Extrapolation Towards Imaginary 0-Nearest Neighbour and Its Improved Convergence Rate

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Abstract

k-nearest neighbour (k-NN) is one of the simplest and most widely-used methods for supervised classification, that predicts a query’s label by taking weighted ratio of observed labels of k objects nearest to the query. The weights and the parameter k ∈ N regulate its bias-variance trade-off, and the trade-off implicitly affects the convergence rate of the excess risk for the k-NN classifier; several existing studies considered selecting optimal k and weights to obtain faster convergence rate. Whereas k-NN with non-negative weights has been developed widely, it was proved that negative weights are essential for eradicating the bias terms and attaining optimal convergence rate. However, computation of the optimal weights requires solving entangled equations. Thus, other simpler approaches that can find optimal real-valued weights are appreciated in practice. In this paper, we propose multiscale k-NN (MS-k-NN), that extrapolates unweighted k-NN estimators from several k ≥ 1 values to k = 0, thus giving an imaginary 0-NN estimator. MS-k-NN implicitly corresponds to an adaptive method for finding favorable real-valued weights, and we theoretically prove that the MS-k-NN attains the improved rate, that coincides with the existing optimal rate under some conditions.

1 Introduction

Supervised classification has been a fundamental problem in machine learning and statistics over the years. It is widely used in a number of applications, such as spam-mail filtering (Cristianini & Shawe-Taylor, 2000), music-genre categorization (Li et al., 2003), semantic scene classification (Boutell et al., 2004), medical diagnosis (Soni et al., 2011), speaker recognition (Ge et al., 2017) and so forth. Moreover, vast amounts of data have become readily available for anyone, along with the rapid development of information technology; taking it into account, potential demands for better classification methods have been still growing.

One of the simplest and most widely-used methods for supervised classification is k-nearest neighbour (k-NN; Fix & Hodges (1951) and Cover & Hart (1967)), where the k-NN estimator predicts a query’s label probability by taking the weighted ratio of observed labels of k objects nearest to the query, and the corresponding classifier specifies the class of objects via the predicted label probabilities. k-NN has strengths in its simplicity and flexibility over and above its statistical consistency (as k = k_n → ∞, k_n/n → 0, n → ∞), that is proved by Fix & Hodges (1951), Cover & Hart (1967) and Stone (1977). However, performance of such a simple k-NN heavily depends on the selection of parameters, i.e., the weights and k therein; inexhaustible discussions on optimal parameter selection have been developed for long decades (Györfi, 1981; Devroye et al., 1996; Boucheron et al., 2005; Audibert & Tsybakov, 2007; Samworth, 2012; Chaudhuri & Dasgupta, 2014; Anava & Levy, 2016; Cannings et al., 2017; Balsubramani et al., 2019).

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Thus the rate for unweighted $k$-NN with larger dimensionality values are computed and plotted for squared radius $r(k)^2 := \|X(k) - X\|^2$, where $X(k)$ is the $k$-th nearest point to the query $X_\ast$. Experiments are conducted 20 times. Dotted line represents the underlying true conditional expectation $\mathbb{E}(Y_\ast \mid X_\ast)$ of the query’s label $Y_\ast \in \{0,1\}$. Bias-variance trade-off is observed; larger bias and smaller variance as $k$ increases. (b) In an instance of the 20 experiments, proposed multiscale $k$-NN (MS-$k$-NN) extrapolates the 4 $k$-NN estimators to $k = 0$ through regression (18) via $r = r(k)$ with $r(0) := 0$. The imaginary 0-NN estimator predicts the true value very well.

A prevailing line of research in the parameter selection focuses on misclassification error rate of classifiers as the sample size $n$ grows asymptotically. They attempt to minimize the convergence rate of the excess risk, i.e., the difference of error rates between the classifier and Bayes-optimal classifier. The convergence rate depends on the functional form of the conditional expectation $\eta(x) := \mathbb{E}(Y \mid X = x)$ of the binary label $Y \in \{0,1\}$ given its feature vector $X \in \mathcal{X}(\subset \mathbb{R}^d)$, and its function class is specified by (i) $\alpha$-margin condition, (ii) $\beta$-Hölder condition, (iii) $\gamma$-neighbour average smoothness, that will be formally described in Definition 1, 2 and 3 later in Section 2. Roughly speaking, classification problems with larger $\alpha \geq 0, \beta > 0, \gamma > 0$ values are easier to solve, and the corresponding convergence rate becomes faster. On the other hand, classification problems with larger dimensionality $d > 0$ are harder, and the convergence rate becomes slower. The convergence rates for specific cases are summarized in Table 1.

| Classifier               | Convergence rate     |
|-------------------------|----------------------|
| Nadaraya-Watson         | $n^{-4/(4+d)}$       |
| Local polynomial†       | $n^{-2\beta/(2\beta+d)}$ |
| $k$-NN (unweighted)     | $n^{-4/(4+d)}$       |
| $k$-NN (with weights $\geq 0$) | $n^{-4/(4+d)}$   |
| $k$-NN (with weights $\in \mathbb{R}$) | $n^{-2\beta/(2\beta+d)}$ |
| **Multiscale $k$-NN**   | $n^{-2\beta/(2\beta+d)}$ |

†convergence rate of the uniform bound; others are non-uniform.

Györfi (1981) is the first work that proves the convergence rate $O(n^{-\gamma/(2\gamma+d)})$ for unweighted $k$-NN classifier by assuming the $\gamma$-neighbour average smoothness. However, this rate does not consider the margin condition; Chaudhuri & Dasgupta (2014) proves that the rate is further improved to $O(n^{-(1+\alpha)\gamma/(2\gamma+d)})$ by additionally imposing the $\alpha$-margin condition. Whereas the rate seems favorable, $\gamma$ is in fact upper-bounded by 2 due to the asymptotic bias of $k$-NN, even if highly-smooth function is considered ($\beta \geq 2$; see Theorem 1). Thus the rate for unweighted $k$-NN is $O(n^{-(1+\alpha)/(4+d)})$ at best.

