Finite-Sample Analysis of Fixed-\(k\) Nearest Neighbor Density Functional Estimators

Shashank Singh  
Statistics & Machine Learning Departments  
Carnegie Mellon University  
Pittsburgh, PA 15213  
sss1@andrew.cmu.edu

Barnabás Póczos  
Machine Learning Departments  
Carnegie Mellon University  
Pittsburgh, PA 15213  
bapoczos@cs.cmu.edu

Abstract

We provide finite-sample analysis of a general framework for using \(k\)-nearest neighbor statistics to estimate functionals of a nonparametric continuous probability density, including entropies and divergences. Rather than plugging a consistent density estimate (which requires \(k \to \infty\) as the sample size \(n \to \infty\)) into the functional of interest, the estimators we consider fix \(k\) and perform a bias correction. This is more efficient computationally, and, as we show in certain cases, statistically, leading to faster convergence rates. Our framework unifies several previous estimators, for most of which ours are the first finite sample guarantees.

1 Introduction

Estimating entropies and divergences of probability distributions in a consistent manner is of importance in a number problems in machine learning. Entropy estimators have applications in goodness-of-fit testing [Goria et al., 2005], parameter estimation in semi-parametric models [Wolsztynski et al., 2005], studying fractal random walks [Alemany and Zanette, 1994], and texture classification [Hero et al., 2002a,b]. Divergence estimators have been used to generalize machine learning algorithms for regression, classification, and clustering from inputs in \(\mathbb{R}^D\) to sets and distributions [Póczos et al., 2012, Oliva et al., 2013].

Divergences also include mutual informations as a special case; mutual information estimators have applications in feature selection [Peng and Ding, 2005], clustering [Aghagolzadeh et al., 2007], causality detection [Hlaváčková-Schindler et al., 2007], optimal experimental design [Lewi et al., 2007, Póczos and Lörincz, 2009], fMRI data analysis [Chai et al., 2009], prediction of protein structures [Adam et al., 2004], and boosting and facial expression recognition [Schan et al., 2005]. Both entropy estimators and mutual information estimators have been used for independent component and subspace analysis [Learned-Miller and Fisher, 2003, Szabó et al., 2007, Póczos and Lörincz, 2005, Hulle, 2008], as well as for image registration [Kybic, 2006, Hero et al., 2002a,b]. Further applications can be found in Leonenko et al. [2008].

This paper considers the more general problem of using \(n\) IID samples from \(P\) to estimate functionals of the form

\[
F(P) := \mathbb{E}_{X \sim P} [f(p(X))],
\]

where \(P\) is an unknown probability measure with smooth density function \(p\) and \(f\) is a known smooth function. We are interested in analyzing a class of nonparametric estimators based on \(k\)-nearest neighbor (\(k\)-NN) distance statistics. Rather than plugging a consistent estimator of \(p\) into (1), which requires \(k \to \infty\) as \(n \to \infty\), these estimators derive a bias correction for the plug-in estimator with fixed \(k\); hence, we refer to this type of estimator as a fixed-\(k\) estimator. Compared to plug-in estimators, fixed-\(k\) estimators are faster to compute. As we show, fixed-\(k\) estimators can also exhibit superior rates of convergence.
As shown in Table 1, several authors have derived bias corrections necessary for fixed-k estimators of entropies and divergences, including, most famously, the Shannon entropy estimator of Kozachenko and Leonenko [1987]. The estimators in Table 1 are known to be weakly consistent. However, for most of these estimators, no finite sample bounds are known. The main goal of this paper is to provide finite-sample analysis of these estimators, via a unified analysis of the estimator after bias correction. Specifically, we will show conditions under which, for β-Hölder continuous (β ∈ (0, 2]) densities on D dimensional space, the bias of fixed-k estimators decays as \( O(n^{-β/D}) \) and the variance decays as \( O(n^{-1}) \), giving a mean squared error of \( O(n^{-2β/D + 1}) \). Hence, the estimators converge at the parametric \( O(n^{-1}) \) rate when \( β ≥ D/2 \), and at the slower rate \( O(n^{-2β/D}) \) otherwise. A modification of the estimators would be necessary to leverage additional smoothness for \( β > 2 \), but we do not pursue this here. Along the way, we also prove a finite-sample version of the useful fact [Leonenko et al., 2008] that (appropriately normalized) k-NN distances have an asymptotic Erlang distribution, which may be of independent interest.

We present our results for distributions \( P \) supported on the unit cube in \( \mathbb{R}^D \) because this significantly simplifies the statements of our results, but, as we discuss in the supplement, our results generalize fairly naturally, for example to distributions supported on a smooth compact manifold. In this context, it is worth noting that our results would scale with the intrinsic dimension of the manifold. As we discuss later, we believe that deriving finite sample rates for distributions with unbounded support may require a truncated modification of the estimators we study (as in Tsybakov and van der Meulen [1996]), but we do not pursue this modification here.

### Table 1: Table of functionals with known bias-corrected k-NN estimators, the type of bias correction necessary, the correction constant, and references. All expectations are over \( X \sim P \).

| Functional Name | Functional Form | Correction | Reference |
|-----------------|-----------------|------------|-----------|
| Shannon Entropy | \( \mathbb{E} \left[ \log p(X) \right] \) | Additive constant: \( \psi(n) - \psi(k) + \log(k/n) \) | Kozachenko and Leonenko [1987], Goria et al. [2005] |
| Rényi-\( α \) Entropy | \( \mathbb{E} \left[ p^\alpha(X) \right] \) | Multiplicative constant: \( \frac{\Gamma(k)}{\Gamma(k+1-\alpha)} \) | Leonenko et al. [2008], Leonenko and Pronzato [2010] |
| KL Divergence   | \( \mathbb{E} \left[ \log \left( \frac{p(X)}{q(X)} \right) \right] \) | None* | Wang et al. [2009] |
| \( α \)-Divergence | \( \mathbb{E} \left[ \left( \frac{p(X)}{q(X)} \right)^{\alpha-1} \right] \) | Multiplicative constant: \( \frac{\Gamma^2(k)}{\Gamma(k-\alpha+1)\Gamma(k+\alpha-1)} \) | Poczos and Schneider [2011] |

\*For KL divergence, the bias corrections for \( p \) and \( q \) exactly cancel.

As shown in Table 1, several authors have derived bias corrections necessary for fixed-k estimators of entropies and divergences, including, most famously, the Shannon entropy estimator of Kozachenko and Leonenko [1987]. The estimators in Table 1 are known to be weakly consistent. However, for most of these estimators, no finite sample bounds are known. The main goal of this paper is to provide finite-sample analysis of these estimators, via a unified analysis of the estimator after bias correction. Specifically, we will show conditions under which, for \( β \)-Hölder continuous (\( β ∈ (0, 2] \)) densities on \( D \) dimensional space, the bias of fixed-k estimators decays as \( O(n^{-β/D}) \) and the variance decays as \( O(n^{-1}) \), giving a mean squared error of \( O(n^{-2β/D + 1}) \). Hence, the estimators converge at the parametric \( O(n^{-1}) \) rate when \( β ≥ D/2 \), and at the slower rate \( O(n^{-2β/D}) \) otherwise. A modification of the estimators would be necessary to leverage additional smoothness for \( β > 2 \), but we do not pursue this here. Along the way, we also prove a finite-sample version of the useful fact [Leonenko et al., 2008] that (appropriately normalized) k-NN distances have an asymptotic Erlang distribution, which may be of independent interest.

We present our results for distributions \( P \) supported on the unit cube in \( \mathbb{R}^D \) because this significantly simplifies the statements of our results, but, as we discuss in the supplement, our results generalize fairly naturally, for example to distributions supported on a smooth compact manifold. In this context, it is worth noting that our results would scale with the intrinsic dimension of the manifold. As we discuss later, we believe that deriving finite sample rates for distributions with unbounded support may require a truncated modification of the estimators we study (as in Tsybakov and van der Meulen [1996]), but we do not pursue this modification here.

