that \( q < C\sqrt{N} \) for sufficiently small constant \( C > 0 \).

B Proof of Theorem 2

Recall that \( \hat{H}_{KL}(X) = \frac{1}{N} \sum_{i=1}^{N} \xi_{k,i}(X) \) and \( \xi_{k,i}(X) \) are identically distributed, therefore, we obtain
\[
\text{Var} \left[ \hat{H}_{KL}(X) \right] = \frac{1}{N^2} \sum_{i=1}^{N} \text{Var} \left[ \xi_{k,i}(X) \right] + \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j \neq i} \text{Cov} \left[ \xi_{k,i}(X), \xi_{k,j}(X) \right]
= \frac{1}{N} \text{Var} \left[ \xi_{k,1}(X) \right] + \frac{N(N - 1)}{N^2} \text{Cov} \left[ \xi_{k,1}(X), \xi_{k,2}(X) \right]
\leq \frac{1}{N} \text{Var} \left[ \xi_{k,1}(X) \right] + \text{Cov} \left[ \xi_{k,1}(X), \xi_{k,2}(X) \right]. \tag{89}
\]

We claim the following two lemmas:

**Lemma 6. Under the Assumption 7**
\[
\text{Var} \left[ \xi_{k,1}(X) \right] = O \left( (\log \log N)^2 \right), \tag{90}
\]

**Lemma 7. Under the Assumption 7**
\[
\text{Cov} \left[ \xi_{k,1}(X), \xi_{k,2}(X) \right] = O \left( (\log \log N)^2 (\log N)^{(2k+2)(1+\delta)} N^{-1} \right). \tag{91}
\]

Combining the two lemmas, we obtain the desired statement.
B.1 Proof of Lemma 6

Recall that in the proof of Theorem 1, we have defined the following distributions:

$$F_{N,x}(u) = \mathbb{P} \left( e^{\xi_{k,1}(X)} < u \mid X_1 = x \right) = \mathbb{P} \left( \rho_{k,1} < r_N(u) \mid X_1 = x \right);$$  

$$F_x(u) = 1 - \exp\{-ue^{\psi(k)}f(x)\} \sum_{j=0}^{k-1} \frac{(ue^{\psi(k)}f(x))^j}{j!},$$  

and their corresponding pdfs $f_{N,x}(u)$ and $f_x(u)$. The variance of $\xi_{k,1}(X)$ is upper bounded by:

$$\text{Var} \left[ \xi_{k,1}(X) \right] \leq \mathbb{E} \left[ (\xi_{k,1}(X))^2 \right] - \mathbb{E} \left[ (\xi_{k,1}(X))^2 \mid X_1 = x \right] \leq \int \left( \int_0^{b_N} (\log u)^2 f_{N,x}(u)du \right) f(x)dx$$  

$$= \int \left( \int_0^{b_N} (\log u)^2 f_{N,x}(u)du + \int_1^{b_N} (\log u)^2 f_{N,x}(u)du \right) f(x)dx. \quad (94)$$

For $u < 1$, Lemma 2 told us that there exists some $C_1 > 0$ such that

$$|f_{N,x}(u) - f_x(u)| \leq C_1 \left( N^{-2/d} + N^{-1} \right) \leq C_1, \quad (95)$$

and the closed form of $f_x(u)$ is given by:

$$f_x(u) = \frac{1}{(k-1)!} e^{\psi(k)}f(x) \exp\{-ue^{\psi(k)}f(x)\}(ue^{\psi(k)}f(x))^{k-1}. \quad (96)$$

Since $\frac{1}{(k-1)!} t^{k-1} e^{-t} < 1$ for all $t > 0$, we know that $f_x(u) < e^{\psi(k)}f(x)$. Therefore, $f_{N,x}(u) \leq C_1 + e^{\psi(k)}f(x)$ by triangle inequality, therefore,

$$\int_0^1 (\log u)^2 f_{N,x}(u)du \leq \left( C_1 + e^{\psi(k)}f(x) \right) \int_0^1 (\log u)^2 du = 2 \left( C_1 + e^{\psi(k)}f(x) \right). \quad (97)$$

For $1 \leq u \leq b_N$, we have $(\log u)^2 \leq (\log b_N)^2 = \log^2((\log N)^{1+\delta}) = (1 + \delta)^2(\log \log N)^2$ for sufficiently large $N$. Therefore,

$$\int_1^{b_N} (\log u)^2 f_{N,x}(u)du \leq (1 + \delta)^2(\log \log N)^2 \int_1^{b_N} f_{N,x}(u)du \leq (1 + \delta)^2(\log \log N)^2. \quad (98)$$

Combine these two results into (94), and we obtain:

$$\text{Var} \left[ \xi_{k,1}(X) \right] \leq \int \left( \int_0^1 (\log u)^2 f_{N,x}(u)du + \int_1^{b_N} (\log u)^2 f_{N,x}(u)du \right) f(x)dx$$  

$$\leq \int \left( 2 \left( C_1 + e^{\psi(k)}f(x) \right) + (1 + \delta)^2(\log \log N)^2 \right) f(x)dx$$  

$$\leq 2C_1 + 2e^{\psi(k)}C_\alpha + (1 + \delta)^2(\log \log N)^2$$  

$$= O \left( (\log \log N)^2 \right), \quad (99)$$

where we used the assumption that $f(x) \leq C_\alpha$. 

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The covariance can be rewritten as:

\[
\text{Cov} [\xi_k(X), \xi_{k'}(X)] \\
= \mathbb{E}[(\xi_k(X) - \mathbb{E} [\xi_k(X)])(\xi_{k'}(X) - \mathbb{E} [\xi_{k'}(X)])] \\
= \int_{x,y} \mathbb{E}[(\xi_k(X) - \mathbb{E} [\xi_k(X)])(\xi_{k'}(X) - \mathbb{E} [\xi_{k'}(X)]) | X_1 = x, X_2 = y] f(x)f(y) dx dy \\
= \int_{||x-y|| \leq 2a_N} \mathbb{E}[(\xi_k(X) - \mathbb{E} [\xi_k(X)])(\xi_{k'}(X) - \mathbb{E} [\xi_{k'}(X)]) | X_1 = x, X_2 = y] f(x)f(y) dx dy \\
+ \int_{||x-y|| > 2a_N} \mathbb{E}[(\xi_k(X) - \mathbb{E} [\xi_k(X)])(\xi_{k'}(X) - \mathbb{E} [\xi_{k'}(X)]) | X_1 = x, X_2 = y] f(x)f(y) dx dy
\]

We split the covariance into two separate cases: If \(||x - y|| \leq 2a_N\), the first term of (100) can be bounded by Cauchy-Schwarz inequality as:

\[
\int_{||x-y|| \leq 2a_N} \mathbb{E}[(\xi_k(X) - \mathbb{E} [\xi_k(X)])(\xi_{k'}(X) - \mathbb{E} [\xi_{k'}(X)]) | X_1 = x, X_2 = y] f(x)f(y) dx dy \\
\leq \int_{||x-y|| \leq 2a_N} \text{Var} [\xi_k(X) | X_1 = x, X_2 = y]^{1/2} \text{Var} [\xi_{k'}(X) | X_1 = x, X_2 = y]^{1/2} f(x)f(y) dx dy. (101)
\]

Consider the following CDF:

\[
F_{N,x}(u) = \mathbb{P} \left( e^{\xi_k(X)} < u | X_1 = x, X_2 = y \right) = \mathbb{P} \left( \rho_{k,1} < r_N(u) | X_1 = x, X_2 = y \right);
\]

and the corresponding pdf \(f_{N,x,y}(u)\), which is given by order statistic [37]:

\[
f_{N,x,y}(u) = \begin{cases} \frac{(N-2)!}{(k-2)!(N-k-1)!} p^{k-2} (1-p)^{N-k-1} \frac{dp}{du} , & ||x-y|| \leq u , \\ \frac{(N-2)!}{(k-1)!(N-k-2)!} p^{k-1} (1-p)^{N-k-2} \frac{dp}{du} , & ||x-y|| > u \end{cases}
\]

where \(p = P(x, r_N(u)) = \int_{t \in B(x, r_N(u))} f(t) dt\). Since \(f(x) \leq C_a\) almost everywhere, we have:

\[
p \leq \text{Vol}(B(x, r_N(u))) \left( \sup_{t \in B(x, r_N(u))} f(t) \right) = c_d r_N(u)^d \cdot C_a \leq \frac{2u C_a e^{\psi(k)}}{N}.
\]

\[
\frac{dp}{du} = \frac{dp}{dr_N(u)} \frac{dr_N(u)}{du} \leq S(B(x, r_N(u))) \left( \sup_{t \in B(x, r_N(u))} f(t) \right) r_N(u) \frac{r_N(u)}{ud} \\
\leq C_d r_N(u)^{d-1} \cdot C_a \cdot \frac{r_N(u)^d C_a}{ud} \leq \frac{2u C_a e^{\psi(k)}}{N}.
\]

Therefore, for any \(u \leq 1\), we have:

\[
f_{N,x,y}(u) \leq \begin{cases} \frac{1}{(k-1)!} N^{k-1} p^{k-2} \frac{dp}{du} \leq \frac{1}{(k-1)!} (2u C_a e^{\psi(k)})^{k-2} (2C_a e^{\psi(k)}) \leq \frac{1}{(k-1)!} (2C_a e^{\psi(k)})^{k-1} , & ||x-y|| \leq u \\ \frac{1}{(k-1)!} N^{k-1} p^{k-1} \frac{dp}{du} \leq \frac{1}{(k-1)!} (2u C_a e^{\psi(k)})^{k-1} (2C_a e^{\psi(k)}) \leq \frac{1}{(k-1)!} (2C_a e^{\psi(k)})^k , & ||x-y|| > u \end{cases}
\]

So there exists some \(C_2\) not depend on \(N\) such that \(f_{N,x,y}(u) \leq C_2\) for all \(u \leq 1\). Therefore, we can bound \(\text{Var} [\xi_k(X) | X_1 = x, X_2 = y]\) as:
Therefore, we know that the first term of (100) is upper bounded by $C$ since $C_{1}$ for some constant $a$ in $N,x,y = (\log(\log(\log(N)))/N$.