As is widely known, $k$-NN estimator has much in common with Nadaraya-Watson (NW) estimator (Tsybakov, 2009). Hall & Kang (2005) considers a classifier based on the NW-estimator and obtains its convergence rate $O(n^{-4/(4+d)})$ for $\alpha = 1$ and twice-differentiable $\eta$; this rate is the same as the case $\alpha = 1$ of the unweighted...
$k$-NN. It is also widely known that the convergence rate of local polynomial (LP)-estimator (Tsybakov, 2009) is drastically improved from that of the NW-estimator, when approximating highly smooth functions; Audibert & Tsybakov (2007) considers a classifier based on the LP-estimator and a slightly different type of convergence rate, i.e., the uniform bound of the excess risk over all the possible $\eta$ and the distribution of $X$; the rate is $O(n^{-(1+\alpha)/\beta/(2\beta+d)})$. Audibert & Tsybakov (2007) also proves that the rate $O(n^{-(1+\alpha)/\beta/(2\beta+d)})$ is optimal among all the classifiers; thus the LP-classifier is proved to be an optimal classifier. However, caution is required to compare it with other rates, as non-uniform bound is only considered in this paper. Furthermore, the LP estimator is composed of polynomials of degree $|\beta| := \max\{β′ ∈ \mathbb{N}_0 | β′ < β\}$; it requires estimating coefficients of $1 + d d^2 + \cdots + d^{|\beta|}$ terms, resulting in high computational cost and difficulty in implementation.

Returning back to $k$-NN classifiers, which do not require such a large number of coefficients therein, Samworth (2012) considers the exact asymptotic expansion of the non-uniform bound of the excess risk, and finds the optimal weights for weighted $k$-NN. The exact convergence rate for the optimal $k$-NN classifier with non-negative weights is $O(n^{-4/(4+d)})$, where the rate is still same as the case $\alpha = 1$ of the unweighted $k$-NN. However, interestingly, Samworth (2012) also proves that real-valued weights including negative weights are essential for eradicating the bias and attaining the exact optimal rate $O(n^{-2\beta/(2\beta+d)})$ for $\eta ∈ \mathcal{C}_\beta$ with $\alpha = 1, \beta = 2u (u ∈ \mathbb{N})$.

**Current issue:** For the weighted $k$-NN, Samworth (2012) gives the asymptotic expansion of the excess risk and shows equations of the optimal real-valued weights to be satisfied. Although theories can be constructed without solving the equations, determining the weights explicitly is rather burdensome, where explicit solutions are shown for limited cases ($\beta = 2, 4$). Therefore, other simpler approaches to determine optimal weights are appreciated in practice.

**Contribution of this paper** is as follows. We propose multiscale $k$-NN (MS-$k$-NN), consisting of two simple steps: (1) unweighted $k$-NN estimators are computed for several $k \geq 1$ values, and (2) extrapolating them to $k = 0$ via regression, as explained in Figure 1. This algorithm computes an imaginary 0-NN estimator. Whereas the MS-$k$-NN is computed quite simply, it is expected to reduce the bias, and it implicitly corresponds to finding favorable real-valued weights for the weighted $k$-NN (Figure 2). Although the obtained weights are different from Samworth (2012), we prove that the MS-$k$-NN attains the improved convergence rate $O(n^{-(1+\alpha)/\beta/(2\beta+d)})$, that coincides with the optimal rate obtained in Samworth (2012), if $\alpha = 1, \beta = 2u (u ∈ \mathbb{N})$. Numerical experiments are conducted for performing MS-$k$-NN. Note that the regression of MS-$k$-NN requires only $1 + \lfloor \beta/2 \rfloor$ terms, much fewer than $1 + d_d^2 + \cdots + d^{|\beta|}$ terms used in the LP classifier.

**Organization** is as follows. After preliminaries in Section 2, existing classifiers and their convergence rates are revisited in Section 3. Proposed MS-$k$-NN and its properties are shown in Section 4 with numerical experiments in Section 5. We conclude this paper in Section 6. Related works are also listed in Supplement A.

Figure 2: Amongst all the experiments, $n = 1000, d = 10, u = C = 2, k_\ast = 100$. In (a), optimal non-negative (15) and real-valued (17) weights for weighted $k$-NN (14) considered in Samworth (2012) are plotted. In (b)–(d), real-valued weights (22), that are implicitly computed in the proposed MS-$k$-NN, are plotted for $k_v = k_v/V, r_v := (k_v/n)^{1/d} (v ∈ [V])$. $V$ is the number of k used for regression.

![Figure 2](image_url)
2 Preliminaries

Here we describe the problem setting in Section 2.1, notation in Section 2.2, and the conditions in Section 2.3.

2.1 Problem Setting

For a non-empty compact set $\mathcal{X} \subset \mathbb{R}^d$, $d \in \mathbb{N}$, a pair of random variables $(X,Y)$ takes values in $\mathcal{X} \times \{0,1\}$ with joint distribution $Q$, where $X$ represents a feature vector of an object, and $Y$ represents its binary class label to which the object belongs. $\mu$ represents the probability density function of $X$ and $\eta$ is the conditional expectation

$$\eta(x) = \mathbb{E}(Y \mid X = x).$$

Later in Section 2.3, $\alpha$-margin condition (Def. 1), $\beta$-Hölder condition (Def. 2) and $\gamma$-neighbour average smoothness (Def. 3) will be defined for the function $\eta$.

$D_n := \{(X_i,Y_i)\}_{i=1}^n$, $n \in \mathbb{N}$, and $(X_s,Y_s)$ are considered throughout this paper, where they are independent copies of $(X,Y)$; $D_n$ is called a sample, and $X_s$ is called a query. Given a query $X_s \in \mathcal{X}$, we consider predicting the corresponding label $Y_s$ by a classifier $\hat{g}_n : \mathcal{X} \to \{0,1\}$ using the sample $D_n$. The performance of a classifier $g$ is evaluated by the misclassification error rate

$$L(g) := \mathbb{P}_{X_s,Y_s}(g(X_s) \neq Y_s).$$

Under some mild assumptions, excess risk

$$\mathcal{E}(\hat{g}_n) := \mathbb{E}_{D_n}(L(\hat{g}_n)) - \inf_{g : \mathcal{X} \to \{0,1\}} L(g)$$

for various classifiers is proved to approach $0$ as $n \to \infty$. Note that the classifier $g_s(X) := 1(\eta(X) \geq 1/2)$ satisfies $L(g_s) = \inf_{g : \mathcal{X} \to \{0,1\}} L(g)$, and it is said to be Bayes-optimal (see, e.g., Devroye et al., 1996, Section 2.2).

Then, the asymptotic order of the excess risk $\mathcal{E}(\hat{g}_n)$ with respect to the sample size $n$ is called convergence rate; the goal of this study is to propose a classifier that (i) is practically easy to implement, and (ii) attains the optimal convergence rate.