### 2 Problem statement and notation

Let \( X := [0, 1]^D \) denote the unit cube in \( \mathbb{R}^D \), and let \( μ \) denote the Lebesgue measure. Suppose \( P \) is an unknown \( μ \)-absolutely continuous Borel probability measure supported on \( X \), and let \( p : X → [0, ∞) \) denote the density of \( P \). Consider a (known) differentiable function \( f : (0, ∞) → \mathbb{R} \). Given \( n \) samples \( X_1, ..., X_n \) drawn IID from \( P \), we are interested in estimating the functional

\[
F(P) := \mathbb{E}_{X \sim P} [f(p(X))].
\]

Somewhat more generally (as in divergence estimation), we may have a function \( f : (0, ∞)^2 → \mathbb{R} \) of two variables and a second unknown probability measure \( Q \), with density \( q \) and \( n \) IID samples \( Y_1, ..., Y_n \). Then, we are interested in estimating

\[
F(P, Q) := \mathbb{E}_{X \sim P} [f(p(X), q(X))].
\]

\[\text{MATLAB implementations of many of these estimators can be found in the Information Theoretical Estimators toolbox available at } \text{https://bitbucket.org/szzoli/ite/} \text{ [Szabó 2014].}
\[\text{Several of these proofs contain errors regarding the use of integral convergence theorems when their conditions do not hold, as described in Poczos and Schneider [2011].}\]
Fix \( r \in [1, \infty] \) and a positive integer \( k \). We will work with distances induced by the \( r \)-norm
\[
\|x\|_r := \left( \sum_{i=1}^{D} x_i^r \right)^{1/r}
\]
and define \( c_{D,r} := \frac{(2\Gamma(1+1/r))^D}{\Gamma(1+D/r)} = \mu(B(0,1)) \), where \( B(x, \varepsilon) := \{ y \in \mathbb{R}^D : \|x - y\|_r < \varepsilon \} \) denotes the open radius-\( \varepsilon \) ball centered at \( x \). Our estimators use \( k \)-nearest neighbor (\( k \)-NN) distances:

**Definition 1.** (\( k \)-NN distance): Suppose we have \( n \) samples \( X_1, \ldots, X_n \) drawn IID from \( P \). For any \( x \in \mathbb{R}^D \), we define the \( k \)-nearest neighbor distance \( \varepsilon_k(x) \) by \( \varepsilon_k(x) = \|x - X_i\|_r \), where \( X_i \) is the \( k \)-th-nearest element (in \( \| \cdot \|_r \) of the set \( \{ X_1, \ldots, X_n \} \) to \( x \). For divergence estimation, if we also have \( n \) samples \( Y_1, \ldots, Y_n \) drawn IID from \( Q \), then we similarly define \( \delta_k(x) = \|x - Y_i\|_r \), where \( Y_i \) is the \( k \)-th-nearest element of \( \{ Y_1, \ldots, Y_n \} \) to \( x \).

Note that the \( \mu \)-absolute continuity of \( P \) precludes the existence of atoms (i.e., for all \( x \in \mathbb{R}^D \), \( P(\{ x \}) = \mu(\{ x \}) = 0 \)). Hence, for all \( x \in \mathbb{R}^D \), \( \varepsilon_k(x) > 0 \) almost surely. This is important, since we will consider quantities such as \( \log \varepsilon_k(x) \) and \( \frac{1}{\varepsilon_k(x)} \).

3 Estimator

3.1 \( k \)-NN density estimation and plug-in functional estimators

The \( k \)-NN density estimator
\[
\hat{p}_k(x) = \frac{k/n}{\mu(B(x, \varepsilon_k(x)))} = \frac{k/n}{c_{D,r} \varepsilon_k(x)}
\]
is well-studied nonparametric density estimator (originally due to [Loftsgaarden and Quesenberry 1965](#)), motivated by the observations that, for small \( \varepsilon > 0 \),
\[
p(x) \approx \frac{P(B(x, \varepsilon))}{\mu(B(x, \varepsilon))}.
\]
and that, \( P(B(x, \varepsilon_k(x))) \approx k/n \). One can show that, for \( x \in \mathbb{R}^D \) at which \( p \) is continuous, if \( k \to \infty \) and \( k/n \to 0 \) as \( n \to \infty \), then \( \hat{p}_k(x) \to p(x) \) in probability ([Loftsgaarden and Quesenberry 1965](#)). Thus, a natural approach for estimating \( F(P) \) is the plug-in estimator
\[
\hat{F}_{PI} := \frac{1}{n} \sum_{i=1}^{n} f(\hat{p}_k(X_i)).
\]

Since \( \hat{p}_k \to p \) in probability pointwise as \( k, n \to \infty \) and \( f \) is smooth, one can show \( \hat{F}_{PI} \) is consistent, and in fact derive finite sample convergence rates (depending on how \( k \to \infty \)). For example, [Sricharan et al. 2010](#) show a convergence rate of \( O \left( n^{-\min\left\{ \frac{1}{p-1}, 1 \right\}} \right) \) for \( \beta \)-Hölder continuous densities (after sample splitting and boundary correction) by setting \( k \approx n^{\frac{1}{p}} \).

Unfortunately, while necessary to ensure \( \mathbb{V} [\hat{p}_k(x)] \to 0 \), the requirement \( k \to \infty \) is computationally burdensome. Furthermore, increasing \( k \) can increase the bias of \( \hat{p}_k \) due to over-smoothing (see § below), suggesting that this may be sub-optimal for estimating \( F(P) \). Indeed, similar work based on kernel density estimation ([Singh and Poczos 2014](#)) suggests that, for plug-in functional estimators, under-smoothing may be preferable, since the empirical mean results in additional smoothing.

3.2 Fixed-\( k \) functional estimators

An alternative approach is to fix \( k \) as \( n \to \infty \). Since \( \hat{F}_{PI} \) is itself an empirical mean, unlike \( \mathbb{V} [\hat{p}_k(x)] \), \( \mathbb{V} \left[ \hat{F}_{PI} \right] \to 0 \) as \( n \to \infty \).

A more critical complication of fixing \( k \) is bias. Since \( f \) is typically non-linear, the non-vanishing variance of \( \hat{p}_k \) translates into asymptotic bias. A solution adopted by several papers is to derive a bias correction function \( B \) (depending only on known factors) such that
\[
E \left[ B \left( f \left( \frac{k/n}{\mu(B(x, \varepsilon_k(x)))} \right) \right) \right] = E \left[ f \left( \frac{P(B(x, \varepsilon_k(x)))}{\mu(B(x, \varepsilon_k(x)))} \right) \right].
\]
For continuous \( p \), the quantity

\[
p_{\varepsilon_k}(x) := \frac{P(B(x, \varepsilon_k(x)))}{\mu(B(x, \varepsilon_k(x))} \tag{4}
\]

is a consistent estimate of \( p(x) \) with \( k \) fixed, but it is not computable, since \( P \) is unknown. The bias correction \( B \) gives us an asymptotically unbiased estimator

\[
\hat{F}_B(P) := \frac{1}{n} \sum_{i=1}^{n} B \left( f \left( \hat{p}_k(X_i) \right) \right) = \frac{1}{n} \sum_{i=1}^{n} B \left( f \left( \frac{k/n}{\mu(B(x, \varepsilon_k(x)))} \right) \right).
\]

that uses \( k/n \) in place of \( P(B(x, \varepsilon_k(x))) \). This estimate extends naturally to divergences:

\[
\hat{F}_B(P, Q) := \frac{1}{n} \sum_{i=1}^{n} B \left( f \left( \hat{p}_k(X_i), \hat{q}_k(X_i) \right) \right).
\]

As an example, if \( f = \log \) (as in Shannon entropy), then it can be shown that, for any continuous \( p \),

\[
\mathbb{E} \left[ \log P(B(x, \varepsilon_k(x))) \right] = \psi(k) - \psi(n).
\]

Hence, for \( B_{n,k} := \psi(k) - \psi(n) + \log(n) - \log(k) \),

\[
\mathbb{E}_{X_1, \ldots, X_n} \left[ f \left( \frac{k/n}{\mu(B(x, \varepsilon_k(x)))} \right) \right] + B_{n,k} = \mathbb{E}_{X_1, \ldots, X_n} \left[ f \left( \frac{P(B(x, \varepsilon_k(x)))}{\mu(B(x, \varepsilon_k(x)))} \right) \right],
\]

giving the estimator of [Kozachenko and Leonenko 1987]. Other examples of functionals for which the bias correction is known are given in Table I.

In general, deriving an appropriate bias correction can be quite a difficult problem specific to the functional of interest, and it is not our goal presently to study this problem; rather, we are interested in bounding the error of \( \hat{F}_B(P) \), assuming the bias correction is known. Hence, our results apply to all of the estimators in Table I as well as any estimators of this form that may be derived in the future.

4 Related work

4.1 Estimating information theoretic functionals

Quite recently, there has been much work on analyzing new estimators for entropy, mutual information, divergences, and other functionals of densities. Besides bias-corrected fixed-\( k \) estimators, most of this work has been along one of three approaches. One series of papers [Liu et al. 2012, Singh and Poczos 2014b,a] studied a boundary-corrected plug-in approach based on under-smoothed kernel density estimation. This approach has strong finite sample guarantees, but requires prior knowledge of the support of the density and can necessitate computationally demanding numerical integration. A second approach [Krishnamurthy et al. 2014, Kandasamy et al. 2015] uses von Mises expansion to correct the bias of optimally smoothed density estimates. This approach shares the difficulties of the previous approach, but is statistically more efficient. A final line of work [Sricharan et al. 2010, Sricharan et al. 2012, Moon and Hero 2014b,a] has studied entropy estimation based on plugging in consistent, boundary corrected \( k \)-NN density estimates (i.e., with \( k \to \infty \) as \( n \to \infty \)). There is also a divergence estimator [Nguyen et al. 2010] based on convex risk minimization, but this is framed in the context of an RKHS and results are difficult to compare.