Now consider the case that $C_{1}$ for some $(x,y) = (\log(\log(\log(N)))/N,1)$:

\[
C \int_{0}^{1} (\log u)^{2} f_{N,x,y}(u) du = C_{2} \int_{0}^{1} (\log u)^{2} du + (\log b_{N})^{2}
\]

\[
= C_{2} \int_{0}^{1} (\log u)^{2} du + (\log b_{N})^{2}
\]

\[
= C_{2} + (1 + \delta)(\log \log N)^{2} \leq C_{2}^{*}(\log \log N)^{2}
\]

(105)

for some $C_{2}^{*} > 0$. Similarly, we know that $\text{Var}[\xi_{1,2}(X) | X_{1} = x, X_{2} = y] \leq C_{2}^{*}(\log \log N)^{2}$. Therefore,

\[
\int_{\|x-y\| \leq 2a_{N}} \text{Var}[\xi_{1,2}(X) | X_{1} = x, X_{2} = y]^{1/2} \text{Var}[\xi_{1,2}(X) | X_{1} = x, X_{2} = y]^{1/2} f(x)f(y) dx dy
\]

\[
\leq C_{2}^{*}(\log \log N)^{2} \int_{\|x-y\| \leq 2a_{N}} f(x)f(y) dx dy
\]

\[
\leq C_{2}^{*}(\log \log N)^{2} \mathbb{P}[\|x-y\| \leq 2a_{N}]
\]

\[
= C_{2}^{*}(\log \log N)^{2} \int \left( \int_{y \in B(x,2a_{N})} f(y) dy \right) f(x) dx.
\]

(106)

Notice that by Lemma 3, we know that

\[
|\int_{y \in B(x,2a_{N})} f(y) dy - f(x)c_{d}(2a_{N})dy| \leq C_{3}a_{N}^{d+2} \leq C_{3}a_{N}^{d},
\]

(107)

for some constant $C_{3} > 0$. So we have $\int_{y \in B(x,2a_{N})} f(y) dy \leq f(x)c_{d}(2a_{N})^{d} + C_{3}a_{N}^{d}$. Therefore, by plugging in $a_{N} = (\log(N)^{1+\delta}/N)^{1/d}$, we obtain that

\[
\int \left( \int_{y \in B(x,2a_{N})} f(y) dy \right) f(x) dx \leq \int \left( f(x)c_{d}(2a_{N})^{d} + C_{3}a_{N}^{d} \right) f(x) dx
\]

\[
\leq (C_{6}a_{N}^{2d} + C_{3}) \left( \log N \right)^{1+\delta} / N.
\]

(108)

Therefore, we know that the first term of (100) is upper bounded by $C_{4}(\log \log N)^{2}(\log N)^{1+\delta}/N$ for some $C_{4}$.

Now consider the case that $\|x-y\| > 2a_{N}$. Then the two balls $B(x,\rho_{k,1})$ and $B(y,\rho_{k,2})$ are disjoint since $\rho_{k,1} \leq a_{N}$. Therefore, consider the following joint distribution:

\[
F_{N,x,y}(u,v) = \mathbb{P}(e^{\xi_{1}(X)} < u, e^{\xi_{2}(X)} < v | X_{1} = x, X_{2} = y) = \mathbb{P}(\rho_{k,1} < r_{N}(u), \rho_{k,2} < r_{N}(v) | X_{1} = x, X_{2} = y)
\]

(109)
Therefore, the covariance can be written as:

\[
\int_{\|x-y\|>2aN} E \left[ (\xi_{k,1}(X) - E[\xi_{k,1}(X)]) (\xi_{k,2}(X) - E[\xi_{k,2}(X)]) \mid X_1 = x, X_2 = y \right] f(x)f(y)dx dy
\]

\[
= \int_{\|x-y\|>2aN} \left( \int_0^{bN} \int_0^{bN} \log u \log v f_{N,x,y}(u,v) du dv \right) - \left( \int_0^{bN} \log u f_{N,x}(u) du \right) \left( \int_0^{bN} \log v f_{N,y}(v) dv \right) f(x)f(y)dx dy
\]

\[
= \int_{\|x-y\|>2aN} \left( \int_0^{bN} \int_0^{bN} \log u \log v \left( f_{N,x,y}(u,v) - f_{N,x}(u) f_{N,y}(v) \right) du dv \right) f(x)f(y)dx dy
\]

\[
\leq \int_{\|x-y\|>2aN} \left( \int_0^{bN} \int_0^{bN} \left| \log u \log v \right| \left| f_{N,x,y}(u,v) - f_{N,x}(u) f_{N,y}(v) \right| du dv \right) f(x)f(y)dx dy.
\]

(110)

Here by the pdf of order statistic \[\text{[37]},\] the pdf of \(f_{N,x,y}(u,v)\) and \(f_{N,x}(u)\) and \(f_{N,y}(v)\) is given by:

\[
f_{N,x,y}(u,v) = \frac{(N-2)!}{(N-2k-2)!((k-1)!)^2} 2^{k-1} q^{k-1} (1 - p - q)^{N-2k-2} \frac{dp}{du} \frac{dq}{dv}, \quad (111)
\]

\[
f_{N,x}(u) = \frac{(N-2)!}{(N-k-2)!((k-1)!)^2} p^{k-1} (1 - p)^{N-k-1} \frac{dp}{du}, \quad (112)
\]

\[
f_{N,y}(v) = \frac{(N-2)!}{(N-k-2)!((k-1)!)^2} q^{k-1} (1 - q)^{N-k-1} \frac{dq}{dv}. \quad (113)
\]

where \(p = P(x, r_N(u)) = \int_{t \in B(x, r_N(u))} f(t) dt\) and \(q = P(y, r_N(v))\) for short. Since \(f(x) \leq C_a\) almost everywhere, we have

\[
p \leq Vol(B(x, r_N(u))) \left( \sup_{t \in B(x, r_N(u))} f(t) \right) = c_a r_N(u)^d \cdot C_a \leq \frac{2u C_a e^{\psi(k)}}{N}. \quad (114)
\]

\[
\frac{dp}{du} = \frac{dr_N(u)}{du} \frac{dr_N(u)}{du} \leq S(B(x, r_N(u))) \left( \sup_{t \in B(x, r_N(u))} f(t) \right) \frac{r_N(u)}{ud} \leq \frac{2C_a e^{\psi(k)}}{N}. \quad (115)
\]

Denote \(C_5 = 2C_a e^{\psi(k)}\) for short, then \(p \leq C_5 u/N\) and \(\frac{dp}{du} \leq C_5/N\). Similarly, \(q \leq C_5 v/N\) and \(\frac{dq}{dv} \leq C_5/N\). Then we can upper bound the difference of \(|f_{N,x,y}(u,v) - f_{N,x}(u) f_{N,y}(v)|\) by:

\[
\left| f_{N,x,y}(u,v) - f_{N,x}(u) f_{N,y}(v) \right| = \frac{1}{((k-1)!)^2} 2^{k-1} q^{k-1} \frac{(N-2)!}{(N-2k-2)!} (1 - p - q)^{N-2k-2} - \frac{(N-2)!}{(N-k-2)!} (1 - p)^{N-k-1} (1 - q)^{N-k-1} \left| \frac{dp}{du} \right| \frac{dq}{dv}
\]

\[
\leq \frac{1}{((k-1)!)^2} \frac{(C_5 u)^{k-1} (C_5 v)^{k-1} (C_5)^2}{N^{k-1}} \frac{(N-2)!}{(N-2k-2)!} (1 - p - q)^{N-2k-2} - \frac{(N-2)!}{(N-k-2)!} (1 - p)^{N-k-1} (1 - q)^{N-k-1} \left| \frac{dp}{du} \right| \frac{dq}{dv}
\]

\[
\leq \frac{1}{((k-1)!)^2} \frac{C_5^2 u^{k-1} v^{k-1}}{N^{2k}} (Q_1 + Q_2 + Q_3), \quad (116)
\]
where

\[
Q_1 = \frac{(N-2)!}{(N-2k-2)!} \left( (1-p-q)^{N-2k-2} - (1-p-q)^{N-k-1} \right),
\]

\[
Q_2 = \left| \frac{(N-2)!}{(N-k-2)!} \right|^2 \left| (1-p-q)^{N-k-1} \right|,
\]

\[
Q_3 = \left( \frac{(N-2)!}{(N-k-2)!} \right)^2 \left( (1-p)^{N-k-1} - (1-p-q)^{N-k-1} \right).
\]

We will bound the three terms separately. For \(Q_1\), notice that \((N-2)!/(N-2k-2)! \leq N^{2k}\) and

\[
(1-p-q)^{N-k-1} - (1-p-q)^{N-2k-2} \leq 1 - (1-p-q)^{k+1} \leq (k+1)(p+q) \leq \frac{(k+1)C_5(u+v)}{N}.
\]

So \(Q_1 \leq (k+1)C_5(u+v)N^{2k-1}\). For \(Q_2\), notice that both \((N-2)!/(N-2k-2)!\) and \((N-2)!/(N-k-2)!\) are polynomial of \(N\) with 2k order, moreover, the coefficient of \(N^{2k}\) are both 1. So they differs at most \(C_6N^{2k-1}\), where \(C_6\) is some constant relevant to \(k\). \((1-p-q)^{N-k-1}\) is simply upper bounded by 1. For \(Q_3\), notice that \((N-2)!/(N-k-2)!\) \(\leq N^{2k}\) and

\[
(1-p)^{N-k-1} - (1-p-q)^{N-k-1} - (1-p-q)^{N-k-1} - (1-p-q)^{N-k-1} \leq (N-k-1)pq(1-p-q) \leq Npq \leq \frac{C^2 uv}{N}.
\]

Therefore, \(Q_3 \leq C^2 uvN^{2k-1}\). Combine the upper bounds of \(Q_1, Q_2, Q_3\) into \((116)\), we obtain:

\[
\frac{1}{\((k-1)!)^2} C^2 u^{k-1} v^{k-1} N^{2k} (k+1)C_5(u+v)N^{2k-1} + C_6N^{2k-1} + C^2 uvN^{2k-1}
\]

\[
\leq \frac{C_7}{N} u^{k-1} v^{k-1} (1 + u + v + uv),
\]

for some \(C_7 > 0\). Plug this in \((116)\), we obtain:

\[
\int_{\|x-y\|>2aN} E \left[ \left( \xi_{k,1}(X) - E \left[ \xi_{k,1}(X) \right] \right) \left( \xi_{k,2}(X) - E \left[ \xi_{k,2}(X) \right] \right) \right] |X_1 = x, X_2 = y| f(x)f(y)dx\ dy
\]

\[
\leq \int_{\|x-y\|>2aN} \left( \int_0^{b_N} \int_0^{b_N} \log u \log v |f_{N,x,y}(u,v) - f_{N,x,y}(u,v)\,|\,dudv \right) f(x)f(y)\,dx\ dy
\]

\[
\leq \int_{\|x-y\|>2aN} \left( \frac{C_7}{N} \int_0^{b_N} \int_0^{b_N} |\log u \log v| \cdot u^{k-1} v^{k-1} (1 + u + v + uv)\,dudv \right) f(x)f(y)\,dx\ dy
\]

\[
\leq \int_{\|x-y\|>2aN} \left( \frac{C_7}{N} (\log b_N)^2 b^{2k+2}_N \right) f(x)f(y)\,dx\ dy
\]

\[
\leq \frac{C^2}{N} (\log b_N)^2 b^{2k+2}_N.
\]

By substituting \(b_N = (\log N)^{1+\delta}\), we obtain the desired claim.
C Proof of Theorem 3

The proof is based on the standard Le Cam’s method \[61\]. First we will prove the \(\Omega(1/N)\) lower bound. Consider two Gaussian distributions \(P = \mathcal{N}(0, I_d)\) and \(Q = \mathcal{N}(0, (1 + \delta)I_d)\). The norm of Hessian matrix of \(P\) and \(Q\) are both bounded, so \(P, Q \in \mathcal{F}_d\). Then we claim that: \(H(P) = d\log(2\pi e)/2\) and \(H(Q) = d\log(2\pi e)/2 + d\log(1 + \delta)/2\). Applying Le Cam’s method, the minimax lower bound is bounded by:

\[
\inf_{\hat{H}, f \in \mathcal{F}_d} \mathbb{E} \left[ \left( \hat{H}_n(X) - H(X) \right)^2 \right] \geq \frac{1}{2} \left( d\log(1 + \delta)/2 \right)^2 \left( 1 - \sqrt{2 - 2 \left( 1 - d_h(P, Q)^2 \right)^N} \right), \tag{124}
\]

where \(d_h(P, Q) = \int \left( \sqrt{p(x)} - \sqrt{q(x)} \right)^2 dx = 2 - \frac{1}{2} \int \sqrt{p(x)}q(x) dx\) is the Hellinger distance of \(P\) and \(Q\), and \(\|P - Q\|_{TV}\) is the total variation between \(P\) and \(Q\). We claim that \(d_h(P, Q)^2\) is bounded as:

\[
d_h(P, Q)^2 = O(d\delta^2). \tag{125}
\]