2.2 Notation

For any given query $X_s \in \mathcal{X}(\subset \mathbb{R}^d)$ and a sample $D_n$, the index $1, 2, \ldots, n$ is re-arranged to be $(1),(2),\ldots,(n)$ s.t.

$$\|X_s - X(1)\|_2 \leq \|X_s - X(2)\|_2 \leq \cdots \leq \|X_s - X(n)\|_2$$

where Euclidean norm $\|\cdot\|_2 = (\sum_{i=1}^d x_i^2)^{1/2}$ is employed throughout this paper. Note that the re-arranged index $(1),(2),\ldots,(n)$ depends on the query $X_s$; we may also denote the index by $(1; X_s),(2; X_s),\ldots,(n; X_s)$.

$$B(X; r) := \{X' \in \mathcal{X} \mid \|X - X'\|_2 \leq r\} \subset \mathcal{X}$$

represents the $d$-dimensional closed ball centered at $x \in \mathcal{X}$ whose radius is $r > 0$.

$f(n) \asymp g(n)$ indicates that the asymptotic order of $f, g$ are the same, $\text{tr}A = \sum_{i=1}^d a_{ii}$ represents the trace of the matrix $A = (a_{ij}) \in \mathbb{R}^{d \times d}$, $1 = (1,1,\ldots,1)^T$ is a vector and $\mathbb{1}(\cdot)$ represents an indicator function. $[\beta] := \max\{\beta' \in \mathbb{N} \mid \beta' \leq \beta\}$ for $\beta > 0$, $[n] := \{1,2,\ldots,n\}$ for any $n \in \mathbb{N}$, and $\|x\|_\infty := \max_{i \in [d]} |x_i|$ for $x = (x_1,x_2,\ldots,x_d)$. Let $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$. For $q \in \mathbb{N}_0$, $C^q = C^q(\mathcal{X})$ represents a set of $q$-times continuously differentiable functions $f : \mathcal{X} \to \mathbb{R}$. 


2.3 Conditions

We first list three different types of conditions on the conditional expectation (1), in Definition 1, 2 and 3 below; they are considered in a variety of existing studies (Györfi, 1981; Devroye et al., 1996; Audibert & Tsybakov, 2007; Tsybakov, 2009; Chaudhuri & Dasgupta, 2014).

Definition 1 (α-margin condition). If there exist constants $L_\alpha \geq 0$, $\tilde{\alpha} > 0$ and $\alpha \geq 0$ such that

$$\mathbb{P}(|\eta(X) - 1/2| \leq t) \leq L_\alpha t^{\alpha},$$

for all $t \in (0, \tilde{\alpha}]$ and $X \in \mathcal{X}$, then $\eta$ is said to be satisfying α-margin condition, where $\alpha$ is called margin exponent.

The above margin condition represents how rapidly the function $\eta$ varies near the classification boundary. In addition, the following Hölder condition specifies the smoothness of functions by a user-specified parameter $\beta > 0$.

Definition 2 ($\beta$-Hölder condition). Let $T_{q,X_*}[\eta]$ be the Taylor expansion of a function $\eta$ of degree $q \in \mathbb{N}_0$ at $X_* \in \mathcal{X}$ (See, Definition 9 in Supplement for details). A function $\eta \in C^{[\beta]}(\mathcal{X})$ is said to be $\beta$-Hölder, where $\beta > 0$ is called Hölder exponent, if there exists $L_\beta > 0$ such that

$$|\eta(X) - T_{[\beta],X_*}[\eta](X)| \leq L_\beta \|X - X_*\|^{\beta}$$

for any $X, X_* \in \mathcal{X}$. Note that a function $\eta \in C(\mathcal{X})^\beta$ for $\beta \in \mathbb{N}$ and compact $\mathcal{X}$ is also $\beta$-Hölder.

The above definition (6) of Hölder continuity is employed in many studies, e.g., Audibert & Tsybakov (2007), and it reduces to

$$|\eta(X) - \eta(X_*)| \leq L_\beta \|X - X_*\|^{\beta}$$

for $0 < \beta \leq 1$. However, (6) and (7) are different for $\beta > 1$, where the latter is considered in Chaudhuri & Dasgupta (2014).

For describing the next condition, we consider $\eta^{(\infty)}(B) := \mathbb{E}(Y|X \in B)$, that is the conditional expectation of $Y$ given the event $X \in B$ for the set $B \subset \mathbb{R}^d$. It is expressed as

$$\eta^{(\infty)}(B) = \frac{\int_{B \cap \mathcal{X}} \eta(X) \mu(X) dX}{\int_{B \cap \mathcal{X}} \mu(X) dX},$$

where Chaudhuri & Dasgupta (2014) Lemma 9 proves that $\eta^{(\infty)}(B(X_*;r))$ asymptotically approximates the $k$-NN estimator (with roughly $r = \|X(k) - X_*\|_2$), that will be formally defined in Definition 5. Note that $\eta^{(\infty)}(B(X;r))$ is properly defined for any $X \in S(\mu)$, where

$$S(\mu) := \left\{X \in \mathcal{X} \mid \int_{B(X;r)} \mu(X) dX > 0, \forall r > 0\right\}$$

is the support of $\mu$. In this paper, we assume that $S(\mu)$ is compact. We then introduce a condition related to the smoothness of function $\eta^{(\infty)}$ as follows.

Definition 3 ($\gamma$-neighbour average smoothness). If there exists $L_\gamma, \gamma > 0$ such that

$$|\eta^{(\infty)}(B(X;r)) - \eta(X)| \leq L_\gamma r^{\gamma}$$

for all $r > 0$ and $X \in S(\mu)$, then the function $\eta$ is said to be $\gamma$-neighbour average smooth with respect to $\mu$, where $\gamma$ is called neighbour average exponent. A weaker version of this condition is used in Györfi (1981), where the constant $L_\gamma$ is replaced by a function $L_\gamma(X)$. A related but different condition called “($\alpha, L$)-smooth” is used in Chaudhuri & Dasgupta (2014); see Supplement C.

We last define an assumption on the density of $X$, that is also employed in Audibert & Tsybakov (2007).

Definition 4 (Strong density assumption). If there exist $\mu_{\min}, \mu_{\max} \in (0, \infty)$ such that $\mu_{\min} \leq \mu(X) \leq \mu_{\max}$ for all $X \in \mathcal{X}$, $\mu$ is said to be satisfying strong density assumption.
3 Existing Classifiers and Convergence Rates

In this section, we first define plug-in classifiers, including \( k \)-NN, Nadaraya-Watson and local polynomial (LP) classifiers in Section 3.1. Subsequently, we review existing studies on convergence rates for LP classifier in Section 3.2, unweighted \( k \)-NN classifier in Section 3.3 and weighted \( k \)-NN classifier in Section 3.4.