Rates of Convergence: For densities over \( \mathbb{R}^D \) satisfying a Hölder smoothness condition parametrized by \( \beta \in (0, \infty) \), the minimax mean squared error rate for estimating functionals of the form \( \int f(p(x)) \, dx \) has been known since [Birge and Massard 1995] to be \( O \left( n^{-\min \{ D/2 + 1, \beta \} } \right) \). [Krishnamurthy et al. 2014] recently derived identical minimax rates for divergence estimation.

Most of the above estimators have been shown to converge at the rate \( O \left( n^{-\min \{ D/2 + 1, \beta \} } \right) \). Only the von Mises approach of [Krishnamurthy et al. 2014] is known to achieve the minimax rate for general \( \beta \) and \( D \), but due to its high computational demand (\( O(2^D n^3) \)), the authors suggest the
use of other statistically less efficient estimators for moderately sized datasets. In this paper, we show that, for $\beta \in (0, 2]$, bias-corrected fixed-$k$ estimators converge at the relatively fast rate of $O\left(n^{-\min\left(\frac{\beta}{D}, 1\right)}\right)$. For $\beta > 2$, modifications are needed for the estimator to leverage the additional smoothness of the density. It is also worth noting the relative computational efficiency of the fixed-$k$ estimators ($O(\sqrt{Dn^2})$, or $O(2^D n \log n)$ using k-d trees for small $D$).

### 4.2 Prior analysis of fixed-$k$ estimators

To our knowledge, the only finite-sample results for $\hat{F}_B(P)$ are the recent results of Biau and Devroye [2015] for the Kozachenko-Leonenko (KL) \[\text{Shannon entropy estimator.}\]

Kozachenko and Leonenko [1987] Theorem 7.1 of Biau and Devroye [2015] shows that, if the density $p$ has compact support, then the variance of the KL estimator decays as $O(n^{-1})$. They also claim (Theorem 7.2) to bound the bias of the KL estimator by $O(n^{-\beta})$, under the assumptions that $p$ is $\beta$-Hölder continuous ($\beta \in (0, 1]$), bounded away from 0 and supported on the interval $[0, 1]$. However, in their proof Biau and Devroye [2015] neglect to bound the additional bias incurred near the boundaries of $[0, 1]$, where the density cannot simultaneously be bounded away from 0 and continuous. In fact, because the KL estimator does not attempt to correct for boundary bias, it is not clear that the bias should decay as $O(n^{-\beta})$ under these conditions; we will require additional conditions at the boundary of $\mathcal{X}$.

Tybakov and van der Meulen [1996] studied a closely related entropy estimator for which they prove $\sqrt{n}$-consistency. Their estimator is identical to the KL estimator, except that it truncates $k$-NN distances at $\sqrt{n}$, replacing $\hat{\varepsilon}_k(x)$ with $\min\{\varepsilon_k(x), \sqrt{n}\}$. This sort of truncation may be necessary for certain fixed-$k$ estimators to satisfy finite-sample bounds for densities of unbounded support, although consistency can be shown regardless.

### 5 Discussion of assumptions

The lack of finite-sample results for fixed-$k$ estimators is due to several technical challenges. Here, we discuss some of these challenges, motivating the assumptions we make to overcome them.

First, these estimators are sensitive to regions of low probability (i.e., $p(x)$ small), for two reasons:

1. Many functions $f$ of interest (e.g., $f = \log$ or $f(z) = z^\alpha$, $\alpha < 0$) have singularities at 0.
2. The $k$-NN estimate $\hat{p}_k(x)$ of $p(x)$ is highly biased when $p(x)$ is small. For example, for $p$ $\beta$-Hölder continuous ($\beta \in (0, 2]$), one has (Mack and Rosenblatt [1979], Theorem 2)

$$\text{Bias}(\hat{p}_k(x)) \asymp \left(\frac{k}{np(x)}\right)^{\beta/D}.$$  

(5)

For these reasons, it has been common in the analysis of $k$-NN estimators to make the following assumption: Poczos and Schneider, 2011, Biau and Devroye 2015

(A1) $p$ is bounded away from zero on its support. That is, $p_* := \inf_{x \in \mathcal{X}} p(x) > 0$.

Second, unlike many functional estimators (see e.g., Pál et al., 2010, Sricharan et al., 2012b, Singh and Poczos, 2014a), the fixed-$k$ estimators we consider do not attempt correct for boundary bias (i.e., bias incurred due to discontinuity of $p$ on the boundary $\partial \mathcal{X}$ of $\mathcal{X}$). The boundary bias of the density estimate $\hat{p}_k(x)$ does vanish at $x$ in the interior $\mathcal{X}^o$ of $\mathcal{X}$ as $n \to \infty$, but additional assumptions are needed to obtain finite-sample rates. Either of the following assumptions would suffice:

(A2) $p$ is continuous not only on $\mathcal{X}^o$ but also on $\partial \mathcal{X}$ (i.e., $p(x) \to 0$ as $\text{dist}(x, \partial \mathcal{X}) \to 0$).

(A3) $p$ is supported on all of $\mathbb{R}^D$. That is, the support of $p$ has no boundary. This is the approach of Tybakov and van der Meulen [1996], but we reiterate that, to handle an unbounded domain, they require truncating $\varepsilon_k(x)$.

\footnote{Not to be confused with Kullback-Leibler (KL) divergence, for which we also analyze an estimator.}

\footnote{This complication appears to have been omitted in the bias bound (Theorem 7.2) of Biau and Devroye [2015] for entropy estimation.}
Unfortunately, both assumptions (A2) and (A3) are inconsistent with (A1). Our approach is to assume (A2) and replace assumption (A1) with a much milder assumption that $p$ is locally lower bounded on its support in the following sense:

(A4) There exist $\rho > 0$ and a function $p_* : \mathcal{X} \to (0, \infty)$ such that, for all $x \in \mathcal{X}, r \in (0, \rho],$

$$p_*(x) \leq \frac{P(B(x,r))}{\mu(B(x,r))}.$$  

We will show (Lemma 2) that assumption (A4) is in fact very mild; in a metric measure space of positive dimension $D$, as long as $p$ is continuous on $\mathcal{X}$, such a $p_*$ exists for any desired $\rho > 0$. For simplicity, we will use $\rho = \sqrt{D} = \text{diam}(\mathcal{X})$.

As hinted by (5) and the fact that $F(P)$ is an expectation, our bounds will contain terms of the form

$$\mathbb{E}_{X \sim P} \left[ \frac{1}{(p_*(X))^{\beta/D}} \right] = \int_{\mathcal{X}} \frac{p(x)}{(p_*(x))^{\beta/D}} d\mu(x)$$

(with an additional $f'(p_*(x))$ factor if $f$ has a singularity at zero). Hence, the real non-trivial assumptions we make will be that these quantities are finite. This depends primarily on how quickly $p$ can be allowed to approach zero near $\partial \mathcal{X}$ (which may be $\infty$ if $\mathcal{X}$ is unbounded). For many functionals, Lemma 6 will give a simple sufficient condition.

6 Preliminary lemmas

Here, we present some lemmas, both as a means of summarizing our proof techniques and also because they may be of independent interest for proving finite-sample bounds for other $k$-NN methods. Due to space constraints, all proofs are given in the appendix. Our first lemma states that, if $p$ is continuous, then it is locally lower bounded as described in the previous section.

Lemma 2. (Existence of Local Bounds) If $p$ is continuous on $\mathcal{X}$ and strictly positive on the interior $\mathcal{X}^\circ$ of $\mathcal{X}$, then, for $\rho := \sqrt{D} = \text{diam}(\mathcal{X})$, there exists a continuous function $p_* : \mathcal{X}^\circ \to (0, \infty)$ and a constant $p^* \in (0, \infty)$ such that

$$0 < p_*(x) \leq \frac{P(B(x,r))}{\mu(B(x,r))} \leq p^* < \infty, \quad \forall x \in \mathcal{X}, r \in (0, \rho].$$

We now show that the existence of local lower and upper bounds implies concentration of the $k$-NN distance of around a term of order $\left( \frac{k}{p(x)} \right)^{1/D}$. Related lemmas, also based on multiplicative Chernoff bounds, have been used by Kpotufe and von Luxburg (2011), Chaudhuri et al. (2014) and Chaudhuri and Dasgupta (2014), Kontorovich and Weiss (2015) to prove finite-sample bounds on $k$-NN methods for cluster tree pruning and classification, respectively. For cluster tree pruning, the relevant inequalities bound the error of the $k$-NN density estimate, and, for classification, they lower bound the probability of nearby samples of the same class. Unlike in cluster tree pruning, we are not using a consistent density estimate, and, unlike in classification, our estimator is a function of $k$-NN distances themselves (rather than their ordering). Hence, our statement is somewhat different, bounding the $k$-NN distances themselves:

Lemma 3. (Concentration of $k$-NN Distances) Suppose $p$ is continuous on $\mathcal{X}$ and strictly positive on $\mathcal{X}^\circ$. Let $p_*$ and $p^*$ be as in Lemma 2. Then, for any $x \in \mathcal{X}^\circ$,

1. if $r > \left( \frac{k}{p_*(x)n} \right)^{1/D}$, then $\mathbb{P} [e_k(x) > r] \leq e^{-p_*(x)r^D n} \left( \frac{p_*(x)r^D n}{k} \right)^k$.