Therefore, by choose \(\delta = \Theta(\sqrt{1/dN})\) such that \(1 - \sqrt{2 - 2 \left( 1 - d_h(P, Q)^2 \right)^N} > 1/2\) the minimax lower bound is given by:

\[
\inf_{\hat{H}, f \in \mathcal{F}_d} \mathbb{E} \left[ \left( \hat{H}_n(X) - H(X) \right)^2 \right] \geq \frac{1}{4} \left( d\log(1 + \sqrt{1/dN})/2 \right)^2 = \Omega(d/N). \tag{126}
\]

We are now left to prove \(125\):

\[
dl_h(P, Q)^2 = 2 - 2 \int \sqrt{p(x)}q(x) dx
\]

\[
= 2 - 2 \int \frac{1}{(2\pi)^{d/2}} \exp \left\{ - \frac{x^2}{2} \right\} \frac{1}{(2\pi)^{d/2}(1 + \delta)^{d/2}} \exp \left\{ - \frac{x^2}{2(1 + \delta)} \right\} dx
\]

\[
= 2 - 2 \int \frac{1}{(2\pi)^{d/2}(1 + \delta)^{d/2}} \exp \left\{ - \frac{x^2}{2} \left( \frac{1 + \delta}{2 + \delta} \right) \right\} dx
\]

\[
= 2 - 2 \left( \frac{(2\pi)^{d/2} \left( \frac{1 + \delta}{2 + \delta} \right)^{d/2}}{(2\pi)^{d/2}(1 + \delta)^{d/4}} \right)
\]

\[
= 2 - 2 \left( \frac{1 + \delta}{(1 + \delta/2)^2} \right)^{d/4}
\]

\[
\leq 2 - 2 \left( 1 - \frac{d}{4} \cdot \frac{\delta^2/4}{(1 + \delta/2)^2} \right) \leq \frac{d\delta^2}{8}, \tag{127}
\]

where we use the fact that \((1 - x)^N \leq 1 - Nx\) for \(x \leq 1\) to obtain the inequality.

The proof of the \(\Omega(N^{-16/(d+8)})\) lower bound follows closely the proof of lower bound in \[29\]. We will use the following lemma, which is an extension of Lecam’s method:

**Lemma 8.** Let \(H\) be a functional defined on some class of functions \(\mathcal{F}\). We have \(u \in \mathcal{F}\) and \(v_\lambda \in \mathcal{F}\) for any \(\lambda\) in some finite index set \(\Lambda\). Define \(\bar{v}^N = \frac{1}{|\Lambda|} \sum_{\lambda \in \Lambda} v_\lambda^N\). If we have:

1. For any \(v_\lambda\), we have \(H(u) - H(v_\lambda) > \alpha\).
Then the minimax lower bound is given by:

\[
\inf_{\hat{H}} \sup_{f \in F} \mathbb{E} \left[ \left( \hat{H}(X) - H(X) \right)^2 \right] \geq K \cdot \alpha^2 (1 - \beta)
\]  

for some constant $K > 0$.

Now let $u$ be the uniform distribution over $[0,1]^d$. To construct the $v_\lambda$ functions, we partition the space $[0,1]^d$ to $m^d$ hypercubes denoted by $R_1, \ldots, R_{m^d}$. Let $t_j : R_j \to [0,1]^d$ maps the small hypercube $R_j$ to $[0,1]^d$. We pick a function $g$ supported on $[0,1]^d$ such that:

1. $\int_{[0,1]^d} g(x) dx = 0$
2. $\int_{[0,1]^d} g^2(x) dx = 1$
3. $g$ belongs to the smoothness class $\mathcal{F}_d$.

We define $u(x)$ to be the uniform distribution on $[0,1]^d$ and $v_\lambda$ by adding an appropriately chosen perturbation:

\[
v_\lambda(x) = u(x) + m^{-\gamma} \sum_{j=1}^{m^d} \lambda_j \mathbb{1}\{x \in R_j\} g(t_j(x))
\]  

for any $\lambda \in \Lambda = \{\pm 1\}^{m^d}$. Here we need $\gamma \geq 2$ to make sure that $v_\lambda \in \mathcal{F}_d$. We claim the following:

**Lemma 9.**

\[
H(u) - H(v_\lambda) \geq \frac{1}{3} m^{-2\gamma}, \forall \lambda \in \{\pm 1\}^{m^d}.
\]  

**Lemma 10.**

\[
\|u^N - \frac{1}{|\Lambda|} v_{\lambda^N}\|_{TV}^2 \leq O(N^2 m^{-d-4\gamma}).
\]  

Therefore, let $m = \Theta(N^{2/(d+4\gamma)})$ such that $\|u^N - \frac{1}{|\Lambda|} v_{\lambda^N}\|_{TV} \leq 1/2$, and by applying Lemma 8, we know that:

\[
\inf_{\hat{H}} \sup_{f \in \mathcal{F}_d} \mathbb{E} \left[ \left( \hat{H}(X) - H(X) \right)^2 \right] \geq \Omega(N^{-8\gamma/(d+4\gamma)}).
\]  

We obtain the minimax lower bound of $N^{-16/(d+8)}$ by plugging in $\gamma = 2$. 


C.1 Proof of Lemma 9

It is obvious that the entropy of uniform distribution is highest. So \( H(u) > H(v_\lambda) \). Their difference is given by:

\[
H(u) - H(v_\lambda) = -\int_{[0,1]^d} u(x) \log u(x) dx + \int_{[0,1]^d} v_\lambda(x) \log v_\lambda(x) dx
\]

\[
= \sum_{j=1}^{m^d} \int_{\mathcal{R}_j} v_\lambda(x) \log v_\lambda(x) dx
\]

\[
= \sum_{j=1}^{m^d} \int_{\mathcal{R}_j} \left( u(x) + m^{-\gamma} \lambda_j g(t_j(x)) \right) \log \left( u(x) + m^{-\gamma} \lambda_j g(t_j(x)) \right) dx
\]

\[
\geq \sum_{j=1}^{m^d} \int_{\mathcal{R}_j} \left( m^{-\gamma} \lambda_j g(t_j(x)) + \frac{1}{3} (m^{-\gamma} \lambda_j g(t_j(x)))^2 dx \right)
\]

\[
= m^{-\gamma} \sum_{j=1}^{m^d} \lambda_j \int_{\mathcal{R}_j} g(t_j(x)) dx + \frac{1}{3} m^{-2\gamma} \sum_{j=1}^{m^d} \lambda_j^2 \int_{\mathcal{R}_j} g^2(t_j(x)) dx
\]

\[
= \frac{1}{3} m^{-2\gamma} \sum_{j=1}^{m^d} m^{-d} = \frac{1}{3} m^{-2\gamma}.
\] (133)

Here the inequality comes from the fact that \( x \log x \geq (x - 1) + \frac{1}{3} (x - 1)^2 \) for \( x \in (0.5, 1.5) \).
C.2 Proof of Lemma 10

The proof uses the fact that \( \|p(x) - q(x)\|_{TV}^2 \leq \mathbb{E}_P[(\frac{q(x)}{p(x)})^2] - 1 \), which comes immediately from Cauchy-Schwarz inequality. So

\[
\mathbb{E}_{\lambda,u,N}[\left( \frac{\hat{v}^N(x)}{u(x)} \right)^2] = \mathbb{E}_{\lambda,u} \left[ \frac{1}{|\Lambda|^2} \sum_{\lambda,\mu \in \Lambda} \frac{v^N(x) v^N_\mu(x)}{(u^N(x))^2} \right] \\
= \frac{1}{|\Lambda|^2} \sum_{\lambda,\mu \in \Lambda} \mathbb{E}_{\lambda,u} \left[ \frac{v^N(x) v^N_\mu(x)}{(u^N(x))^2} \right] \\
= \frac{1}{|\Lambda|^2} \sum_{\lambda,\mu \in \Lambda} \left( \mathbb{E}_{\lambda,u} \left[ \frac{v^N(x) v^N_\mu(x)}{(u^N(x))^2} \right] \right)^N \\
= \frac{1}{|\Lambda|^2} \sum_{\lambda,\mu \in \Lambda} \left( \sum_{j=1}^{m^d} \int_{R_j} (1 + m^{-\gamma} \lambda_j g(t_j(x))(1 + m^{-\gamma} \mu_j g(t_j(x))) dx \right)^N \\
= \frac{1}{|\Lambda|^2} \sum_{\lambda,\mu \in \Lambda} \left( 1 + m^{-\gamma} \sum_{j=1}^{m^d} (\lambda_j + \mu_j) \int_{R_j} g(t_j(x)) dx + m^{-2\gamma} \sum_{j=1}^{m^d} \lambda_j \mu_j \int_{R_j} g^2(t_j(x)) dx \right)^N \\
= \frac{1}{|\Lambda|^2} \sum_{\lambda,\mu \in \Lambda} \left( 1 + m^{-d-2\gamma} \sum_{j=1}^{m^d} \lambda_j \mu_j \right)^N \\
\leq \frac{1}{|\Lambda|^2} \sum_{\lambda,\mu \in \Lambda} \exp \left\{ N m^{-d-2\gamma} \sum_{j=1}^{m^d} \lambda_j \mu_j \right\} \\
\leq \frac{1}{|\Lambda|^2} \sum_{\lambda,\mu \in \Lambda} \left( 1 + N m^{-d-2\gamma} \sum_{j=1}^{m^d} \lambda_j \mu_j + n^2 m^{-2d-4\gamma} \sum_{j=1}^{m^d} \lambda_j \mu_j \right)^2 \\
= 1 + N m^{-d-2\gamma} \sum_{j=1}^{m^d} \lambda_j \mu_j + N^2 m^{-2d-4\gamma} \sum_{j=1}^{m^d} \sum_{k=1}^{m^d} \lambda_j \mu_j \lambda_k \mu_k \\
= 1 + N^2 m^{-2d-4\gamma} \sum_{j=1}^{m^d} \sum_{\lambda_j, \mu_j \in \{\pm 1\}} \lambda_j^2 \mu_j^2 \\
= 1 + 4N^2 m^{-2d-4\gamma} \tag{134}
\]

where the first inequality comes from the fact that \( 1 + x \leq e^x \) and the second comes from \( e^x \leq 1 + x + x^2 \) for \( x \leq 2 \). Therefore, we have \( \|u^n - \frac{1}{|\Lambda|^2} v^N_\lambda \|_{TV}^2 \leq O(N^2 m^{-d-4\gamma}) \).