3.1 Plug-in Classifiers

In this paper, we consider only a plug-in classifier (Audibert & Tsybakov, 2007)

\[
g^{\text{(plug-in)}}(X; \hat{\eta}_n) := \mathbb{1}(\hat{\eta}_n(X) \geq 1/2),
\]

where \( \hat{\eta}_n(X) \) is an estimator of \( \eta(X) \), that leverages the sample \( D_n \). Given a query \( X_\ast \in \mathcal{X} \), some archetypal examples of the function value \( \hat{\eta}_n(X_\ast) \) are listed in the following.

**Definition 5.** (Unweighted) \( k \)-nearest neighbour (\( k \)-NN) estimator is defined as

\[
\hat{\eta}^{(k\text{NN})}_{n,k}(X_\ast) := \frac{1}{k} \sum_{i=1}^{k} Y_i \mathbb{1}(X_i \geq X_\ast),
\]

where \( (1; X_\ast), (2; X_\ast), \ldots, (n; X_\ast) \) is the re-arranged index defined in Section 2.2 and \( k \in \mathbb{N} \) is a user-specified parameter. Then, \( g^{(k\text{NN})}_{n,k}(X) := g^{\text{(plug-in)}}(X; \hat{\eta}^{(k\text{NN})}_{n,k}) \) is called \( k \)-nearest neighbour (\( k \)-NN) classifier.

Weighted \( k \)-NN will be similarly defined in Definition 8 in Section 3.4. In what follows, \( K : \mathcal{X} \to \mathbb{R} \) represents a kernel function, e.g., Gaussian kernel \( K(X) := \exp(-\|X\|^2) \), and \( h > 0 \) represents a bandwidth.

**Definition 6.** Nadaraya-Watson (NW) estimator is

\[
\hat{\eta}^{(NW)}_{n,h}(X_\ast) := \frac{\sum_{i=1}^{n} Y_i K\left(\frac{X_i - X_\ast}{h}\right)}{\sum_{i=1}^{n} K\left(\frac{X_i - X_\ast}{h}\right)}
\]

if the denominator is nonzero, and it is zero otherwise. \( g^{(NW)}_{n,h}(X) := g^{\text{(plug-in)}}(X; \hat{\eta}^{(NW)}_{n,h}) \) is called NW-classifier.

Here, we define a loss function

\[
\mathcal{L}_{n,h}(f, X_\ast) := \sum_{i=1}^{n} (Y_i - f(X_i - X_\ast))^2 K\left(\frac{X_i - X_\ast}{h}\right)
\]

for \( f : \mathcal{X} \to \mathbb{R} \); Using a constant function \( f(x) \equiv \theta \), NW estimator can be regarded as a minimizer \( \theta \in \mathbb{R} \) of (12). NW estimator is then generalized to the local polynomial (LP) estimator when \( Y_i \) is predicted by a polynomial function.

**Definition 7.** Let \( \mathcal{F}_q \) denotes the set of polynomial functions \( f : \mathcal{X} \to \mathbb{R} \) of degree \( q \in \mathbb{N}_0 \). Considering the function

\[
\hat{f}^{X_\ast}_{n,h,q} := \min_{f \in \mathcal{F}_q} \mathcal{L}_{n,h}(f, X_\ast),
\]

local polynomial (LP) estimator of degree \( q \) is defined as

\[
\hat{\eta}^{(LP)}_{n,h,q}(X_\ast) := \hat{f}^{X_\ast}_{n,h,q}(0)
\]

if \( \hat{f}^{X_\ast}_{n,h,q} \) is the unique minimizer of (13) and it is zero otherwise. The corresponding \( g^{(LP)}_{n,h,q}(X) := g^{\text{(plug-in)}}(X; \hat{\eta}^{(LP)}_{n,h,q}) \) is called LP classifier.

Note that LP classifier is computed via polynomial function of degree \( q \); they contain \( 1 + d + d^2 + \cdots + d^q \) terms therein, and it results in high computational cost if \( d, q \) are large.
3.2 Convergence Rate for LP Classifier

**Proposition 1** (Audibert & Tsybakov (2007) Th. 3.3). Let \( \mathcal{X} \) be a compact set, and assuming that (i) \( \eta \) satisfies \( \alpha \)-margin condition and is \( \beta \)-Hölder, and (ii) \( \mu \) satisfies strong density assumption, then the convergence rate of the LP classifier with the bandwidth \( h_n = h_n \preceq n^{-1/(2\beta+d)} \) is

\[
\mathcal{E}(\hat{g}_{n,h_n,X,*}) = O(n^{-(1+\alpha)/\beta + (2\beta+d)}).
\]

The above Proposition 1 indicates that, the convergence rate for the LP classifier is faster than \( O(n^{-1/2}) \) for \( \alpha\beta > d/2 \), and the rate is even faster than \( O(n^{-1}) \) for \( (\alpha-1)\beta > d \), though such inequalities are rarely satisfied since the dimension \( d \) is large in many practical situations.

Rigorously speaking, Audibert & Tsybakov (2007) considers the uniform bound of the excess risk over all the possible \((\eta,\mu)\), and Audibert & Tsybakov (2007) Theorem 3.5 proves the optimality of the rate, i.e., \( \sup_{(\eta,\mu)} \mathcal{E}(g) \geq 3C \cdot n^{-(1+\alpha)\beta/(2\beta+d)} \) for any classifier \( g \) when \( \alpha\beta < d \). LP classifier is thus proved to be an optimal classifier in this sense. However, the optimality is for uniform evaluation \( \sup_{(\eta,\mu)} \mathcal{E}(\cdot) \), but not the non-uniform evaluation \( \mathcal{E}(\cdot) \), that is considered in this paper; it remains unclear whether the (non-uniform) evaluation is still lower-bounded by \( n^{-(1+\alpha)\beta/(2\beta+d)} \) if sup is removed. In particular, the uniform bound of NW classifier (i.e., LP classifier with \( [\beta] = 0 \)) is \( O(n^{-2/(2\beta+d)}) \) for \( \alpha = \beta = 1 \), but it is slower than the convergence rate \( O(n^{-4/(4+d)}) \) of NW classifier.