2. if $r \in \left[ 0, \left( \frac{k}{p^*n} \right)^{1/D} \right)$, then $\mathbb{P} [e_k(x) < r] \leq e^{-p_*(x)r^D n} \left( \frac{p^*r^D n}{k} \right)^{kp_*(x)/p^*}.$

It is worth noting the asymmetry of the upper and lower bounds; perhaps counter-intuitively, the lower bound also depends on $p_*$. It is this asymmetry that causes the large (over-estimation) bias of $k$-NN density estimators when $p$ is small (as in (5)).
The following theorem uses Lemma 3 to bound expectations of monotone functions of \( \hat{p}_k \) normalized by \( p_\ast \). As suggested by the form of the integral in the bounds, this can be thought of as a finite-sample statement of the fact that (appropriately normalized) \( k \)-NN distances have an asymptotic Erlang distribution; this asymptotic statement is central to the consistency proofs of Leonenko et al. [2008] and Poczos and Schneider [2011] for their \( \alpha \)-entropy and divergence estimators, respectively.

**Lemma 4.** Suppose \( p \) is continuous on \( X \) and strictly positive on \( X^\circ \). Let \( p_\ast \) and \( p^\ast \) be as in Lemma 2. Let \( f : (0, \infty) \to \mathbb{R} \) be differentiable, and define \( M_{f, p} : X \to [0, \infty) \) by

\[
M_{f, p}(x) := \sup_{z \in \lbrack p_\ast(x), p^\ast \rbrack} \left| \frac{d}{dz} f(z) \right|
\]

Assume

\[
C_f := \mathbb{E}_{X \sim p} \left[ \frac{M_{f, p}(X)}{(p_\ast(X))^{\frac{1}{D}}} \right] < \infty.
\]

Then, \( \hat{F}_B(P) \) is \( D \)-Hölder continuous with constant \( L > 0 \) on \( X \), and \( M_{f, p}(x) \) is strictly positive on \( X^\circ \).

**Theorem 5. (Bias Bound)** Suppose that, for some \( \beta \in (0, 2] \), \( p \) is \( \beta \)-Hölder continuous with constant \( L > 0 \) on \( X \), and \( p_\ast \) is strictly positive on \( X^\circ \). Let \( p_\ast \) and \( p^\ast \) be as in Lemma 2. Let \( f : (0, \infty) \to \mathbb{R} \) be differentiable, and define \( M_{f, p} : X \to [0, \infty) \) by

\[
M_{f, p}(x) := \sup_{z \in \lbrack p_\ast(x), p^\ast \rbrack} \left| \frac{d}{dz} f(z) \right|
\]

Assume

\[
C_f := \mathbb{E}_{X \sim p} \left[ \frac{M_{f, p}(X)}{(p_\ast(X))^{\frac{1}{D}}} \right] < \infty.
\]

Then, \( \left| \hat{F}_B(P) - F(P) \right| \leq C_f L \left( \frac{k}{n} \right)^{\frac{1}{D}} \).

The statement for divergences is similar, assuming that \( q \) is also \( \beta \)-Hölder continuous with constant \( L \) and strictly positive on \( X^\circ \). Specifically, we get the same bound if we replace \( M_{f, p} \) with

\[
M_{f, q}(x) := \sup_{(w, z) \in \lbrack p_\ast(x), p^\ast \rbrack \times \lbrack q_\ast(x), q^\ast \rbrack} \left| \frac{\partial}{\partial w} f(w, z) \right|
\]

and define \( M_{f, q} \) similarly (i.e., with \( \frac{\partial}{\partial z} \) and we assume that

\[
C_f := \mathbb{E}_{X \sim p} \left[ \frac{M_{f, p}(X)}{(p_\ast(X))^{\frac{1}{D}}} \right] + \mathbb{E}_{X \sim p} \left[ \frac{M_{f, q}(X)}{(q_\ast(X))^{\frac{1}{D}}} \right] < \infty.
\]

\( f_+ (x) := \max \{ 0, f(x) \} \) and \( f_- (x) := - \min \{ 0, f(x) \} \) denote the positive and negative parts of \( f \). Recall that \( \mathbb{E} [f(X)] = \mathbb{E} [f_+(X)] - \mathbb{E} [f_-(X)] \).
As an example of the applicability of Theorem 5, consider estimating the Shannon entropy. Then, if $f(z) = \log(x)$, and we need $f \int_X p_*^\beta d\mu(x) < \infty$.

The assumption $f \int_X p_*^\beta d\mu(x) < \infty$ is not immediately transparent. For the functionals in Table 1, $C_f$ has the form $\int_X p(x)^c dx$, for some $c > 0$, and hence $C_f < \infty$ intuitively means $p(x)$ cannot approach zero too quickly as $\text{dist}(x, \partial \mathcal{X}) \to 0$. The following lemma gives a formal sufficient condition:

**Lemma 6. (Boundary Condition)** Let $c > 0$. Suppose there exist $b_0 \in (0, \frac{1}{c})$, $c_\theta, \rho_0 > 0$ such that, for all $x \in \mathcal{X}$ with $\epsilon(x) := \text{dist}(x, \partial \mathcal{X}) < \rho_0$, $p(x) \geq c_\theta \epsilon^\theta(x)$. Then, $\int_X p(x)^c d\mu(x) < \infty$.

Now, we turn to bounding the variance. Although the fixed-$k$ estimator is an empirical mean, because the terms being averaged (functions of $k$-NN distances) are dependent, it is not obvious how to go about bounding the variance of the estimator. We generalize the approach used by Biau and Devroye [2015] to prove a variance bound on the KL estimator of Shannon entropy. The key insight is to use the geometric fact that, in $(\mathbb{R}^d, \| \cdot \|_p)$, there exists a constant $N_{k,D}$ (independent of $n$) such that any sample $X_i$ can be amongst the $k$-nearest neighbors of at most $N_{k,D}$ other samples. Hence, at most $N_{k,D} + 1$ of the terms in (2) can change when a single $X_i$ is added, leading to a variance bound via the Efron-Stein inequality [Efron and Stein, 1981], which bounds the variance of a function of random variables in terms of its changes when its arguments are resampled.

**Theorem 7. (Variance Bound)** Suppose that $B \circ f$ is continuously differentiable and strictly monotone. Assume that $C_{f,p} := \mathbb{E}_{X \sim P}[\mathbb{B}^2(f(p_*(X)))] < \infty$, and that $C_f := \int_0^\infty e^{-y} k f(y) < \infty$. Then, for

$$C_V := 2 + N_{k,D} (3 + 4k) (C_{f,p} + C_f), \quad \text{we have} \quad \mathbb{V} \left[ \hat{F}_B(P) \right] \leq \frac{C_V}{n}.$$ 

As an example, if $f = \log$ (as in Shannon entropy), then, since $B$ is an additive constant, we simply require $\int_X p(x) \log^2(p_*^\beta(x)) < \infty$.

In general, $N_{k,D}$ is of the order $k 2^c D$, for some $c > 0$. Our bound is likely quite loose in $k$; in practice, $\mathbb{V} \left[ \hat{F}_B(P) \right]$ typically decreases somewhat with $k$.

### 8 Conclusions and discussion

In this paper, we gave finite-sample bias and variance error bounds for a class of fixed-$k$ estimators of functionals of probability density functions, including the entropy and divergence estimators in Table 1. The bias and variance bounds in turn imply a bound on the mean squared error (MSE) of the bias-corrected estimator via the usual decomposition into squared bias and variance:

**Corollary 8. (MSE Bound)** Under the conditions of Theorems 5 and 7,

$$\mathbb{E} \left[ (\hat{H}_k(X) - H(X))^2 \right] \leq C_f^2 L^2 \left( \frac{k}{n} \right)^{2\beta/D} + \frac{C_V}{n}. \quad (9)$$

**Choice of $k$:** It is worth noting that, contrary to the name, fixing $k$ is not required for “fixed-$k$” estimators. Indeed, Pérez-Cruz [2008] empirically studied the effects of changing $k$ with $n$, finding that fixing $k = 1$ gave the best results for estimating $F(P)$. However, it appears there has been no formal theoretical justification for fixing $k$ in estimation problems. Assuming the tightness of our bias bound in $k$, we provide this in a worst-case sense: since the bias bound is nondecreasing in $k$ and our variance bound is no larger than the minimax MSE rate for most such estimation problems, we cannot improve the (worst-case) convergence rate of estimators by reducing variance (i.e., by increasing $k$). It is worth noting, however, that Pérez-Cruz [2008] found increasing $k$ quickly (e.g., $k = n/2$) was best for certain hypothesis tests based on these estimators. Intuitively, this is because minimizing is somewhat less important that minimizing variance problematic for testing problems.