D Proof of Theorem 4

Note that

\[
\hat{I}_{KSG}(X;Y) = \hat{H}_{KSG}(X) + \hat{H}_{KSG}(Y) - \hat{H}_{KL} inf(X,Y) , \\
\hat{I}_{BI-KSG}(X;Y) = \hat{H}_{BI-KSG}(X) + \hat{H}_{BI-KSG}(Y) - \hat{H}_{KL} inf(X,Y) ,
\]

37
where
\[
\hat{H}_{KL,\infty}(X,Y) \equiv -\psi(k) + \log N + \log c_{d_x,\infty}c_{d_y,\infty} + (d_x + d_y) \log \rho_{k,i,\infty},
\]
\[
\hat{H}_{KSG}(X) \equiv -\frac{1}{N} \sum_{i=1}^{N} \psi(n_{x,i,\infty} + 1) + \log N + \log c_{d_x,\infty} + d_x \log \rho_{k,i,\infty},
\]
\[
\hat{H}_{KSG}(Y) \equiv -\frac{1}{N} \sum_{i=1}^{N} \psi(n_{y,i,\infty} + 1) + \log N + \log c_{d_y,\infty} + d_y \log \rho_{k,i,\infty},
\]
and
\[
\hat{H}_{KL,2}(X,Y) \equiv -\psi(k) + \log N + \log c_{d_x+d_y,2} + (d_x + d_y) \log \rho_{k,i,2},
\]
\[
\hat{H}_{BI-KSG}(X) \equiv -\frac{1}{N} \sum_{i=1}^{N} \log n_{x,i,2} + \log N + \log c_{d_x,2} + d_x \log \rho_{k,i,2},
\]
\[
\hat{H}_{BI-KSG}(Y) \equiv -\frac{1}{N} \sum_{i=1}^{N} \log n_{y,i,2} + \log N + \log c_{d_y,2} + d_y \log \rho_{k,i,2}.
\]

We prove the following technical lemma that shows the convergence of the marginal entropy estimate (136) and (139). The convergence of (137) and (140) is immediate by interchanging X and Y. The convergence in probability of the joint entropy estimate (135) and (138) are known from [28]. This proves the desired claim.

**Lemma 11.** Under the hypotheses of Theorem 5, the estimated marginal entropy converges to the true entropy, i.e. for all \( \varepsilon > 0 \)
\[
\lim_{N \to \infty} P \left( \left| \hat{H}_{KSG}(X) - H(X) \right| > \varepsilon \right) = 0,
\]
\[
\lim_{N \to \infty} P \left( \left| \hat{H}_{BI-KSG}(X) - H(X) \right| > \varepsilon \right) = 0.
\]

**D.1 Proof of Lemma 11**

Define
\[
\hat{f}^{KSG}_X(X_i) \equiv \frac{\exp\{\psi(n_{x,i,\infty} + 1)\}}{Nc_{d_x,\infty}\rho^{d_x}_{k,i,\infty}},
\]
and
\[
\hat{f}^{BI-KSG}_X(X_i) \equiv \frac{n_{x,i,2}}{Nc_{d_x,2}\rho^{d_x}_{k,i,2}},
\]
such that \( \hat{H}_{KSG}(X) = -\frac{1}{N} \sum_{i=1}^{N} \log \hat{f}^{KSG}_X(X_i) \) and \( \hat{H}_{BI-KSG}(X) = -\frac{1}{N} \sum_{i=1}^{N} \log \hat{f}^{KSG}_X(X_i) \). From now on we will skip the subscript KSG or BI-KSG and the subscript 2 or \( \infty \) if the formula holds for both. We will
specify it whenever necessary. Now we write \(|\hat{H}(X) - H(X)|\) as:

\[
\begin{align*}
|\hat{H}(X) - H(X)| &= \left| -\frac{1}{N} \sum_{i=1}^{N} \log \hat{f}_X(X_i) - \left( -\int f_X(x) \log f_X(x) dx \right) \right| \\
&\leq \left| \frac{1}{N} \sum_{i=1}^{N} \log f_X(X_i) - \int f_X(x) \log f_X(x) dx \right| + \frac{1}{N} \sum_{i=1}^{N} \log \hat{f}_X(X_i) - \log f_X(X_i) \right|.
\end{align*}
\]

(145)

The first term is the error from the empirical mean. Notice that \(\log f_X(X_i)\) are i.i.d. random variables, satisfying

\[
\mathbb{E} |\log f_X(X_i)| = \int f_X(x) |\log f_X(x)| dx < +\infty
\]

(146)

where the mean is given by:

\[
\mathbb{E} (\log f_X(X_i)) = \int f_X(x) \log f_X(x) dx.
\]

(147)

Therefore, by weak law of large numbers, we have:

\[
\lim_{N \to \infty} P \left( \left| \frac{1}{N} \sum_{i=1}^{N} \log f_X(X_i) - \int f_X(x) \log f_X(x) dx \right| > \varepsilon \right) = 0
\]

(148)

for any \(\varepsilon > 0\).

The second term comes from density estimation. We denote \(Z = (X, Y)\) and \(f(z) = f(x, y)\) for short, then for any fixed \(\varepsilon > 0\), we obtain:

\[
\begin{align*}
\mathbb{P} \left( \frac{1}{N} \sum_{i=1}^{N} |\log \hat{f}_X(X_i) - \log f_X(X_i)| > \varepsilon \right) &\leq \mathbb{P} \left( \bigcup_{i=1}^{N} \{ |\log \hat{f}_X(X_i) - \log f_X(X_i)| > \varepsilon \} \right) \\
&\leq N \cdot \mathbb{P} \left( |\log \hat{f}_X(X_i) - \log f_X(X_i)| > \varepsilon \right) \\
&= N \int \mathbb{P} \left( \frac{|\log \hat{f}_X(X_i) - \log f_X(X_i)|}{\varepsilon} > \frac{1}{\varepsilon} \right) f(z) dz
\end{align*}
\]

(149)

where

\[
I_1(z) = \mathbb{P} \left( \rho_{k,i} > \log N(Nf(z)c_{d_x+d_y})^{-\frac{1}{c_{d_x+d_y}}} |Z_i = z\right)
\]

(150)

\[
I_2(z) = \mathbb{P} \left( \rho_{k,i} < (\log N)^2(Nf_X(x)c_{d_x})^{-\frac{1}{d_x}} |Z_i = z = (x,y) \right)
\]

(151)

\[
I_3(z) = \int_{r=(\log N)^2(Nf_X(x)c_{d_x})^{-\frac{1}{d_x}}} \mathbb{P} \left( |\log \hat{f}_X(X_i) - \log f_X(X_i)| > \varepsilon |\rho_{k,i} = r, Z_i = z\right) f_{\rho_{k,i}}(r) dP
\]

(152)

where \(f_{\rho_{k,i}}(r)\) is the pdf of \(\rho_{k,i}\) given \(Z_i = z\). We will consider the three terms separately, and show that each is bounded by \(o(N^{-1})\).
$I_1$: Let $B_Z(z, r) = \{Z : \|Z - z\| < r\}$ be the $(d_x + d_y)$-dimensional ball centered at $z$ with radius $r$. Since the Hessian matrix of $H(f)$ exists and $\|H(f)\| < C$ almost everywhere, then for sufficiently small $r$, there exists $z'$ such that

$$
P(u \in B_Z(z, r)) = \int_{\|u - z\| \leq r} f(u)du
$$

$$
\geq \int_{\|u - z\| \leq r} f(z) + (u - z)^T \nabla f(z) + (u - z)^T H_f(z')(u - z)du
$$

$$
\geq \left[ f(z)c_{d_x + d_y}r_{d_x + d_y}(1 - C r^2), f(z)c_{d_x + d_y}r_{d_x + d_y}(1 + C r^2) \right].
$$

Then for sufficiently large $N$,

$$
p_1 = P\left( u \in B_Z(z, \log N(f(z)c_{d_x + d_y})^{-\frac{1}{\|z\| + r}}) \right)
$$

$$
\geq f(z)c_{d_x + d_y}\left( \log N(f(z)c_{d_x + d_y})^{-\frac{1}{\|z\| + r}} \right)^{d_x + d_y}\left( 1 - C(\log N(f(z)c_{d_x + d_y})^{-\frac{1}{\|z\| + r}})^2 \right)
$$

$$
\geq \frac{(\log N)^{d_x + d_y}}{2N}
$$

Therefore, $I_1(z)$ is upper bounded by:

$$
I_1(z) = P\left( \rho_{k,i} > \log N(f(z)c_{d_x + d_y})^{-\frac{1}{\|z\| + r}} \mid Z_i = z \right)
$$

$$
= \sum_{m=0}^{k-1} \binom{N}{m} p_1^m (1 - p_1)^{N-1-m}
$$

$$
\leq \sum_{m=0}^{k-1} N^m (1 - p_1)^{N-1-m}
$$

$$
\leq kN^{k-1}(1 - \frac{(\log N)^{d_x + d_y}}{2N})^{N-k-1}
$$

$$
\leq kN^{k-1} \exp\left\{ -\frac{(\log N)^{d_x + d_y}(N-k-1)}{2N} \right\}
$$

$$
\leq kN^{k-1} \exp\left\{ -\frac{(\log N)^{d_x + d_y}}{4} \right\}
$$

for any $d_x, d_y \geq 1$.

$I_2$: For sufficiently large $N$, we have

$$
p_2 = P\left( u \in B_Z(z, (\log N)^2(f(x)c_{d_x})^{-\frac{1}{\|x\|}}) \right)
$$

$$
\leq f(z)c_{d_x + d_y}\left( \log N \right)^2(f(x)c_{d_x})^{-\frac{1}{\|x\|}} \left( 1 + C(\log N(f(x)c_{d_x})^{-\frac{1}{\|x\|}})^2 \right)
$$

$$
\leq \frac{2f(z)c_{d_x + d_y}(\log N)^2(d_x + d_y)N^{-\frac{d_x + d_y}{d_x}}}{(f(x)c_{d_x})^{-\frac{1}{\|x\|}}} \left( \log N \right)^2(d_x + d_y)N^{-\frac{d_x + d_y}{d_x}}
$$

$$
\leq 2f_N(y|x) \frac{c_{d_x + d_y}d_x}{c_{d_x}} (\log N)^2(d_x + d_y)N^{-\frac{d_x + d_y}{d_x}}
$$

$$
\leq 2C(c_{d_x + d_y}d_x) (\log N)^2(d_x + d_y)N^{-\frac{d_x + d_y}{d_x}}.
$$


$I_2$ is upper bounded by:

\[
I_2(z) = \mathbb{P}\left( \rho_{k,i} < \log N(Nf_X(x)c_{d_x})^{-\frac{1}{m}} | Z_i = z \right)
\]

\[
= \sum_{m=k}^{N-1} \binom{N-1}{m} p_2^m (1 - p_2)^N - 1 - m
\]

\[
\leq \sum_{m=k}^{N-1} N^m p_2^m
\]

\[
\leq \sum_{m=k}^{N-1} (2C e^{c_{d_x+d_y}} (\log N)^{2(d_x+d_y)} N^{-\frac{d_y}{m^2}})^m
\]

\[
\leq (4C e^{c_{d_x+d_y}})^k (\log N)^{2K(d_x+d_y)} N^{-\frac{k d_y}{m^2}},
\]

for any $d_x, d_y \geq 1$ and $k \geq 1$.