We last note that the LP classifier leverages the polynomial of degree \( q \), that is defined in eq. (13); it contains \( 1 + d + d^2 + \cdots + d^q \) terms, resulting in high computational cost as the dimension \( d \) of feature vectors is usually not that small.

3.3 Convergence Rate for Unweighted \( k \)-NN Classifier

Here, we consider the simpler (unweighted) \( k \)-NN; the following Proposition 2 shows the convergence rate.

**Proposition 2** (A slight modification of Chaudhuri & Dasgupta (2014) Th. 4). Let \( \mathcal{X} \) be a compact set, and assuming that (i) \( \eta \) satisfies \( \alpha \)-margin condition and is \( \gamma \)-neighbour average smooth, and (ii) \( \mu \) satisfies strong density assumption. Then, the convergence rate of the unweighted \( k \)-NN classifier with \( k_* = k_n \approx n^{2\gamma/(2\gamma+1)} \) is

\[
\mathcal{E}(\hat{g}_{n,k_*}^{(kNN)}) = O(n^{-(1+\alpha)\gamma/(2\gamma+d)}).
\]

**Proof** Chaudhuri & Dasgupta (2014) Theorem 4(b) shows the convergence rate; see Supplement C for the correspondence of the assumption and symbols. \( \square \)

So our current concern is whether the convergence rate \( O(n^{-(1+\alpha)\gamma/(2\gamma+d)}) \) of the unweighted \( k \)-NN classifier can be associated to the rate \( O(n^{-(1+\alpha)\beta/(2\beta+d)}) \) of the LP classifier, that is already obtained in Proposition 1.

Chaudhuri & Dasgupta (2014) asserts that these two rates are the same, i.e., \( \gamma = \beta \), if there exists \( L_\beta > 0 \) such that (7) holds for any \( X, X_* \in \mathcal{X} \). Unfortunately, however, only constant functions can satisfy the condition (7) for \( \beta > 1 \) (Mittmann & Steinwart, 2003, Lemma 2.3); only an extremely restricted function class is considered in Chaudhuri & Dasgupta (2014).

We here return back to the \( \beta \)-Hölder condition (6) considered in this paper and Audibert & Tsybakov (2007), that is compatible with the condition (7) for \( \beta \leq 1 \) but is different for \( \beta > 1 \). Whereas a variety of functions besides constant functions satisfy the \( \beta \)-Hölder condition (6), our following Theorem 1 shows that \( \gamma = 2 \) even if \( \eta \) is highly smooth (\( \beta \gg 2 \)); the convergence rate for unweighted \( k \)-NN is bounded, regardless of the smoothness of \( \eta \).

**Theorem 1.** Let \( \mathcal{X} \) be a compact set, and let \( \beta > 0 \). Assuming that (i) \( \mu \) and \( \eta \mu \) are \( \beta \)-Hölder, and (ii) \( \mu \) satisfies the strong density assumption, there exist constants \( L_\beta > 0, \bar{r} > 0 \) and continuous functions \( b_1^*, b_2^*, \ldots, b_{[\beta/2]}^*, \delta_{\beta,r} : \mathcal{X} \to \mathbb{R} \) such that

\[
\eta^{(\infty)}(B(X_*;r)) - \eta(X_*) = \sum_{c=1}^{[\beta/2]} b_c^*(X_*) r^{2c} + \delta_{\beta,r}(X_*), \quad |\delta_{\beta,r}(X_*)| \leq L_\beta r^\beta
\]
for all $r \in (0, \bar{r}], X_\ast \in \mathcal{S}(\mu)$ defined in (9). Moreover, for $\beta > 2$, $b_\ast^1(X_\ast) = \frac{1}{2(d+4)\mu(X_\ast)}(\Delta[\eta(X_\ast)\mu(X_\ast)] - \eta(X_\ast)\Delta\mu(X_\ast))$ with $\Delta := \frac{\partial^2}{\partial x_1^2} + \cdots + \frac{\partial^2}{\partial x_d^2}$; if $\eta$ is $\beta(\geq 2)$-Hölder, $\eta$ is $(\gamma = 2)$-neighbour average smooth and

$$\mathcal{E}(\hat{g}^{(kNN)}_{\ast,n}) = O(n^{-2(1+\alpha)/(4+d)}).$$

Proof. The numerator and denominator of $\eta^{(\infty)}(B(X_\ast;r))$ are obtained via integrating Taylor expansions of $\eta\mu$ and $\mu$, respectively; division of the obtained polynomials proves the assertion. See, Supplement F for the detailed proof. \hfill \square

Note that, the rate with $\alpha = 1$ coincides with the rate $O(n^{-4/(4+d)})$ of NW-classifier (Hall & Kang, 2005) proved for the case $\alpha = 1$.

### 3.4 Weighted $k$-NN Classifier and Convergence Rate

We here consider weighted $k$-NN defined as follows.

**Definition 8.** Similarly to the unweighted $k$-NN (Def. 5), weighted $k$-NN estimator and classifier are defined as

$$\hat{g}^{(kNN)}_{\ast,n,k,w}(X_\ast) := \sum_{i=1}^k w_i Y_{(i)},$$

and $\hat{g}^{(kNN)}_{\ast,n,k,w}(X) := g^{(plug-in)}(X;\hat{g}^{(kNN)}_{\ast,n,k,w})$, respectively, where $w = (w_1, w_2, \ldots, w_k) \in \mathbb{R}^k$ represents a user-specified weight vector. It reduces to unweighted $k$-NN if $w = 1/k$.

Samworth (2012) first considers non-negative weights for the weighted $k$-NN; they find optimal weights

$$w_\ast^i := \frac{1}{k_\ast} \left(1 + \frac{d}{2} - \frac{d}{2k_\ast^2/d}(i^1+2/d - (i-1)^{1+2/d})\right)$$

for $i \in [k_\ast]$ and 0 otherwise, where $k_\ast \asymp n^{4/(d+4)}$, through the asymptotic expansion of the excess risk. However, the obtained rate is still $O(n^{-4/(4+d)})$ (Samworth (2012) Theorem 2), that is the same as the case $\alpha = 1$ of unweighted $k$-NN (Theorem 1); convergence evaluation of the $k$-NN still remains slow, even if arbitrary weights can be specified.

For further improving the convergence rate, Samworth (2012) also considers **real-valued weights** allowing negative values. The improved convergence rate is given in the following Proposition 3. Formal descriptions, i.e., definition of the weight set $\mathcal{W}_{n,s}$ and conditions for their rigorous proof, are described in Supplement D due to the space limitation.