**Acknowledgments**

Omitted for anonymity.
References

C. Adam. Information theory in molecular biology. *Physics of Life Reviews*, 1:3–22, 2004.
M. Agaholzadeh, H. Soltanani-Zadeh, B. Araabi, and A. Aghaholzadeh. A hierarchical clustering based on mutual information maximization. In *Proc. of IEEE International Conference on Image Processing*, pages 277–280, 2007.
P. A. Alemany and D. H. Zanette. Fractal random walks from a variational formalism for Tsallis entropies. *Phys. Rev. E*, 49(2):R956–R958, Feb 1994. doi: 10.1103/PhysRevE.49.R956.
Gérard Biau and Luc Devroye. Entropy estimation. In *Lectures on the Nearest Neighbor Method*, pages 75–91. Springer, 2015.
L. Birge and P. Massart. Estimation of integral functions of a density. *A. Statistics*, 23:11–29, 1995.
B. Chai, D. B. Walther, D. M. Beck, and L. Fei-Fei. Exploring functional connectivity of the human brain using multivariate information analysis. In *NIPS*, 2009.
Kamalika Chaudhuri and Sanjoy Dasgupta. Rates of convergence for nearest neighbor classification. In *Advances in Neural Information Processing Systems*, pages 3437–3445, 2014.
Kamalika Chaudhuri, Samory Kpotufe, and Ulrike von Luxburg. Consistent procedures for cluster tree estimation and pruning. *Information Theory, IEEE Transactions on*, 60(12):7900–7912, 2014.
Bradley Efron and Charles Stein. The jackknife estimate of variance. *The Annals of Statistics*, pages 586–596, 1981.
M. N. Goria, N. N. Leonenko, V. V. Merger, and P. L. Novi Inverardi. A new class of random vector entropy estimators and its applications in testing statistical hypotheses. *J. Nonparametric Statistics*, 17:277–297, 2005.
A. O. Hero, B. Ma, O. Michel, and J. Gorman. Alpha-divergence for classification, indexing and retrieval, 2002a. Communications and Signal Processing Laboratory Technical Report CSPL-328.
A. O. Hero, B. Ma, O. J. J. Michel, and J. Gorman. Applications of entropic spanning graphs. *IEEE Signal Processing Magazine*, 19(5):85–95, 2002b.
K. Hlaváčkova-Schindler, M. Paluš, M. Vejmelka, and J. Bhattacharya. Causality detection based on information-theoretic approaches in time series analysis. *Physics Reports*, 441:1–46, 2007.
M. M. Van Hulle. Constrained subspace ICA based on mutual information optimization directly. *Neural Computation*, 20:964–973, 2008.
Kirthivasan Kandasamy, Akshay Krishnamurthy, Barnabas Poczos, Larry Wasserman, et al. Nonparametric von mises estimators for entropies, divergences and mutual informations. In *Advances in Neural Information Processing Systems*, pages 397–405, 2015.
Arich Kontorovich and Reu Weiss. A bayes consistent 1nn classifier. In *Proceedings of the Eighteenth International Conference on Artificial Intelligence and Statistics*, pages 480–488, 2015.
L. F. Kozachenko and N. N. Leonenko. A statistical estimate for the entropy of a random vector. *Problems of Information Transmission*, 23:9–16, 1987.
Samory Kpotufe and Ulrike von Luxburg. Pruning nearest neighbor cluster trees. *arXiv preprint arXiv:1105.0540*, 2011.
A. Krishnamurthy, K. Kandasamy, B. Poczos, and L. Wasserman. Nonparametric estimation of renyi divergence and friends. *In International Conference on Machine Learning (ICML), 2014.*
K. Kybic. Incremental updating of nearest-neighbor-based high-dimensional entropy estimation. In *Proc. Acoustics, Speech and Signal Processing*, 2006.
E. G. Learned-Miller and J. W. Fisher. ICA using spacings estimates of entropy. *J. Machine Learning Research*, 4:1271–1295, 2003.
Henri Lebesgue. Sur l’intégration des fonctions discontinues. In *Annales scientifiques de l’École normale supérieure*, volume 27, pages 361–450. Société mathématique de France, 1910.
N. Leonenko and L. Pronzato. Correction of ‘a class of Rényi information estimators for multidimensional densities’ *Ann. Statist.*, 36(2):2153–2182, 2010.
N. Leonenko, L. Pronzato, and V. Savani. A class of Rényi information estimators for multidimensional densities. *Annals of Statistics*, 35(5):2153–2182, 2007.
J. Lewi, R. Butera, and L. Paninski. Real-time adaptive information-theoretic optimization of neurophysiology experiments. In *Advances in Neural Information Processing Systems*, volume 19, 2007.
H. Liu, J. Laflerty, and L. Wasserman. Exponential concentration inequality for mutual information estimation. In *Neural Information Processing Systems (NIPS)*, 2012.
D. O. Loftsgaarden and C. P. Quesenberry. A nonparametric estimate of a multivariate density function. *Ann. Math. Statist.*, 36:1049–1051, 1965.
Jouni Lunnikainen and Eero Saksman. Every complete doubling metric space carries a doubling measure. *Proceedings of the American Mathematical Society*, 126(2):531–534, 1998.
YP Mack and Murray Rosenblatt. Multivariate k-nearest neighbor density estimates. *Journal of Multivariate Analysis*, 9(1):1–15, 1979.
Kevin Moon and Alfred Hero. Multivariate f-divergence estimation with confidence. In *Advances in Neural Information Processing Systems*, pages 2429–2438, 2014a.
Kevin R Moon and Alfred O Hero. Ensemble estimation of multivariate f-divergence. In *Information Theory (ISIT), 2014 IEEE International Symposium on*, pages 356–360. IEEE, 2014b.
N. Nguyen, M. J. Wainwright, and M. I. Jordan. Estimating divergence functionals and the likelihood ratio by convex risk minimization. *IEEE Transactions on Information Theory, To appear.*, 2010.
J. Oliwa, B. Poczos, and J. Schneider. Distribution to distribution regression. In *International Conference on Machine Learning (ICML), 2013*.
D. Pál, B. Poczos, and Cs. Szepesvári. Estimation of Rényi entropy and mutual information based on generalized nearest-neighbor graphs. In *Proceedings of the Neural Information Processing Systems*, 2010.
H. Peng and C. Drid. Feature selection based on mutual information: Criteria of max-dependency, max-relevance, and min-redundancy. *IEEE Trans On Pattern Analysis and Machine Intelligence*, 27, 2005.
P. Pérez-Cruz. Estimation of information theoretic measures for continuous random variables. In *Advances in Neural Information Processing Systems 21*, 2008.
B. Poczos and A. Lörincz. Independent subspace analysis using geodesic spanning trees. In *ICML*, pages 673–680, 2005.
B. Poczos and A. Lörincz. Identification of recurrent neural networks by Bayesian interrogation techniques. *J. Machine Learning Research*, 10:515–554, 2009.
B. Poczos and J. Schneider. On the estimation of alpha-divergences. In *International Conference on AI and Statistics (AISTATS)*, volume 15 of *JMLR Workshop and Conference Proceedings*, pages 609–617, 2011.
B. Poczos, L. Xiong, D. Sutherland, and J. Schneider. Nonparametric kernel estimators for image classification. In *25th IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, 2012.
C. Shan, S. Gong, and P. W. Mcowen. Conditional mutual information based boosting for facial expression recognition. In *British Machine Vision Conference (BMVC)*, 2005.
S. Singh and B. Poczos. Exponential concentration of a density functional estimator. In *Neural Information Processing Systems (NIPS)*, 2014a.
S. Singh and B. Poczos. Generalized exponential concentration inequality for Rényi divergence estimation. In *International Conference on Machine Learning (ICML)*, 2014b.
K. Sritharan, R. Raich, and A. Hero. Empirical estimation of entropy functions with confidence. Technical Report, [http://arxiv.org/abs/1012.4188](http://arxiv.org/abs/1012.4188) 2010.
K. Sritharan, D. Wei, and A. Hero. Ensemble estimators for multivariate entropy estimation, 2012a. [http://arxiv.org/abs/1203.5629](http://arxiv.org/abs/1203.5629).
Kumar Sritharan, Raúl Raich, and Alfred O Hero III. Estimation of nonlinear functionals of densities with confidence. *Information Theory, IEEE Transactions on*, 58(7):4135–4159, 2012b.
Z. Szabo, B. Poczos, and A. Lörincz. Undercomplete blind subspace deconvolution. *J. Machine Learning Research*, 8:1063–1095, 2007.
Zoltán Szabó. Information theoretic estimators toolbox. *Journal of Machine Learning Research*, 15:283–287, 2014.

[https://bitbucket.org/szzoli/ite/](https://bitbucket.org/szzoli/ite/)
A More General Setting

In the main paper, for the sake of clarity, we discussed only the setting of distributions on the $D$-dimensional unit cube $[0, 1]^D$. For sake of generality, we prove our results in the significantly more general setting of a set equipped with a metric, a base measure, a probability density, and an appropriate definition of dimension. This setting subsumes Euclidean spaces, in which $k$-NN methods are usually analyzed, but also includes, for instance, Riemannian manifolds.