$I_3$: Now we will consider KSG and BI-KSG separately. Also we need to specify whether we are considering $\ell_2$ or $\ell_\infty$ norm. For KSG, given that $Z_i = z = (x, y)$ and $\rho_{k,i,\infty} = r$, we have:

\[
\mathbb{P}\left( \log \hat{f}_\chi^{KS}(X_i) - \log f_X(X_i) > \varepsilon | \rho_{k,i,\infty} = r, Z_i = z \right)
\]

\[
= \mathbb{P}\left( |\psi(n_{x,i,\infty} + 1) - \log N - \log c_{d_x,\infty} - d_x \log \rho_{k,i,\infty} - \log f_X(x) | > \varepsilon | \rho_{k,i,\infty} = r, Z_i = z \right).
\]

Notice that for any integer $x \geq 2$, we have $\log(x-1) < \psi(x) < \log(x)$. Therefore

\[
\mathbb{P}\left( \psi(n_{x,i,\infty} + 1) - \log N - \log c_{d_x,\infty} - d_x \log \rho_{k,i,\infty} - \log f_X(x) < -\varepsilon | \rho_{k,i,\infty} = r, Z_i = z \right)
\]

\[
\leq \mathbb{P}\left( \log n_{x,i,\infty} - \log N - \log c_{d_x,\infty} - d_x \log \rho_{k,i,\infty} - \log f_X(x) < -\varepsilon | \rho_{k,i,\infty} = r, Z_i = z \right)
\]

\[
= \mathbb{P}\left( n_{x,i,\infty} < N c_{d_x,\infty} r^{d_y} f_X(x) e^{-\varepsilon} | \rho_{k,i,\infty} = r, Z_i = z \right).
\]

In the other direction,

\[
\mathbb{P}\left( \psi(n_{x,i,\infty} + 1) - \log N - \log c_{d_x,\infty} - d_x \log \rho_{k,i,\infty} - \log f_X(x) > \varepsilon | \rho_{k,i,\infty} = r, Z_i = z \right)
\]

\[
\leq \mathbb{P}\left( \log n_{x,i,\infty} + 1 - \log N - \log c_{d_x,\infty} - d_x \log \rho_{k,i,\infty} - \log f_X(x) > \varepsilon | \rho_{k,i,\infty} = r, Z_i = z \right)
\]

\[
= \mathbb{P}\left( n_{x,i,\infty} > N c_{d_x,\infty} r^{d_y} f_X(x) e^\varepsilon - 1 | \rho_{k,i,\infty} = r, Z_i = z \right).
\]

For BI-KSG, we have:

\[
\mathbb{P}\left( \log \hat{f}_\chi^{BI-KSG}(X_i) - \log f_X(X_i) > \varepsilon | \rho_{k,i,2} = r, Z_i = z \right)
\]

\[
= \mathbb{P}\left( |\log n_{x,i,2} - \log N - \log c_{d_x,2} - d_x \log \rho_{k,i,2} - \log f_X(x) | > \varepsilon | \rho_{k,i,2} = r, Z_i = z \right)
\]

\[
= \mathbb{P}\left( |\log n_{x,i,2} - \log N c_{d_x,2} r^{d_y} f_X(x) | > \varepsilon | \rho_{k,i,2} = r, Z_i = z \right)
\]

\[
= \mathbb{P}\left( n_{x,i,2} > N c_{d_x,2} r^{d_y} f_X(x) e^\varepsilon | \rho_{k,i,2} = r, Z_i = z \right)
\]

\[
+ \mathbb{P}\left( n_{x,i,2} < N c_{d_x,2} r^{d_y} f_X(x) e^{-\varepsilon} | \rho_{k,i,2} = r, Z_i = z \right).
\]
Combine them together, we have:

\[
\mathbb{P}\left( \left| \log \hat{f}_X(X_i) - \log f_X(X_i) \right| > \varepsilon \mid \rho_{k,i} = r, Z_i = z \right) \\
\leq \mathbb{P} \left( n_{x,i} < N \alpha \varepsilon f_X(x) e^{-\varepsilon} \mid \rho_{k,i} = r, Z_i = z \right) \\
+ \mathbb{P} \left( n_{x,i} > N \alpha \varepsilon f_X(x) e^{\varepsilon} - 1 \mid \rho_{k,i} = r, Z_i = z \right). 
\] (162)

holds for both KSG and BI-KSG estimates. Recall that in Theorem 5 given that \( \rho_{k,i} = r \) and \( Z_i = z \), \( n_{x,i} - k \) is distributed as \( \sum_{l=k+1}^{N-1} U_i \), where \( U_i \) are i.i.d Bernoulli random variables with mean \( p \) satisfying

\[
r^{-d_x} \left| p - f_X(x) c_d x r^{d_x} \right| \leq C_1 (r^2 + r^{d_v}). 
\] (164)

For small enough \( r \) such that \( C_1 (r^2 + r^{d_v}) \leq \varepsilon / 2 \), we obtain

\[
\mathbb{P} \left( n_{x,i} > (N - 1) c_d x r^{d_x} f_X(x) e^{\varepsilon} - 1 \mid \rho_{k,i} = r, Z_i = z \right) \\
= \mathbb{P} \left( \sum_{l=k+1}^{N-1} U_i > (N - 1) c_d x r^{d_x} f_X(x) e^{\varepsilon} - k - 1 \right) \\
= \mathbb{P} \left( \sum_{l=k+1}^{N-1} U_i - (N - k - 1) \mathbb{E}[U_i] > (N - 1) c_d x r^{d_x} f_X(x) e^{\varepsilon} - k - 1 - (N - k - 1) \mathbb{E}[U_i] \right), 
\] (165)

and the right-hand side in the probability is lower bounded by

\[
N \alpha \varepsilon f_X(x) e^{\varepsilon} - k - 1 - (N - k - 1) \mathbb{E}[U_i] \\
\geq N \alpha \varepsilon f_X(x) e^{\varepsilon} - k - 1 - (N - k - 1) f_X(x) c_d x r^{d_x} (1 + \varepsilon / 2) \\
\geq (N - k - 1) c_d x r^{d_x} f_X(x) (e^{\varepsilon} - 1 - \varepsilon / 2) - k - 1 \\
\geq (N - k - 1) c_d x r^{d_x} f_X(x) \varepsilon / 4 
\] (166)

for sufficiently large \( N \) such that \( (N - k - 1) c_d x r^{d_x} f_X(x) (e^{\varepsilon} - 1 - \varepsilon / 4) > k + 1 \). Since \( U_i \) is Bernoulli, we have \( \mathbb{E}[U_i^2] = \mathbb{E}[U_i] \). Now applying Bernstein’s inequality, [166] is upper bounded by:

\[
\mathbb{P} \left( \sum_{l=k+1}^{N-1} U_i - (N - k - 1) \mathbb{E}[U_i] > (N - 1) c_d x r^{d_x} f_X(x) e^{\varepsilon} - k - (N - k - 1) \mathbb{E}[U_i] \right) \\
\leq \exp \left\{ - \frac{(N - k - 1) c_d x r^{d_x} f_X(x) \varepsilon / 4)^2}{2 \left( (N - k - 1) \mathbb{E}[U_i^2] + \frac{1}{3} ((N - k - 1) c_d x r^{d_x} f_X(x) \varepsilon / 4)) \right) \right\} \\
\leq \exp \left\{ - \frac{(N - k - 1) c_d x r^{d_x} f_X(x) \varepsilon / 4)^2}{2 \left( (N - k - 1) c_d x r^{d_x} f_X(x) (1 + \varepsilon / 2) + \frac{1}{3} ((N - k - 1) c_d x r^{d_x} f_X(x) \varepsilon / 4)) \right) \right\} \\
= \exp \left\{ - \frac{\varepsilon^2}{32(1 + 7\varepsilon / 12)} (N - k - 1) c_d x r^{d_x} f_X(x) \right\}. 
\] (167)
Similarly, the tail bound on the other way is given by:

\[
\mathbb{P} \left( n_{x, \ell} < Nc_d, r^{d_x} f_X(x)e^{-\varepsilon} \mid \rho_{k, \ell} = r, Z_i = z \right) = \mathbb{P} \left( \sum_{i=k+1}^{N-1} U_i < Nc_d, r^{d_x} f_X(x)e^{-\varepsilon} - k \right) = \mathbb{P} \left( \sum_{i=k+1}^{N-1} U_i - (N - k - 1)\mathbb{E}[U_i] < Nc_d, r^{d_x} f_X(x)e^{-\varepsilon} - k - (N - k - 1)\mathbb{E}[U_i] \right),
\]

(168)

and the right hand side in the probability is upper bounded by

\[
Nc_d, r^{d_x} f_X(x)e^{-\varepsilon} - k - (N - k - 1)\mathbb{E}[U_i] \\
\leq Nc_d, r^{d_x} f_X(x)e^{-\varepsilon} - k - (N - k - 1)f_X(x)c_d, r^{d_x}(1 - \varepsilon/2) \\
\leq (N - k - 1)c_d, r^{d_x} f_X(x)e^{-\varepsilon} - (N - k - 1)f_X(x)c_d, r^{d_x}(1 - \varepsilon/2) \\
= (N - k - 1)c_d, r^{d_x} f_X(x) \left( e^{-\varepsilon} - 1 + \varepsilon/2 \right) \\
\leq -(N - k - 1)c_d, r^{d_x} f_X(x)e^{\varepsilon/4}
\]

(169)

for sufficiently small \( r \) such that \((k + 1)c_d, r^{d_x} f_X(x)e^{-\varepsilon} \leq k \) and sufficiently small \( \varepsilon \) such that \( e^{-\varepsilon} - 1 + \varepsilon/2 \leq -\varepsilon/4 \). Similarly, by applying Bernstein’s inequality, (168) is upper bounded by:

\[
\mathbb{P} \left( \sum_{i=k+1}^{N-1} U_i - (N - k - 1)\mathbb{E}[U_i] < Nc_d, r^{d_x} f_X(x)e^{-\varepsilon} - k - (N - k - 1)\mathbb{E}[U_i] \right) \\
\leq \mathbb{P} \left( \sum_{i=k+1}^{N-1} U_i - (N - k - 1)\mathbb{E}[U_i] > -(N - k - 1)c_d, r^{d_x} f_X(x)e^{\varepsilon/4} \right) \\
\leq \exp \left\{ - \frac{((N - k - 1)c_d, r^{d_x} f_X(x)e^{\varepsilon/4})^2}{2 \left( (N - k - 1)\mathbb{E}[U_i]^2 + \frac{3}{4}((N - k - 1)c_d, r^{d_x} f_X(x)e^{\varepsilon/4}) \right) } \right\} \\
\leq \exp \left\{ - \frac{((N - k - 1)c_d, r^{d_x} f_X(x)e^{\varepsilon/4})^2}{2 \left( (N - k - 1)c_d, r^{d_x} f_X(x)(1 + \varepsilon/2) + \frac{3}{4}((N - k - 1)c_d, r^{d_x} f_X(x)e^{\varepsilon/4}) \right)} \right\} \\
= \exp \left\{ - \frac{\varepsilon^2}{32(1 + 7\varepsilon/12)}(N - k - 1)c_d, r^{d_x} f_X(x) \right\}.
\]