**Proposition 3** (Samworth (2012) Th. 6). Let $\mathcal{W}_{n,s}$ be a set of real-valued weights defined in Supplement D, where we assume the conditions (i)–(iv) therein. Note that the condition (ii) implies $\eta \in C^\beta$, $\beta = 2u$ for $u \in \mathbb{N}$. If $(\alpha = 1)$-1-margin condition is assumed, then

$$\mathcal{E}(\hat{g}^{(kNN)}_{n,k,w}) \asymp \left\{B_1 \sum_{i=1}^n w_i^2 + B_2 \left(\sum_{i=1}^n \frac{d_i^{(u)}}{w_i \mu^{\ell/d}}\right)^2\right\} + o(1)$$

holds for $w \in \mathcal{W}_{n,s}$, where $B_1, B_2$ are some constants and $d_{\ell}^{(u)} := i^{1+2/\ell} - (i-1)^{1+2/\ell}$ if $\ell \in [u]$.

Following Proposition 3, Samworth (2012) shows that the asymptotic minimizer of (16) with the weight constraint $\sum_{i=1}^n w_i = 1, \sum_{i=1}^n d_i^{(u)} w_i = 0$ for all $\ell \in [u-1]$, and $w_i = 0$ for $i = k^*+1, \ldots, n$ with $k^* \asymp n^{2\beta/(2\beta+d)}$ is in the form of

$$w_\ast^i := (a_0 + a_1 d_1^{(1)} + \cdots + a_u d_i^{(u)})/k_\ast$$

(17)
for \( i = 1, 2, \ldots, k_s \), where \( \mathbf{a} = (a_0, a_1, \ldots, a_u) \in \mathbb{R}^{u+1} \) are unknowns. Samworth (2012) proposes to find optimal \( \mathbf{a} \) so that (17) satisfies the weight constraint. Then, the obtained weights lead to the following optimal rate.

**Corollary 1.** Symbols and assumptions are the same as those of Proposition 3. Then, the optimal \( \mathbf{w}_* \) and \( k_* \approx n^{2\beta/(2\beta+d)} \) lead to

\[
\mathcal{E}(\hat{g}_{n,k_*,\mathbf{w}_*}) \approx n^{-2\beta/(2\beta+d)}.
\]

Although only the case \( \alpha = 1 \) is considered in Samworth (2012), the convergence rate in Corollary 1 coincides with the rate for LP-classifier, given in Proposition 1.

Whereas theories can be constructed without solving the equations, solving the equations to determine the optimal real-valued weights explicitly is rather burdensome, where the explicit solution is shown only for \( u = 1, 2 \) (namely, \( \beta = 2, 4 \)) in Samworth (2012); the solution for \( u = 2 \) is

\[
a_1 := \frac{1}{(k_*)^{2/d}} \left\{ \frac{(d+4)^2}{4} - \frac{2(d+4)}{d+2} a_0 \right\}, \quad a_2 = \frac{1 - a_0 - (k_*)^{2/d} a_1}{(k_*)^{4/d}}
\]

(see, Supplement D for more details, and also see Figure 2(a) for the optimal weights computed in an experiment \( (u = 2) \)). Therefore, other simpler approaches to determine optimal real-valued weights are appreciated in practice.

### 4 Multiscale \( k \)-NN

In this section, we propose multiscale \( k \)-NN (MS-\( k \)-NN), that implicitly finds favorable real-valued weights for weighted \( k \)-NN. Note that the obtained weights are different from Samworth (2012), as illustrated in Figure 2. In what follows, we first describe the underlying idea in Section 4.1, and formally define MS-\( k \)-NN in Section 4.2. Subsequently, the weights obtained via MS-\( k \)-NN are shown in Section 4.3, the convergence rate is discussed in Section 4.4.

#### 4.1 Underlying Idea

Similarly to Samworth (2012), we consider eradicating the bias appeared in the conventional \( k \)-NN. In reality, the bias is non-negligible as shown in numerical experiments (Fig. 1).

Since \( \eta^{(\infty)}(B(X_*;r)) \) asymptotically approximates the \( k \)-NN estimator \( \hat{\eta}^{(\text{NN})}_{n,k}(X_*) \) for roughly \( r = r(k) := \|X(k) - X_*\| \) (see, e.g., Chaudhuri & Dasgupta (2014) Lemma 9), asymptotic expansion in Theorem 1 indicates that

\[
\hat{\eta}^{(\text{NN})}_{n,k}(X_*) \approx \eta(X_*) + \sum_{c=1}^{[\beta/2]} b^c r^{2c},
\]

for some \( \{b^c\} \subset \mathbb{R} \). Here, we consider estimating a regression function \( f_{X_*}(r) := b_0 + \sum_{c=1}^{[\beta/2]} b_c r^{2c} \) to predict the unweighted \( k \)-NN estimator \( \hat{\eta}^{(\text{NN})}_{n,k}(X_*) \); then, extrapolating the estimators from \( k > 0 \) to \( k = 0 \) via \( r = r(k) \) with \( r(0) := 0 \) yields \( \hat{f}_{X_*}(0) = \hat{b}_0 \approx \eta(X_*) \), and it is expected to ignore the bias term \( \sum b^c r^{2c} \).

#### 4.2 Computing Multiscale \( k \)-NN

In this section, we define the algorithm of MS-\( k \)-NN by following the underlying idea explained in the previous Section 4.1.

Let \( V, C \in \mathbb{N} \). Fix any query \( X_* \in \mathcal{X} \). We first compute unweighted \( k \)-NN estimators for \( 1 \leq k_1 < k_2 < \cdots < k_V \leq n \), i.e.,

\[
\hat{\eta}^{(\text{NN})}_{n,k_1}(X_*), \hat{\eta}^{(\text{NN})}_{n,k_2}(X_*), \ldots, \hat{\eta}^{(\text{NN})}_{n,k_V}(X_*).
\]
Then, we compute \( r_v := \|X_{(k_v)} - X_s\|_2 \), and consider a simple regression such that

\[
\hat{\eta}_{n,k_v}^{(k\text{NN})}(X_s) \approx b_0 + b_1 r_v^2 + b_2 r_v^4 + \cdots + b_C r_v^{2C}
\]

for all \( v \in [V] \), where \( b = (b_0, b_1, \ldots, b_C) \) is a regression coefficient vector to be estimated. Note that the regression function is a polynomial of \( r_v^2 \) which contains only terms of even degrees \( r_v^{2c} \), since all the bias terms are of even degrees as shown in Theorem 1. However, it is certainly possible that we employ a polynomial with terms of odd degrees in practical cases.