Definition 1. (Metric Measure Space): A quadruple $(\mathbb{X}, d, \Sigma, \mu)$ is called a metric measure space if $(\mathbb{X}, d)$ is a complete metric space, $(\mathbb{X}, \Sigma, \mu)$ is a $\sigma$-finite measure space, and $\Sigma$ contains the Borel $\sigma$-algebra induced by $d$.

Definition 2. (Scaling Dimension): A metric measure space $(\mathbb{X}, d, \Sigma, \mu)$ has scaling dimension $D \in [0, \infty)$ if there exist constants $\mu_*, \mu^* > 0$ such that, $\forall r > 0, x \in \mathbb{X}$, $\mu_* \leq \frac{\mu(B(x, r))}{r^D} \leq \mu^*$. \[\square\]

Remark 3. The above definition of dimension coincides with $D$ in $\mathbb{R}^D$, where, under the $L^p$ metric and Lebesgue measure,

$$\mu_* = \mu^* = \frac{(2\Gamma(1 + 1/p))^D}{\Gamma(1 + D/p)}$$

is the usual volume of the unit ball. However, it is considerably more general than the vector-space definition of dimension. It includes, for example, the case that $\mathbb{X}$ is a smooth Riemannian manifold, with the standard metric and measure induced by the Riemann metric. In this case, our results scale with the intrinsic dimension of data, rather than the dimension of a space in which the data are embedded. Often, $\mu_* = \mu^*$, but leaving these distinct allows, for example, manifolds with boundary. The scaling dimension is slightly more restrictive than the well-studied doubling dimension of a measure, [Luukkainen and Saksman (1998)] which enforces only an upper bound on the rate of growth.

B Proofs of Lemmas

Lemma 2. Consider a metric measure space $(\mathbb{X}, d, \Sigma, \mu)$ of scaling dimension $D$, and a $\mu$-absolutely continuous probability measure $P$, with density function $p : \mathbb{X} \to [0, \infty)$ supported on

$$\mathcal{X} := \{x \in \mathbb{X} : p(x) > 0\}.$$

If $p$ is continuous on $\mathcal{X}$, then, for any $\rho > 0$, there exists a function $p_* : \mathcal{X} \to (0, \infty)$ such that

$$0 < p_*(x) \leq \inf_{r \in (0, \rho)} \frac{P(B(x, r))}{\mu(B(x, r))}, \quad \forall x \in \mathcal{X},$$

and, if $p$ is bounded above by $p^* := \sup_{x \in \mathcal{X}} p(x) < \infty$, then

$$\sup_{r \in (0, \rho]} \frac{P(B(x, r))}{\mu(B(x, r))} \leq p^* < \infty, \quad \forall r \in (0, \rho].$$

Proof: Let $x \in \mathcal{X}$. Since $p$ is continuous and strictly positive at $x$, there exists $\varepsilon \in (0, \rho]$ such that and, for all $y \in B(x, \varepsilon)$, $p(y) \geq p(x)/2 > 0$. Define

$$p_*(x) := \frac{p(x) \mu_*/2}{\mu^*} \left(\frac{\varepsilon}{\rho}\right)^D.$$
Then, for any \( r \in (0, \rho] \), since \( P \) is a non-negative measure, and \( \mu \) has scaling dimension \( D \),

\[
P(B(x,r)) \geq P(B(x,\varepsilon r/\rho)) \geq \mu(B(x,\varepsilon r/\rho)) \min_{y \in B(x,\varepsilon r/\rho)} p(y)
\]

\[
\geq \mu(B(x,\varepsilon r/\rho)) \frac{p(x)}{2}
\]

\[
\geq \frac{p(x)}{2} \mu^* \left( \frac{\varepsilon r}{\rho} \right)^D = p^*_*(x) \mu^* r^D \geq p^*_*(x) \mu(B(x, r)).
\]

Also, trivially, \( \forall r \in (0, \rho] \),

\[
P(B(x,r)) \leq \mu(B(x,r)) \max_{y \in B(x,\varepsilon r/\rho)} p(y) \leq p^*_*(x) \mu(B(x,r)).
\]

**Lemma 3.** Consider a metric measure space \((X, d, \Sigma, \mu)\) of scaling dimension \( D \), and a \( \mu \)-absolutely continuous probability measure \( P \), with continuous density function \( p : X \to [0, \infty) \) supported on

\[ X := \{ x \in X : p(x) > 0 \}. \]

For \( x \in X \), if \( r > \left( \frac{k}{p^*_*(x)n} \right)^{1/D} \), then

\[
\mathbb{P} \left[ \varepsilon_k(x) > r \right] \leq e^{-p^*_*(x)rDn} \left( e \frac{p^*_*(x)rDn}{k} \right)^k.
\]

and, if \( r \in \left[ 0, \left( \frac{k}{p^*_*(x)n} \right)^{1/D} \right) \), then

\[
\mathbb{P} \left[ \varepsilon_k(x) \leq r \right] \leq e^{-p^*_*(x)rDn} \left( e p^*_*(x)rDn \frac{k}{p^*_*(x)rDn} \right)^{kp^*_*(x)/p^*}.
\]

**Proof:** Notice that, for all \( x \in X \) and \( r > 0 \),

\[
\sum_{i=1}^{n} 1_{\{X_i \in B(x,r)\}} \sim \text{Binomial} \left( n, P(B(x,r)) \right),
\]

and hence that many standard concentration inequalities apply. Since we are interested in small \( r \) (and hence small \( P(B(x,r)) \)), we prefer bounds on relative error, and hence apply multiplicative Chernoff bounds. If \( r > \left( k/(p^*_*(x)n) \right)^{1/D} \), then, by definition of \( p^*_* \), \( P(B(x,r)) < k/n \), and so, applying the multiplicative Chernoff bound with \( \delta := \frac{p^*_*(x)rDn - k}{p^*_*(x)rDn} \geq 0 \) gives

\[
\mathbb{P} \left[ \varepsilon_k(x) > r \right] = \mathbb{P} \left[ \sum_{i=1}^{n} 1_{\{X_i \in B(x,r)\}} < k \right]
\]

\[
\leq \mathbb{P} \left[ \sum_{i=1}^{n} 1_{\{X_i \in B(x,r)\}} < (1 - \delta)n P(B(x,r)) \right]
\]

\[
\leq \left( \frac{e^{-\delta}}{(1 - \delta)^{1-\delta}} \right)^{nP(B(x,r))}
\]

\[
= e^{-p^*_*(x)rDn} \left( e p^*_*(x)rDn \frac{k}{p^*_*(x)rDn} \right)^{kp^*_*(x)/p^*}.
\]
Similarly, if \( r < (k/(p^*n))^{1/D} \), then, applying the multiplicative Chernoff bound with \( \delta := \frac{k-p^*rDn}{p^*rn} > 0 \),

\[
\mathbb{P}[\epsilon_k(x) < r] \leq \mathbb{P} \left[ \sum_{i=1}^n 1_{\{X_i \in B(x,r)\}} \geq k \right] \\
\leq \mathbb{P} \left[ \sum_{i=1}^n 1_{\{X_i \in B(x,r)\}} \geq (1+\delta)nP(B(x,r)) \right] \\
\leq \left( \frac{e^{\delta}}{(1+\delta)^{1+\delta}} \right)^{nP(B(x,r))} \\
\leq e^{-p(x)rDn} \left( \frac{c_{n^*}Dn}{k} \right)^{k_p(x)/p^*}.
\]

The bound we prove below is written in a somewhat different form from the version of Lemma 4 in the main paper. This form follows somewhat more intuitively from Lemma 3 but does not make obvious the connection to the asymptotic Erlang distribution. To derive the form in the paper, one simply integrates the integral below by parts, plugs in the function \( x \mapsto f \left( p_*(x)/\left(\frac{k/n}{eD}\epsilon_n \right) \right) \), and applies the bound \((e/k)^k \leq \frac{e}{\sqrt{k}}\).

**Lemma 4.** Consider the setting of Lemma 3 and assume \( X \) is compact with diameter \( \rho := \sup_{x,y \in X} d(x,y) \). Suppose \( f : (0, \rho) \rightarrow \mathbb{R} \) is continuously differentiable, with \( f' > 0 \). Then, for any \( x \in X \), we have the upper bound

\[
\mathbb{E}[f^+(\epsilon_k(x))] \leq f^+ \left( \left( \frac{k}{p_*(x)n} \right)^{1/k} \right) + \frac{(e/k)^k}{D(nP_*)^k} \int_k^{np_*(x)^\rho} e^{-y} y^D \frac{\rho_0^0 + \rho_1^0}{2} f' \left( \left( \frac{y}{nP_*(x)} \right)^{1/k} \right) dy,
\]

and the lower bound

\[
\mathbb{E}[f^-(\epsilon_k(x))] \leq f^- \left( \left( \frac{k}{p^*n} \right)^{1/k} \right) + \frac{(e/k)^k}{D(nP_*)^k} \int_0^{\kappa(x)} e^{-y} y^D \frac{\rho_0^0 + \rho_1^0}{2} f' \left( \left( \frac{y}{nP_*(x)} \right)^{1/k} \right) dy,
\]

where \( f^+(x) = \max \{0, f(x)\} \) and \( f^-(x) = -\min \{0, f(x)\} \) denote the positive and negative parts of \( f \), respectively, and \( \kappa(x) := kp_*(x)/p^* \).