(170)

Therefore, \( I_3(z) \) is upper bounded by:

\[
I_3(z) = \int_{r = (\log N)^2(N f_X(x)c_{d_x})^{-\frac{1}{2d_x}}}^{\log N(N f(z)c_{d_x} + d_y)^{-\frac{1}{2d_x}}} \mathbb{P} \left( \left| \log f_X(X_i) - \log f_X(X_i) \right| > \varepsilon \mid \rho_{k, i} = r, Z_i = z \right) f_{\rho_{k, i}}(r) dr \\
\leq 2 \exp \left\{ - \frac{\varepsilon^2}{32(1 + 7\varepsilon/12)} (N - k - 1)c_d, r^{d_x} f_X(x) \right\} f_{\rho_{k, i}}(r) dr \\
\leq 2 \exp \left\{ - \frac{\varepsilon^2}{64} Nc_d, f_X(x)((\log N)^2(N f_X(x)c_{d_x})^{-\frac{1}{2d_x}})^{d_x} \right\} \\
\leq 2 \exp \left\{ - \frac{\varepsilon^2}{64} (\log N)^{2d_x} \right\}
\]

(171)

for sufficiently large \( N \) such that \((N - k - 1)/(1 + \frac{7}{12} \varepsilon) > N/2 \) and any \( d_x \geq 1 \). The upper bounds of \( I_1(z), I_2(z) \) and \( I_3(z) \) are all independent of \( z \). Therefore, combine the upper bounds of \( I_1(z), I_2(z) \) and \( I_3(z) \), we
obtain
\[ \mathbb{P}\left( \frac{1}{N} \sum_{i=1}^{N} \left| \log \hat{f}_X(X_i) - \log f_X(X_i) \right| > \varepsilon \right) \]
\[ \leq N \int (I_1(z) + I_2(z) + I_3(z)) f(z) dz \]
\[ = kN^k \exp \left\{ - \frac{\log N d + d_y}{4} \right\} + \left( 4C_{d_x+d_y} \right)^k \left( \log N \right)^{2k(d_x+d_y)} N^{1 - \frac{k d_y}{64} + 2N \exp \left\{ - \frac{\varepsilon^2}{64} \left( \log N \right)^{2d_x} \right\}}. \]

If \( k > d_y/d_x \) as per our assumption, each of the three terms goes to 0 as \( N \to \infty \).
Therefore
\[ \lim_{N \to \infty} \mathbb{P}\left( \frac{1}{N} \sum_{i=1}^{N} \left| \log \hat{f}_X(X_i) - \log f_X(X_i) \right| > \varepsilon \right) = 0 \]  \hspace{1cm} (172)

Therefore, by combining the convergence of error from sampling and error from density estimation, we obtain that \( \tilde{H}(X) \) converges to \( H(X) \) in probability.

### E Proof of Theorem 5

We will introduce some notations first. Let \( Z = (X, Y) \), \( f(x) = f(x, y) \) and \( d = d_x + d_y \) for short. Let \( B(z, r) \) denote the \( d \)-dimensional ball centered at \( z \) with radius \( r \), \( B_X(x, r) \) denote the \( d_x \)-dimensional ball (on \( X \) space) centered at \( x \) with radius \( r \). \( P(z, r) \) denotes the probability mass inside \( B(z, r) \), i.e., \( P(z, r) = \int_{B(z, r)} f(t) dt \). Similarly, \( P_X(x, r) = \int_{B_X(x, r)} f_X(t) dt \) denotes the probability mass inside \( B_X(z, r) \).

Now note that if \( \rho_{k,i} \leq a_N \), we can write \( \iota_{k,i,2} \) and \( \iota_{k,i,\infty} \) as:
\[ \iota_{k,i,\infty} = \xi_{k,i,\infty}(X) + \xi_{k,i,\infty}(Y) - \xi_{k,i,\infty}(Z) \]
\[ \iota_{k,i,2} = \xi_{k,i,2}(X) + \xi_{k,i,2}(Y) - \xi_{k,i,2}(Z) , \]
where
\[ \xi_{k,i,\infty}(Z) \equiv -\psi(k) + \log N + \log c_{d_x,\infty} c_{d_y,\infty} + d \log \rho_{k,i,\infty} , \]  \hspace{1cm} (173)
\[ \xi_{k,i,\infty}(X) \equiv -\psi(n_{x,i,\infty} + 1) + \log N + \log c_{d_x,\infty} + d_x \log \rho_{k,i,\infty} , \]  \hspace{1cm} (174)
\[ \xi_{k,i,\infty}(Y) \equiv -\psi(n_{y,i,\infty} + 1) + \log N + \log c_{d_y,\infty} + d_y \log \rho_{k,i,\infty} . \]  \hspace{1cm} (175)

and
\[ \xi_{k,i,2}(Z) \equiv -\psi(k) + \log N + \log c_{d_x,2} + d \log \rho_{k,i,2} , \]  \hspace{1cm} (176)
\[ \xi_{k,i,2}(X) \equiv -\log(n_{x,i,2}) + \log N + \log c_{d_x,2} + d_x \log \rho_{k,i,2} , \]  \hspace{1cm} (177)
\[ \xi_{k,i,2}(Y) \equiv -\log(n_{y,i,2}) + \log N + \log c_{d_y,2} + d_y \log \rho_{k,i,2} . \]  \hspace{1cm} (178)

If \( \rho_{k,i} > a_N \), just define \( \xi_{k,i,\infty}(X) = \xi_{k,i,\infty}(Y) = \xi_{k,i,\infty}(Z) = 0 \). Similar as the proof of Theorem 4, we drop the superscript KSG or BI-KSG and subscript 2 and \( \infty \) for statements that holds for both. Since \( \iota_{k,i} \)'s are identically distributed, we have \( \mathbb{E}[\tilde{I}(X; Y)] = \mathbb{E}[\iota_{k,1}] \). By triangular inequality, the bias of \( \tilde{I}(X; Y) \) can be
written as:

\[
\begin{align*}
\mathbb{E} \left[ \tilde{f}(X;Y) \right] - I(X;Y) \\
= \mathbb{E} [\hat{f}_{k,1}] - I(X;Y) \\
\leq |\mathbb{E} [\xi_{k,1}(X)] - H(X)| + |\mathbb{E} [\xi_{k,1} - H(Y)]| + |\mathbb{E} [\xi_{k,1}(Z)] - H(Z)| \\
\leq |\mathbb{E} [(\xi_{k,1}(X) - H(X)) \cdot \mathbb{I}\{\rho_{k,1} \leq a_N\}]| + |\mathbb{E} [(\xi_{k,1}(X) - H(X)) \cdot \mathbb{I}\{\rho_{k,1} > a_N\}]| \\
+ |\mathbb{E} [(\xi_{k,1}(Y) - H(Y)) \cdot \mathbb{I}\{\rho_{k,1} \leq a_N\}]| + |\mathbb{E} [(\xi_{k,1}(Y) - H(Y)) \cdot \mathbb{I}\{\rho_{k,1} > a_N\}]| \\
+ |\mathbb{E} [\xi_{k,1}(Z) \cdot \mathbb{I}\{\rho_{k,1} \leq a_N\} - H(Z)]| + |\mathbb{E} [\xi_{k,1}(Z) \cdot \mathbb{I}\{\rho_{k,1} > a_N\}]|
\end{align*}
\]

(179)

The probability that \( \rho_{k,i} > a_N \) is bounded by the following lemma:

**Lemma 12.** Under the Assumption (c) and (d), we have:

\[
\mathbb{P}(\rho_{k,i} > a_N) \leq CN^{k-1} \exp\{-C(\log N)^{1+\delta}\}. \tag{180}
\]

Note \( N^{k-1} \exp\{-C(\log N)^{1+\delta}\} \) decays faster than \( 1/N^c \) for any constant \( c \).

Now we consider the bias of \( \xi_{k,1}(X) \) and \( \xi_{k,1}(Y) \) when \( \rho_{k,i} \leq a_N \). \( \xi_{k,1}(Z) \) is local \( d \)-dimensional Kozachenko-Leonenko entropy estimator \([26]\). Therefore, by Theorem 1, we obtain:

\[
\mathbb{E} [\xi_{k,1}(Z) \cdot \mathbb{I}\{\rho_{k,1} \leq a_N\}] - H(Z) \leq O \left( \frac{\log N}{N^{2/d}} \right), \tag{181}
\]

The following lemma establishes the convergence rate for marginal entropy estimator \( \xi_{k,1}(X) \).

**Lemma 13.** Under the Assumption (c) – (e), the bias of marginal entropy estimator \( \xi_{k,1}(X) \) is given by:

\[
\mathbb{E} \left[ (\xi_{k,1}(X) - H(X)) \cdot \mathbb{I}\{\rho_{k,1} \leq a_N\} \right] = O \left( \frac{\log N}{N^{2/d}} \right), \tag{182}
\]

for \( k \geq d_x/d_y \).

Convergence rate of \( \xi_{k,1}(Y) \) is immediate by exchanging \( X \) and \( Y \) and \( k \geq d_x/d_y \). Combining Theorem 1, Lemma 13 and Lemma 12, we obtain the desired statement.

**E.1 Proof of Lemma 12**

For \( Z_1 = z \), the kNN distance is larger than \( a_N \), i.e. \( \rho_{k,1} > a_N \) when at most \( k-1 \) samples are in \( B(z, a_N) \), which gives

\[
\mathbb{P}(\rho_{k,1} > a_N \mid Z_1 = z) = \frac{1}{m} \binom{N-1}{m} P(z, a_N)^m (1 - P(z, a_N))^{N-1-m}. \tag{183}
\]

Assuming \( f \) is twice continuously differentiable as per Assumption (d) and \( a_N \) vanishes as \( N \) grows, \( f(z)Vol(B(z, a_N)) \) approaches \( P(z, a_N) \). Precisely, by Lemma 4 for sufficiently large \( N \), we have \( P(z, a_N) \geq
Define \( f(z)c_d a_N^k - C_d a_N^{k+2} \). This provide the following upper bound:

\[
\mathbb{P}( \rho_{k,1} > a_N \mid Z_1 = z ) = \sum_{m=0}^{k-1} \binom{N-1}{m} P(z,a_N)^m (1 - P(z,a_N))^{N-1-m} \leq \sum_{m=0}^{k-1} N^m (1 - P(z,a_N))^{N-1-m} \leq kN^{k-1}(1 - P(z,a_N))^{N-k-1} \leq kN^{k-1} \exp\{-(N-k-1)P(z,a_N)\} \leq kN^{k-1} \exp\{-(N-k-1)f(z)c_d a_N^k + (N-k-1)C_d a_N^{k+2}\} \leq kN^{k-1} \exp\{-Cf(z)(\log(N))^{1+\delta}\} \exp\{\log(N)^{(1+\delta)(1+2/d)} / N^{2/d}\} \leq keN^{k-1} \exp\{-Cf(z)(\log(N))^{1+\delta}\}. \tag{184}
\]

The last inequality comes from the fact that \( \log(N)^{(1+\delta)(1+2/d)} / N^{2/d} < 1 \) for sufficiently large \( N \) and \( s \geq 1 \). Taking the expectation over \( Z_1 \),

\[
\mathbb{P}( \rho_{k,1} > a_N ) = \int f(z) \mathbb{P}( \rho_{k,i} > a_N \mid Z_i = z ) \, dz \leq keN^{k-1} \int f(z) \exp\{-Cf(z)(\log(N))^{1+\delta}\} \, dz \leq keCk N^{k-1} \exp\{-CC_0(\log(N))^{1+\delta}\}, \tag{185}
\]

where the last inequality comes from Assumption 3(c).