More formally, we consider a mimimization problem

\[
\hat{b} := \arg \min_{b \in \mathbb{R}^{C+1}} \sum_{v=1}^{V} \left( \hat{\eta}_{n,k_v}^{(k\text{NN})}(X_s) - b_0 - \sum_{c=1}^{C} b_c r_v^{2c} \right)^2.
\]

Then, we propose a multiscale \( k\text{-NN} \) (MS-\( k\text{-NN} \)) estimator

\[
\hat{\eta}_{n,k}^{(\text{MS-}k\text{-NN})}(X_s) := \hat{b}_0 \left( = z(X_s)^\top \hat{\eta}_{n,k}^{(k\text{NN})}(X_s) \right),
\]

where \( k = (k_1, k_2, \ldots, k_V) \in \mathbb{N}^V \), \( \hat{\eta}_{n,k}^{(k\text{NN})}(X_s) := (\hat{\eta}_{n,k_1}^{(k\text{NN})}(X_s), \ldots, \hat{\eta}_{n,k_V}^{(k\text{NN})}(X_s))^\top \in \mathbb{R}^V \) and \( z(X_s) \in \mathbb{R}^V \) will be defined in (21). Since (18) extrapolates \( k\text{-NN} \) estimators to \( r = 0 \), we also call the situation by "extrapolating to \( k = 0 \)" analogously. The corresponding MS-\( k\text{-NN} \) classifier is defined as \( \hat{g}_{n,k}^{(\text{MS-}k\text{-NN})}(X) := \hat{g}^{(\text{plug-in})}(X; \hat{\eta}_{n,k}^{(\text{MS-}k\text{-NN})}) \).

Note that the number of terms in the regression function (18) is \( 1 + C \), and \( C \) will be specified as \( C = \lfloor \beta/2 \rfloor \) under the \( \beta \)-Hölder condition in Theorem 2; overall number of terms is \( 1 + \lfloor \beta/2 \rfloor \), and is much less than the number of coefficients used in LP classifier (\( = 1 + d + d^2 + \cdots + d^{[\beta]} \)).

### 4.3 Corresponding Real-valued Weights

In this section, real-valued weights implicitly obtained via MS-\( k\text{-NN} \) are considered. These weights are only for theoretical interests, and they are not computed in practice.

The vector \( z(X_s) = (z_1(X_s), z_2(X_s), \ldots, z_V(X_s))^\top \in \mathbb{R}^V \) in the definition of MS-\( k\text{-NN} \) (20) is obtained by simply solving the minimization problem (19), as

\[
z(X_s) := \frac{(I - \mathcal{P}_R I(X_s)) \mathbbm{1}}{V - 1 \mathcal{P}_R \mathbbm{1}},
\]

where \( \mathbbm{1} = (1, 1, \ldots, 1)^\top \in \mathbb{R}^V \), \( \mathcal{P}_R = R(R^\top R)^{-1} R \) and \((i, j)\)-th entry of \( R = R(X_s) \) is \( r_i^{2j} \) for \( (i, j) \in [V] \times [C] \); note that the radius \( r_i \) depends on the query \( X_s \). Therefore, the corresponding optimal real-valued weight \( w^*_s(X_s) = (w^*_1(X_s), w^*_2(X_s), \ldots, w^*_{k_V}(X_s)) \) is obtained as

\[
w^*_v(X_s) := \sum_{v = 1}^{k_v} \frac{z_v(X_s)}{k_v} \in \mathbb{R}, \quad (\forall i \in [k_V]),
\]

then \( \hat{\eta}_{n,k_V,w^*_s}^{(k\text{NN})}(X_s) = \hat{g}_{n,k}^{(\text{MS-}k\text{-NN})}(X_s) \). Here, we note that the weight (22) is adaptive to the query \( X_s \), as each entry of the matrix \( R \) used in the definition of \( z \) (21) depends on both sample \( D_n \) and query \( X_s \). See Supplement E for the skipped derivation of the above (21) and (22). Total sum of the weights (22) is then easily proved as

\[
\sum_{i=1}^{k_V} w^*_v(X_s) = \sum_{v=1}^{V} z_v(X_s) = 1^\top z(X_s) \equiv 1.
\]
To give an example, Figure 2(b)–2(d) illustrate the optimal weights (22) for \( V = 5, 10, 20 \). The weights are not monotonically decreasing for \( i \leq k_v (= 100) \), and the weights are smoothly connected to \( w_{k_v+1}^v = 0 \) at \( i \approx k_v \), unlike Samworth (2012) shown in Figure 2(a).

Although the weights (22) can be easily computed, from application perspective, there is no need to calculate (22) explicitly; only a procedure needed for MS-\( k \)-NN is to conduct the regression (19) and specify \( \hat{\eta}_{n,k}^{(MS-kNN)} \) by the intercept \( \hat{b}_0 \) stored in the regression coefficient \( \hat{b} \). Then, MS-\( k \)-NN automatically coincides with the weighted \( k \)-NN using the above optimal weight (22).

### 4.4 Convergence Rate for MS-\( k \)-NN classifier

Here, we consider the convergence rate for MS-\( k \)-NN classifier. Firstly, we specify a vector \( \ell = (\ell_1, \ell_2, \ldots, \ell_V) \in \mathbb{R}^V \) so that \( \ell_1 = 1 < \ell_2 < \cdots < \ell_V < \infty \). We assume that

\[(C-1)\quad k_{1,n} \asymp n^{2\beta/(2\beta+d)},\]

\[(C-2)\quad k_v,n := \min \{k \in [n] \mid \|X(k) - X_*\|_2 \geq \ell_v r_{1,n}\} \quad \text{for} \quad v = 2, 3, \ldots, V, \quad \text{where} \quad r_{1,n} := \|X(k_{1,n}) - X_*\|_2,\]

\[(C-3)\quad \exists L_z > 0 \text{ such that } \|z_\ell\|_\infty < L_z, \text{ where } z_\ell = \frac{(\ell - P R)_1}{R_1} \text{ and } R = (\ell^2)_i j \in \mathbb{R}^{[V] \times [C]},\]

for all \( X_* \in S(\mu) \). Then, regarding the MS-\( k \)-NN estimator (19) and its corresponding MS-\( k \)-NN classifier, the following Theorem 2 holds.