**Proof:** For notational simplicity, we prove the statement for \( g(x) = f \left( np_*(x)^D \right) \); the main result follows by substituting \( f \) back in.

Define

\[
\epsilon_0^+ = f^+ \left( \left( \frac{k}{p_*(x)n} \right)^{1/k} \right) \quad \text{and} \quad \epsilon_0^- = f^- \left( \left( \frac{k}{p^*n} \right)^{1/k} \right).
\]

Writing the expectation in terms of the survival function,

\[
\mathbb{E}[f^+(\epsilon_k(x))] = \int_0^{\infty} \mathbb{P} \left[ f(\epsilon_k(x)) > \epsilon \right] d\epsilon \\
= \int_0^{\epsilon_0^+} \mathbb{P} \left[ f(\epsilon_k(x)) > \epsilon \right] d\epsilon + \int_{\epsilon_0^+}^{f^+(\rho)} \mathbb{P} \left[ f(\epsilon_k(x)) > \epsilon \right] d\epsilon, \\
\leq \epsilon_0^+ + \int_{\epsilon_0^+}^{f^+(\rho)} \mathbb{P} \left[ f(\epsilon_k(x)) > \epsilon \right] d\epsilon,
\]

since \( f \) is non-decreasing and \( \mathbb{P} [\epsilon_k(x) > \rho] = 0 \). By construction of \( \epsilon_0^+ \), for all \( \epsilon > \epsilon_0^+ \), \( f^{-1}(\epsilon) > (k/(p_*(x)n))^{1/D} \). Hence, applying Lemma 3 followed by the change of variables
When applying Lemma 3 followed the change of variables where C together with inequality (13), this gives the result (11). Together with (12), this gives the upper bound (10). Similar steps give

\[ \mathbb{E}[f(\varepsilon_k(x))] \leq \varepsilon_0 + \int_{\varepsilon_0}^{f^{-}(0)} \mathbb{P}[f(\varepsilon_k(x)) < -\varepsilon] \, d\varepsilon. \]  

(13)

Applying Lemma 3 followed the change of variables \( y = np_*(x) (f^{-1}(\varepsilon))^D \) gives

\[ \int_{\varepsilon_0}^{f^{-}(\rho)} \mathbb{P}[\varepsilon_k(x) > f^{-1}(\varepsilon)] \, d\varepsilon \leq \frac{(e/k)^k}{D(np_*(x))^{B}} \int_{k}^{np_*(x)p^D} e^{-y} \frac{e^{y}D_{k+1-D}}{D} f'(\left(\frac{y}{np_*(x)}\right)^{\frac{1}{D}}) \, dy, \]

Together with (12), this gives the upper bound (10). Similar steps give

\[ \mathbb{E}[f(\varepsilon_k(x))] \leq \varepsilon_0 + \int_{\varepsilon_0}^{f^{-}(0)} \mathbb{P}[f(\varepsilon_k(x)) < -\varepsilon] \, d\varepsilon. \]  

(13)

Applying Lemma 3 followed the change of variables \( y = np_*(x) (f^{-1}(\varepsilon))^D \) gives

\[ \int_{\varepsilon_0}^{f^{-}(\rho)} \mathbb{P}[\varepsilon_k(x) < f^{-1}(\varepsilon)] \, d\varepsilon \leq \frac{(e/\kappa(x))^{\kappa(x)}}{D(np_*(x))^\kappa(x)} \int_{0}^{n(x)} e^{-y} \frac{D\kappa(x) + 1}{D} f'(\left(\frac{y}{np_*(x)}\right)^{\frac{1}{D}}) \, dy, \]

Together with inequality (13), this gives the result (11).

B.1 Applications of Lemma 4

When \( f(x) = \log(x) \), (10) gives

\[ \mathbb{E}[\log_+(\varepsilon_k(x))] \leq \frac{1}{D} \log_+\left(\frac{k}{p_*(x)n}\right) + \left(\frac{e}{k}\right)^k \Gamma(k, k) \leq \frac{1}{D} \left(\log_+\left(\frac{k}{p_*(x)n}\right) + 1\right) \]

and (11) gives

\[ \mathbb{E}[\log_-(\varepsilon_k(x))] \leq \frac{1}{D} \left(\log_+\left(\frac{k}{p_*(x)n}\right) + \frac{e}{\kappa(x)} \gamma(\kappa(x), \kappa(x))\right) \]

\[ \leq \frac{1}{D} \left(\log_+\left(\frac{k}{p_*(x)n}\right) + \frac{1}{\kappa(x)}\right). \]  

(14)

(15)

For \( \alpha > 0 \), \( f(x) = x^\alpha \), (10) gives

\[ \mathbb{E}[\varepsilon_k^\alpha(x)] \leq \left(\frac{k}{p_*(x)n}\right)^{\frac{\alpha}{D}} + \left(\frac{e}{\kappa(x)}\right)^k \frac{\alpha \Gamma(k + \alpha/D, k)}{D(np_*(x))^{\alpha/D}} \]

\[ \leq C_2 \left(\frac{k}{p_*(x)n}\right)^{\frac{\alpha}{D}}, \]

(16)

where \( C_2 = 1 + \frac{\alpha}{D}. \) For any \( \alpha \in [-D\kappa(x), 0] \), when \( f(x) = -x^\alpha \), (11) gives

\[ \mathbb{E}[\varepsilon_k^\alpha(x)] \leq \left(\frac{k}{p_*(x)n}\right)^{\frac{\alpha}{D}} + \left(\frac{e}{\kappa(x)}\right)^k \frac{\alpha \gamma(\kappa(x) + \alpha/D, \kappa(x))}{D(np_*(x))^{\alpha/D}} \]

\[ \leq C_3 \left(\frac{k}{p_*(x)n}\right)^{\frac{\alpha}{D}}, \]

(17)

(18)

where \( C_3 = 1 + \frac{\alpha}{D\kappa(x) + \alpha}. \)

---

3 If need not be surjective, but the generalized inverse \( f^{-1} : [-\infty, \infty] \rightarrow [0, \infty] \) defined by \( f^{-1}(\varepsilon) := \inf\{x \in (0, \infty) : f(x) \geq \varepsilon\} \) suffices here.

4 \( \Gamma(s, x) := \int_{s}^{\infty} t^{s-1} e^{-t} \, dt \) and \( \gamma(s, x) := \int_{s}^{x} t^{s-1} e^{-t} \, dt \) denote the upper and lower incomplete Gamma functions respectively. We used the bounds \( \Gamma(s, x), x\gamma(s, x) \leq x^s e^{-x}. \)
C Proof of Bias Bound

Theorem 5. Consider the setting of Lemma 3. Suppose $p$ is $\beta$-Hölder continuous, for some $\beta \in (0, 2]$. Let $f : (0, \infty) \to \mathbb{R}$ be differentiable, and define $M_f : X \to [0, \infty)$ by

$$M_f(x) := \sup_{z \in [\frac{x}{p(x)}, \frac{x}{c}]} \|\nabla f(z)\|$$

(assuming this quantity is finite for almost all $x \in \mathcal{X}$). Suppose that

$$C_M := \mathbb{E}_{X \sim p} \left[ \frac{M_f(X)}{(p_*(X))^{\frac{\beta}{\gamma}}} \right] < \infty.$$  

Then, for $C_B := C_M L$,

$$\mathbb{E}_{X,X_1,\ldots,X_n \sim p} \left[ f(p_{\epsilon_k}(X)) - F(p) \right] \leq C_B \left( \frac{k}{n} \right)^{\frac{\beta}{\gamma}}.$$  

Proof: By construction of $p_*$ and $p^*$,

$$p_*(x) \leq p_*(x) = \frac{P(B(x, \varepsilon))}{\mu(B(x, \varepsilon))} \leq p^*.$$  

Also, by the Lebesgue differentiation theorem [Lebesgue, 1910], for $\mu$-almost all $x \in \mathcal{X}$,

$$p_*(x) \leq p(x) \leq p_*.$$  

For all $x \in \mathcal{X}$, applying the mean value theorem followed by inequality (16),

$$\mathbb{E}_{X_1,\ldots,X_n \sim p} \left[ \|f(p(x)) - f(p_{\epsilon_k}(x))\| \right] \leq \mathbb{E}_{X_1,\ldots,X_n \sim p} \left[ \|\nabla f(\xi(x))\| \|p(x) - p_{\epsilon_k}(x)\| \right]$$

$$\leq M_f(x) \mathbb{E}_{X_1,\ldots,X_n \sim p} \left[ |p(x) - p_{\epsilon_k}(x)| \right]$$

$$\leq \frac{M_f(x)LD}{D + \beta} \mathbb{E}_{X_1,\ldots,X_n \sim p} \left[ \frac{\varepsilon_\beta^k(x)}{p_*(x)n} \right]$$

$$\leq \frac{C_2 M_f(x)LD}{D + \beta} \left( \frac{k}{p_*(x)n} \right)^{\frac{\beta}{\gamma}}.$$  