### E.2 Proof of Lemma 13

Define \( r_N = (\log N)^2 N^{-1/d_x} \), we can split the bias of \( \xi_{k,i}(X) \) into two parts:

\[
|\mathbb{E}[ (\xi_{k,1}(X) - H(X)) \cdot I\{\rho_{k,1} \leq a_N\}] | \leq |\mathbb{E}[ (\xi_{k,1}(X) - H(X)) \cdot I\{\rho_{k,1} < r_N\}] | + |\mathbb{E}[ (\xi_{k,1}(X) - H(X)) \cdot I\{r_N \leq \rho_{k,1} \leq a_N\}] |, \tag{186}
\]

If \( \rho_{k,1} < r_N \), recall that \( \xi_{k,1}(X) = -h(n_{x,1}) + \log c_d + \log N + d_x \log \rho_{k,1} \), where \( h(x) = \log(x) \) or \( \psi(x+1) \). Notice that \( k < n_{x,1} < N \), so \( 0 \leq h(n_{x,1}) \leq 2 \log N \). Therefore, we can bound the first term of (186) by:

\[
\mathbb{E}[ (\xi_{k,1}(X) - H(X)) \cdot I\{\rho_{k,1} < r_N\}] \leq \mathbb{E}[ (\log N + \log c_d + d_x \log \rho_{k,1} - H(X)) \cdot I\{\rho_{k,1} < r_N\}] \leq (\log N + \log c_d - H(X)) \mathbb{P}(\rho_{k,1} < r_N) + d_x \int_0^{r_N} \log r f_{\rho_{k,1}}(r) \, dr, \tag{187}
\]

where \( f_{\rho_{k,1}}(r) \) is the pdf of \( \rho_{k,1} \). Similarly, it can be lower bouded by:

\[
\mathbb{E}[ (\xi_{k,1}(X) - H(X)) \cdot I\{\rho_{k,1} < r_N\}] \geq \mathbb{E}[ (-\log N + \log c_d + d_x \log \rho_{k,1} - H(X)) \cdot I\{\rho_{k,1} < r_N\}] \geq (-\log N + \log c_d - H(X)) \mathbb{P}(\rho_{k,1} < r_N) + d_x \int_0^{r_N} \log r f_{\rho_{k,1}}(r) \, dr, \tag{188}
\]

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Therefore, we obtain:

\[
\mathbb{E} \left[ (\xi_{k,1}(X) - H(X)) \cdot I\{ \rho_{k,1} < r_N \} \right] 
\leq (\log N + |\log c_d - H(X)|) \mathbb{P}(\rho_{k,1} < r_N) + d_2 \int_0^{r_N} |\log r| f_{\rho_{k,1}}(r) dr ,
\]  

(189)

Now we will give an upper bound on the probability \( \mathbb{P}(\rho_{k,1} < r_N) \) for any \( r \leq r_N \). Given that \( Z_1 = z \), let \( p_r \) be the probability inside the \( t_p \) ball centered at \( Z_1 = z = (x, y) \) with radius \( r \). For sufficiently large \( N \), we have

\[
p_r = \mathbb{P}(u \in B_Z(z, r)) \leq \left( \sup_{t \in B_Z(z, r)} f(t) \right) c_d r^d \leq C_a c_d r^d
\]  

(190)

Therefore, \( \mathbb{P}(\rho_{k,1} < r \mid Z_1 = z) \) is upper bounded by:

\[
\mathbb{P}(\rho_{k,1} < r \mid Z_1 = z) = \sum_{m=k}^{N-1} \binom{N-1}{m} p_r^m (1 - p_r)^{N-1-m} 
\leq \sum_{m=k}^{N-1} N^m p_r^m \leq \sum_{m=k}^{N-1} (N c_a d_r^d)^m \leq 2(N c_a d_r^d)^k,
\]

Recall that \( r \leq r_N = (\log N)^2 N^{-1/d_x} \), so for sufficiently large \( N \), we have \( N c_a d_r^d \leq 1/2 \), which gives us the last inequality. Notice that this probability is independent of \( z \), therefore, we have \( \mathbb{P}(\rho_{k,1} < r) \leq 2(N c_a d_r^d)^k \). Plugging in \( r_N = (\log N)^2 N^{-1/d_x} \), we obtain:

\[
\mathbb{P}(\rho_{k,1} < r_N) \leq 2(N c_a d_r^d (\log N)^2 N^{-d/(d_x)})^k = 2C_a^{k} k d_r^d (\log N)^{2kd} N^{-kd/d_x}
\]  

(191)

Let \( F_{\rho_{k,1}}(r) \) be the CDF of \( \rho_{k,1} \) and \( F_0(r) = 2(N c_a d_r^d)^k \) be the upper bound for \( F_{\rho_{k,1}}(r) \). Then using integration by parts, the integral \( \int_0^{r_N} |\log r| f_{\rho_{k,1}}(r) dr \) can be bounded by:

\[
\int_0^{r_N} |\log r| f_{\rho_{k,1}}(r) dr = \int_0^{r_N} (-\log r) dF_{\rho_{k,1}}(r)
= -\log(r_N) F_{\rho_{k,1}}(r_N) + \lim_{r \to 0} (\log(r) F_{\rho_{k,1}}(r)) - \int_0^{r_N} \left( -\frac{F_{\rho_{k,1}}(r)}{r} \right) dr
\leq -\log(r_N) F_0(r_N) + \int_0^{r_N} \left( \frac{F_0(r)}{r} \right) dr
= -2 \log(r_N) (N c_a d_r^d)^k + \int_0^{r_N} \left( \frac{2(N c_a d_r^d)^k}{r} \right) dr
= -2 \log(r_N) (N c_a d_r^d)^k + \frac{2}{kd} (N c_a d_r^d)^k
= \frac{2}{kd} (N c_a d_r^d)^k \frac{k d_r^d}{N} (1 - k d \log(r_N))
= \frac{2}{kd} (N c_a d_r^d)^k (\log N)^{2kd} N^{-\frac{k d_r^d}{d_x}} (1 - k d (\frac{1}{d_x} \log N + 2 \log \log N))
= \frac{2(C_a d_r^d)^k}{kd} (\log N)^{2kd} (1 + \frac{k d_r^d}{d_x} \log N) N^{-\frac{k d_r^d}{d_x}}
\]  

(192)

If \( k \geq d_x/d_y \), then there exists some constant \( C \) such that \( \mathbb{P}(\rho_{k,1} < r_N) \leq C(\log N)^{2kd}/N \) and \( \int_0^{r_N} |\log r| f_{\rho_{k,1}}(r) dr \leq \)
for sufficiently large \( N \).

Now we consider the second term of (186). Recall that

\[
\xi_{k,1,2}(X) = \log \left( \frac{c_{d_x,2} N \rho_{k,1,2}^{d_x}}{n_{x,1,2}} \right)
\]

(194)

\[
\xi_{k,1,\infty}(X) = \log \left( \frac{c_{d_x,\infty} N \rho_{k,1,\infty}^{d_x}}{\exp\{\psi(n_{x,1,\infty} + 1)\}} \right),
\]

(195)

Given that \( r_N \leq \rho_{k,1,2} \leq a_N \), the bias of \( \xi_{k,1,2}(X) \) is upper bounded by:

\[
|E[(\xi_{k,1,2}(X) - H(X)) \cdot I\{r_N \leq \rho_{k,1,2} \leq a_N\}]|
\]

\[
= \left| \int_{r_N}^{a_N} \left[ \left( \xi_{k,1,2}(X) + \int f_X(x) \log f_X(x) dx \right) \cdot I\{r_N \leq \rho_{k,1,2} \leq a_N\} \right] dz \right|
\]

\[
\leq \int_{r_N}^{a_N} \left[ \log \left( f_X(x) c_{d_x,2} N \rho_{k,1,2}^{d_x} \right) - E\left[ \log(n_{x,1,2}) \rho_{k,1,2} = r, Z_1 = z \right] \right] f_{\rho_{k,1,2}}(r) dr \right| (196)
\]

where we applied the Jensen’s inequality. By noticing that \( \log(x) < \psi(x+1) < \log(x+1) \) for any integer \( x \geq 2 \), we have \( |\psi(x+1) - y| \leq \max_{\theta \in [0,1]} |\log(x+\theta) - y| \). So the bias of \( \xi_{k,1,\infty} \) is upper bounded by:

\[
E[(\xi_{k,1,\infty}(X) - H(X)) \cdot I\{r_N \leq \rho_{k,1,\infty} \leq a_N\}]
\]

\[
= \left| \int_{r_N}^{a_N} \left[ \left( \xi_{k,1,\infty}(X) + \int f_X(x) \log f_X(x) dx \right) \cdot I\{r_N \leq \rho_{k,1,\infty} \leq a_N\} \right] dz \right|
\]

\[
\leq \int_{r_N}^{a_N} \left[ \log \left( f_X(x) c_{d_x,\infty} n_{x,1,\infty} \right) - \log \left( f_X(x) c_{d_x,\infty} N \rho_{k,1,\infty}^{d_x} \right) \right] f_{\rho_{k,1,\infty}}(r) dr \right| (197)
\]

Combine the arguments for KSG and BI-KSG, we obtain:

\[
E[(\xi_{k,1}(X) - H(X)) \cdot I\{r_N \leq \rho_{k,1} \leq a_N\}]
\]

\[
\leq \int_{r_N}^{a_N} \left[ \max_{\theta \in [0,1]} E\left[ \log(n_{x,1,\infty} + \theta) | \rho_{k,1,\infty} = r, Z_1 = z \right] \right] f_{\rho_{k,1,\infty}}(r) dr \right| (198)
\]

From now on we drop the subscript 2 or \( r_N \). Recall that in Theorem 6 given that \( \rho_{k,i} = r \) and \( Z_i = z \), \( n_{x,i} - k \) is distributed as \( \sum_{l=k+1}^{N-1} U_i \), where \( U_i \) are i.i.d Bernoulli random variables with mean \( p \) satisfying

\[
r^{-d_x} \left| p - f_X(x) c_{d_x} r^{d_x} \right| \leq C_1(r^2 + r^{d_x}).
\]

(199)

For \( r > r_N = (\log N)^{2N-1/d_x} \), we know that \( p \geq f_X(x) c_{d_x} r^{d_x}/2 = f_X(x) c_{d_x} (\log N)^{2d_x}/(2N) \) for sufficiently large \( N \). Therefore, for any \( \theta \in [0,1] \), using the Taylor expansion of a logarithm, we obtain:

\[
E[\log(n_{x,1} + \theta) | \rho_{k,1} = r, X_1 = x] = \log \left( p(N-k-1) + k + \theta \right) - \frac{1-p}{2p(N-k-1)} + O\left( \frac{1}{p^2(N-k-1)^2} \right)
\]
For sufficiently large $N$, this gives

\[
\left| E(\log(n, x, 1 + \theta) | \rho_{k, 1} = r, X_1 = x) - \log \left( f_X(x) c_{d_*} N^{d_*} \right) \right|
\]
\[
\leq \left| \log \left( p(N - k - 1) + k + \theta \right) - \log \left( f_X(x) c_{d_*} N^{d_*} \right) \right| + \frac{1 - p}{2p(N - k - 1)} + \frac{C_2}{p^2(N - k - 1)^2}
\]
\[
\leq \log(pN) - \log \left( f_X(x) c_{d_*} N^{d_*} \right) + \left| \log(pN) - \log \left( pN + k(1 - p) + \theta - p \right) \right|
\]
\[
+ \frac{1 - p}{2p(N - k - 1)} + \frac{C_2}{p^2(N - k - 1)^2}
\]
\[
\leq \log(pN) - \log \left( f_X(x) c_{d_*} N^{d_*} \right) + \frac{C_3}{pN}, \quad \text{(201)}
\]

For sufficiently large $N$ we have sufficiently small $r$ such that, from Theorem 6, we get $p > f_X(x) c_{d_*} r^{d_*}/2$. Therefore the first term in (201) is bounded by:

\[
\left| \log(pN) - \log \left( f_X(x) c_{d_*} N^{d_*} \right) \right| \leq \left| p - f_X(x) c_{d_*} r^{d_*} \right| \left( \frac{1}{2p} + \frac{1}{2f_X(x) c_{d_*} r^{d_*}} \right)
\]
\[
\leq C_1 \left( r^{d_*+2} + r^{d_*+d_y} \right) \frac{3}{2f_X(x) c_{d_*} r^{d_*}}
\]
\[
\leq \frac{3C_1 (r^2 + r^{d_y})}{2c_{d_*} f_X(x)}, \quad \text{(202)}
\]

where we used the fact that $\log x - \log y \leq |x - y|(1/(2x) + 1/(2y))$ for any positive $x$ and $y$ and the upper bound on $|p - f_X(x) c_{d_*} r^{d_*}|$ from (199). The second term in (201) is bounded by $2C_3/(f_X(x) r^{d_*} N)$, which gives, for $C_4 = \max\{3C_1/2c_{d_*}, 2C_3\}$,

\[
\left| E(\log(n, x, 1 + \theta) | \rho_{k, 1} = r, X_1 = x) - \log \left( f_X(x) c_{d_*} N^{d_*} \right) \right| \leq \frac{C_4}{f_X(x)} \left( \frac{1}{r^{d_*} N} + r^2 + r^{d_y} \right). \quad \text{(203)}
\]

To integrate with respect to $\rho_{k, 1} = r$, note that $\rho_{k, 1}$ is simply the $k^{th}$ order statistic of $N - 1$ i.i.d. random variables $\{\|Z_2 - z\|, \|Z_3 - z\|, \ldots, \|Z_N - z\|\}$. The corresponding pdf satisfies [12]:

\[
f_{\hat{\rho}_{k, 1}^{(N-1)}}(r) = \frac{N - 1}{k - 1} f_{\hat{\rho}_{k-1, 1}^{(N-2)}}(r) P(z, r). \quad \text{(204)}
\]

For any $\theta \in (0, 1)$, we have

\[
\int_0^{a_N} \left| E(\log(n, x, 1 + \theta) | \rho_{k, i} = r, Z_i = z) - \log \left( f_X(x) c_{d_*} N^{d_*} \right) \right| f_{\hat{\rho}_{k, i}^{(N-1)}}(r) dr
\]
\[
\leq C_4 \int_0^{a_N} \frac{1}{f_X(x)} \left( \frac{1}{r^{d_*} N} + r^2 + r^{d_y} \right) f_{\hat{\rho}_{k, i}^{(N-1)}}(r) dr
\]
\[
= C_4 \int_0^{a_N} \frac{(N - 1) P(z, r)}{(k - 1) f_X(x)} \left( \frac{1}{r^{d_*} N} + r^2 + r^{d_y} \right) f_{\hat{\rho}_{k-1, 1}^{(N-2)}}(r) dr
\]
\[
\leq C_4 \max_{r \leq a_N} \frac{N P(z, r)}{(k - 1) f_X(x)} \left( \frac{1}{r^{d_*} N} + r^2 + r^{d_y} \right). \quad \text{(205)}
\]

By Lemma 4 $|P(z, r) - f(z) c_{d_*} r^d| \leq C r^{d+2}$. Therefore, for sufficiently small $a_N$, we have $P(z, r) < 2 f(z) c_{d_*} r^d$
for all \( r \leq a_N \). Then we have:

\[
\max_{r \leq a_N} \frac{NP(z,r)}{(k-1)f_X(x)} \left( \frac{1}{r^{d_s}N} + r^2 + r^{d_y} \right) \leq \max_{r \leq a_N} \frac{2f(z)cd^dN}{(k-1)f_X(x)} \left( \frac{1}{r^{d_s}N} + r^2 + r^{d_y} \right) \\
= \max_{r \leq a_N} \frac{2cf_Y(y|x)}{k-1} \left( r^{d_y} + N r^{d+2} + N r^{d+d_y} \right) \\
\leq C_5 \left( a_N^{d_y} + N a_N^{d+2} + N a_N^{d+d_y} \right).
\]

(206)

Since \( f_Y(y|x) \) is upper bounded by \( C_\varepsilon \), here \( C_5 \) is given by \( C_5 = 2cd/C_\varepsilon/(k-1) \). Now averaging over \( z \), we get:

\[
\mathbb{E} \left[ (\xi_{k,1}(X) - H(X)) \cdot 1\{r_N \leq \rho_{k,1} \leq a_N \} \right] \leq C_4 C_5 \int f(z) \left( a_N^{d_y} + N a_N^{d+2} + N a_N^{d+d_y} \right) dz \\
\leq C_4 C_5 \left( a_N^{d_y} + N a_N^{d+2} + N a_N^{d+d_y} \right).
\]

(207)

Together with Equation (193) and by the choice of \( a_N \) in Equation (19), the proof is completed.

F Proof of Theorem 6

Given that \( Z_1 = z = (x,y) \) and \( \rho_{k,1} = r \), let \( \{2,3,\ldots,N\} = S \cup \{j\} \cup T \) be a partition of the indices with \( |S| = k-1 \) and \( |T| = N-k-1 \). Define an event \( A_{S,j,T} \) associated to the partition as:

\[
A_{S,j,T} = \{ \|Z_s - z\| < \|Z_j - z\|, \forall s \in S, \text{ and } \|Z_t - z\| > \|Z_j - z\|, \forall t \in T \}.
\]

(208)

Since \( Z_j - z \) are i.i.d. random variables each of the events \( A_{S,j,T} \) has identical probability. The number of all partitions is \( \frac{(N-1)!}{(N-k-1)!} \) and thus \( \mathbb{P}(A_{S,j,T}) = \frac{(N-k-1)!}{(N-1)!} \). So the cdf of \( n_{x,i} \) is given by:

\[
\mathbb{P}(n_{x,i} \leq k + m | \rho_{k,1} = r, Z_1 = z) = \sum_{S,j,T} \mathbb{P}(A_{S,j,T}) \mathbb{P}(n_{x,i} \leq k + m | A_{S,j,T}, \rho_{k,1} = r, Z_1 = z) \\
= \frac{(N-k-1)!}{(N-1)!} \sum_{S,j,T} \mathbb{P}(n_{x,i} \leq k + m | A_{S,j,T}, \rho_{k,1} = r, Z_1 = z).
\]

(209)

Now condition on event \( A_{S,j,T} \) and \( \rho_{k,1} = r \), namely \( Z_j \) is the \( k \)-nearest neighbor with distance \( r \), \( S \) is the set of samples with distance smaller than \( r \) and \( T \) is the set of samples with distance greater than \( r \). Recall that \( n_{x,1} \) is the number of samples with \( \|X_j - x\| < r \). For any index \( s \in S \cup \{j\} \), \( \|X_s - x\| < r \) is satisfied. Therefore, \( n_{x,1} \leq k + m \) means that there are no more than \( m \) samples in \( T \) with \( X \)-distance smaller than \( r \). Let \( U_t = \mathbb{I}\{\|X_t - x\| < r \|Z_t - z\| > r\} \). Therefore,

\[
\mathbb{P}(n_{x,1} \leq k + m | A_{S,j,T}, \rho_{k,1} = r, Z_1 = z) \\
= \mathbb{P}\left( \sum_{t \in T} \mathbb{I}\{\|X_t - x\| < r \} \leq m, \|Z_s - z\| < r, \forall s \in S, \|Z_t - z\| > r, \forall t \in T, Z_1 = z \right) \\
= \mathbb{P}\left( \sum_{t \in T} \mathbb{I}\{\|X_t - x\| < r \} \leq m, \|Z_t - z\| > r, \forall t \in T \right) = \mathbb{P}\left( \sum_{i=k+1}^{N-1} U_t \leq m \right).
\]

(210)

We can drop the conditioning of \( Z_t \)'s for \( s \notin T \) since \( Z_s \) and \( X_t \) are independent. Therefore, given that \( \|Z_t - z\| > r \) for all \( t \in T \), the variables \( \mathbb{I}\{\|X_t - x\| < r \} \) are i.i.d. and have the same distribution as \( U_t \). We
conclude:

\[ P(n_{x,1} \leq k + m | \rho_{k,1} = r, Z_i = z) = \frac{(N - k - 1)! (k - 1)!}{(N - 1)!} \sum_{S, j, T} \mathbb{P}(n_{x,i} \leq k + m | A_{S,j,T}, \rho_{k,i} = r, Z_i = z) \]

\[ = \frac{(N - k - 1)! (k - 1)!}{(N - 1)!} \sum_{S, j, T} \mathbb{P} \left( \sum_{l=k+1}^{N} U_l \leq m \right) = \mathbb{P} \left( \sum_{l=k+1}^{N} U_l \leq \{21\} \right) \]

Thus we have shown that \( n_{x,i} - k \) has the same distribution as \( \sum_{l=k+1}^{N-1} U_l \) given \( Z_i = z \) and \( \rho_{k,i} = r \), in other words is a Binomial random variable.

Now we bound the mean of \( U_l \):

\[ p = \mathbb{E}[U_i] = \mathbb{P} \left( \|X_l - x\| < r \mid \|Z_l - z\| > r \right) = \frac{P_X(x, r) - P(z, r)}{1 - P(z, r)}. \quad (212) \]

By Lemma 4, we have:

\[ |P_X(x, r) - f_X(x) c_d x r^d| \leq C r^{d+2}. \quad (213) \]

and

\[ |P(z, r) - f(z) c_d r^d| \leq r^{d+2}. \quad (214) \]

Therefore, the difference of \( p \) and \( f_X(x) c_d x r^d \) is bounded by:

\[ |p - f_X(x) c_d x r^d| \leq \left| \frac{P_X(x, r) - P(z, r)}{1 - P(z, r)} - P_X(x, r) \right| + \left| P_X(x, r) - f_X(x) c_d x r^d \right| \]

\[ \leq \frac{P(z, r)(1 - P_X(x, r))}{1 - P(z, r)} + \left| P_X(x, r) - f_X(x) c_d x r^d \right| \]

\[ \leq P(z, r) + C r^{d+2} \leq C (r^{d+2} + r^{d+\theta}). \quad (215) \]