Hence,

$$\mathbb{E}_{X_1,\ldots,X_n \sim p} \left[ F(p) - \hat{F}(p) \right] = \mathbb{E}_{X \sim p} \left[ \mathbb{E}_{X_1,\ldots,X_n \sim p} \left[ f(p(X)) - f(p_{\epsilon_k}(X)) \right] \right]$$

$$\leq \frac{C_2 LD}{D + \beta} \mathbb{E}_{X \sim p} \left[ \frac{M_f(X)}{(p_*(X))^{\frac{\beta}{\gamma}}} \right] \left( \frac{k}{n} \right)^{\frac{\beta}{\gamma}} = \frac{C_2 C_M LD}{D + \beta} \left( \frac{k}{n} \right)^{\frac{\beta}{\gamma}}.$$  

Lemma 6. Let $c > 0$. Suppose there exist $b_0 \in (0, \frac{1}{c})$, $c_0, \rho_0 > 0$ such that for all $x \in \mathcal{X}$ with $\varepsilon(x) := \text{dist}(x, \partial \mathcal{X}) < \rho_0$, $p(x) \geq c_0 e^{b_0}(x)$. Then,

$$\int_{\mathcal{X}} (p_*(x))^{-c} \, d\mu(x) < \infty.$$  

Proof: Let $\mathcal{X}_0 := \{x \in \mathcal{X} : \text{dist}(x, \partial \mathcal{X}) < \rho_0\}$ denote the region within $\rho_0$ of $\partial \mathcal{X}$. Since $p_*$ is continuous and strictly positive on the compact set $\mathcal{X} \setminus \mathcal{X}_0$, it has a positive lower bound $\ell := \inf_{x \in \mathcal{X} \setminus \mathcal{X}_0} (p_*(x))$ on this set, and it suffices to show

$$\int_{\mathcal{X} \setminus \mathcal{X}_0} (p_*(x))^{-c} \, d\mu(x) < \infty.$$  

14
For all $x \in X_0$,

$$p_*(x) \geq \frac{\min\{\ell, c_0 x^b_0(x)\}}{\mu(B(x, \sqrt{D}))}.

Hence,

$$\int_{X \setminus X_0} (p_*(x))^{-c} \, d\mu(x) \leq \int_{X \setminus X_0} \ell^{-c} \, d\mu(x) + \int_{X \setminus X_0} c_0^{-c} x^{-b_0/c}(x) \, d\mu(x).

The first integral is trivially bounded by $\ell^{-c}$. Since $\partial X$ is the union of $2D$ “squares” of dimension $D - 1$, the second integral can be reduced to the sum of $2D$ integrals of dimension 1, giving the bound

$$2Dc_0^{-c} \int_0^{\rho_0} x^{-b_0/c}(x) \, dx.

Since $b_0/c < 1$, the integral is finite.

\[ \text{D Proof of Variance Bound} \]

**Theorem 7. (Variance Bound)** Suppose that $B \circ f$ is continuously differentiable and strictly monotone. Assume that $C_{f,p} := \mathbb{E}_{X \sim P} \left[ B^2(f(p_*(X))) \right] < \infty$, and that $C_f := \int_0^\infty e^{-y} y^k f(y) < \infty$. Then, for

$$C_V := 2 (1 + N_{k,D}) (3 + 4k) (C_{f,p} + C_f), \quad \text{we have} \quad \mathbb{V} \left[ \hat{F}_B(P) \right] \leq \frac{C_V}{n}.

**Proof:** For convenience, define

$$H_i := B \left( f \left( \frac{k/n}{\mu(B(X_i, \varepsilon_k(X_i)))} \right) \right).

By the Efron-Stein inequality [Efron and Stein, 1981] and the fact that the $\hat{F}_B(P)$ is symmetric in $X_1, \ldots, X_n$,

$$\mathbb{V} \left[ \hat{F}_B(P) \right] \leq \frac{n}{2} \mathbb{E} \left[ (\hat{F}_B(P) - F'_B(P))^2 \right]

\leq n \mathbb{E} \left[ (\hat{F}_B(P) - F_{2:n})^2 + (\hat{F}_B(P) - F'_{2:n})^2 \right]

= 2n \mathbb{E} \left[ (\hat{F}_B(P) - F_{2:n})^2 \right],

where $\hat{F}'_B(P)$ denotes the estimator after $X_1$ is resampled, and $F_{2:n} := \frac{1}{n} \sum_{i=2}^n H_i$. Then,

$$n(\hat{F}_n(P) - F_{2:n}) = H_1 + \sum_{i=2}^n 1_{E_i} (H_i - H'_i),

where $1_{E_i}$ is the indicator function of the event $E_i = \{\varepsilon_k(X_i) \neq \varepsilon'_k(X_i)\}$. By Cauchy-Schwarz followed by the definition of $N_{k,D}$,

$$n^2(\hat{F}_n(P) - \hat{F}_{n-1}(P))^2 = \left( 1 + \sum_{i=2}^n 1_{E_i} \right) \left( H_1^2 + \sum_{i=2}^n 1_{E_i} (H_i - H'_i)^2 \right)

= (1 + N_{k,D}) \left( H_1^2 + \sum_{i=2}^n 1_{E_i} (H_i - H'_i)^2 \right)

\leq (1 + N_{k,D}) \left( H_1^2 + 2 \sum_{i=2}^n 1_{E_i} (H_i^2 + H'_i^2) \right).
Taking expectations, since the terms in the summation are identically distributed, we need to bound

\[
\mathbb{E} \left[ H_1^2 \right], \quad (19)
\]

\[
(n - 1) \mathbb{E} \left[ 1_{E_2} H_2^2 \right], \quad (20)
\]

and \( (n - 1) \mathbb{E} \left[ 1_{E_2} H_2^2 \right] \).

Bounding (19): Note that

\[
\mathbb{E} \left[ H_1^2 \right] = \mathbb{E} \left[ B^2 \left( f \left( \hat{p}_k(X_1) \right) \right) \right] = \mathbb{E} \left[ B^2 \left( g \left( \frac{p_*(x)}{p_0(x)} \right) \right) \right]
\]

for \( g(y) = f \left( p_*(x)/y \right) \). Applying the upper bound in Lemma 4 if \( B^2 \circ g \) is increasing,

\[
\mathbb{E} \left[ H_1^2 \right] \leq B^2(g(1)) + \frac{e\sqrt{k}}{\Gamma(k + 1)} C_1 = B^2(f(p_*(x))) + \frac{e\sqrt{k}}{\Gamma(k + 1)} C_1.
\]

If \( B^2 \circ g \) is decreasing, we instead use the lower bound in Lemma 4, giving a similar result. If \( B^2 \circ g \) is not monotone (i.e., if \( B \circ g \) takes both negative and positive values), then, since \( B \circ f \) is monotone (by assumption), we can apply the above steps to \( (B \circ g)_- \) and \( (B \circ g)_+ \), which are monotone, and add the resulting bounds.

Bounding (20): Since \( \{ \varepsilon_k(X_2) \neq \varepsilon'_k(X_2) \} \) is precisely the event that \( X_1 \) is amongst the \( k \)-NN of \( X_2 \), \( \mathbb{P} \left[ \varepsilon_k(X_1) \neq \varepsilon'_k(X_1) \right] = k/(n - 1) \). Thus, since \( E_2 \) is independent of \( \varepsilon_k(X_2) \) and

\[
(n - 1) \mathbb{E} \left[ 1_{E_2} H_2^2 \right] = (n - 1) \mathbb{E} \left[ 1_{E_2} \right] \mathbb{E} \left[ H_2^2 \right] = k \mathbb{E} \left[ H_2^2 \right] = k \mathbb{E} \left[ H_1^2 \right],
\]

and we can use the bound for (19).

Bounding (21): Since \( E_2 \) is independent of \( \varepsilon_{k+1}(X_2) \) and

\[
(n - 1) \mathbb{E} \left[ 1_{E_2} H_2^2 \right] = (n - 1) \mathbb{E} \left[ 1_{E_2} B^2 \left( f \left( \hat{p}_{k+1}(X_2) \right) \right) \right] = (n - 1) \mathbb{E} \left[ 1_{E_2} \right] \mathbb{E} \left[ B^2 \left( f \left( \hat{p}_{k+1}(X_2) \right) \right) \right] = k \mathbb{E} \left[ B^2 \left( f \left( \hat{p}_{k+1}(X_2) \right) \right) \right].
\]

Hence, we can again use the same bound as for (19), except with \( k + 1 \) instead of \( k \).

Combining these three terms gives the final result.