**Theorem 2** (Convergence rate for MS-\( k \)-NN). Assuming that (i) \( \mu \) and \( \eta \mu \) are \( \beta \)-Hölder, (ii) \( \mu \) satisfies the strong density assumption, (iii) \( C := \lfloor \beta/2 \rfloor \leq V - 1 \), and (iv) the conditions (C-1)–(C-3) are satisfied. Then,

\[\mathcal{E}(\hat{\eta}_{n,k}^{(MS-kNN)}) = O(n^{-(1+\alpha)\beta/(2\beta+d)}).\]

**Proof.** Our proof almost follows that of Chaudhuri & Dasgupta (2014) Theorem 4(b), showing the convergence rate for unweighted \( k \)-NN classifier. However, the bias evaluation is different, as we consider \( \beta \)-Hölder condition and Chaudhuri & Dasgupta (2014) considers \( \gamma \)-neighbour average smoothness. See Supplement G for the detailed proof.

The rate obtained in Theorem 2 coincides with the optimal rate provided in Corollary 1; MS-\( k \)-NN is an optimal classifier, at least for the case \( \alpha = 1, \beta = 2u \ (u \in \mathbb{N}) \).

### 5 Numerical Experiments

In this Section, we conduct numerical experiments.

- **Datasets:** We employ datasets from UCI Machine Learning Repository (Dua & Graff, 2017). Each of datasets consists of \( d \)-dimensional \( n \) feature vectors \( X_i \in \mathcal{X} \), and their labels \( Y_i \in \{1, 2, \ldots, m\} \) representing 1 of \( m \) categories.

- **Preprocessing:** Feature vectors are first normalized, and then randomly divided into 70% for prediction (\( n_{\text{pred}} = \lfloor 0.7n \rfloor \)) and the remaining for test query.

- **Evaluation metric:** By employing some estimators, category of the query is predicted so that the corresponding estimator attains the maximum value. Then, the classification accuracy is evaluated via 30 times experiments. The MS-\( k \)-NN estimated via radius \( r(k) \) and that via log \( k \) described in Supplement B are performed with \( C = 1 \); they are compared with existing unweighted \( k \)-NN, and weighted \( k \)-NN with the optimal non-negative and real-valued weights (Samworth, 2012).

- **Parameter tuning:** For unweighted and weighted \( k \)-NN, we first fix theoretically optimal \( k := \max \{2, \lfloor n_{\text{train}}^{4/(4+d)} \rfloor \} \). For MS-\( k \)-NN, we choose \( k_v := \min_{k \in \mathbb{N}} \{\|X(k) - X_*\|_2 \geq c_v \cdot \|X(1) - X_*\|_2\} \), \( v \in [V], V = 4 \), so that \( r_v \approx c_v r_1 \), where \( c_1 = 1.5, c_2 = 2, c_3 = 2.5, c_4 = 3 \).
• **Results:** Sample mean and the sample standard deviation on 30 experiments are shown in Table 2. Overall, weighted $k$-NN and MS-$k$-NN show better score than unweighted $k$-NN ($w_i = 1/k$). MS-$k$-NN via radius $r(k)$ shows the best score for 8 out of 12 datasets; this number is maximum among all the methods considered. In contrast, MS-$k$-NN via log $k$ sometimes demonstrates slightly lower scores, for instance for Biodegradation dataset; seemingly, using the radius $r(k)$ is better than log $k$. At last, $k$-NN with optimal real-valued weights obtained in Samworth (2012) can be unstable; for instance, it shows much lower score than others, for Ecoli and Yeast datasets; larger sample sizes would be needed for receiving benefits from the asymptotic theory.

Table 2: Each dataset consists of $n$ feature vectors whose dimension is $d$; each object is labeled by 1 of $m$ categories. Sample average and the standard deviation for the prediction accuracy are computed on 30 times experiments. Best score is **colored blue and bolded**.

| Dataset       | $n$  | $d$ | $m$ | $k$-NN $w_i = 1/k$ (11) | $w_i \geq 0$ (15) | $w_i \in \mathbb{R}$ (17) | MS-$k$-NN $r(k)$ (20) | $\log k$ (23) |
|---------------|------|-----|-----|------------------------|-------------------|------------------------|---------------------|--------------|
| Banknote      | 1371 | 4   | 2   | 0.99 ± 0.00            | 0.99 ± 0.01       | 0.99 ± 0.01            | 1.00 ± 0.00         | 1.00 ± 0.00    |
| Diabetes      | 768  | 8   | 2   | 0.73 ± 0.03            | 0.73 ± 0.03       | 0.66 ± 0.03            | 0.73 ± 0.03         | 0.74 ± 0.02    |
| Ionsphere     | 350  | 34  | 2   | 0.43 ± 0.13            | 0.53 ± 0.14       | 0.53 ± 0.14            | 0.54 ± 0.14         | 0.53 ± 0.14    |
| Biodegradation| 1054 | 41  | 2   | 0.80 ± 0.02            | 0.83 ± 0.01       | 0.83 ± 0.01            | 0.86 ± 0.02         | 0.77 ± 0.02    |
| Spambase      | 4600 | 57  | 2   | 0.89 ± 0.01            | **0.91 ± 0.01**   | **0.91 ± 0.01**        | 0.86 ± 0.01         | 0.87 ± 0.01    |
| Iris          | 150  | 4   | 3   | **0.95 ± 0.03**        | **0.95 ± 0.03**   | 0.92 ± 0.04            | **0.95 ± 0.03**     | 0.94 ± 0.03    |
| Wireless      | 2000 | 7   | 4   | **0.98 ± 0.00**        | **0.98 ± 0.00**   | **0.98 ± 0.01**        | **0.98 ± 0.00**     | **0.98 ± 0.00** |
| Robot navigation | 5455 | 24  | 4   | 0.86 ± 0.01            | 0.86 ± 0.01       | 0.85 ± 0.01            | **0.87 ± 0.01**     | 0.81 ± 0.01    |
| Page blocks   | 5473 | 10  | 5   | 0.96 ± 0.00            | **0.97 ± 0.00**   | 0.95 ± 0.00            | 0.96 ± 0.00         | 0.96 ± 0.01    |
| Glass         | 213  | 9   | 6   | 0.65 ± 0.04            | **0.68 ± 0.06**   | **0.68 ± 0.05**        | 0.62 ± 0.05         | 0.59 ± 0.05    |
| Ecoli         | 335  | 7   | 8   | 0.84 ± 0.03            | **0.85 ± 0.03**   | 0.73 ± 0.04            | **0.85 ± 0.03**     | **0.85 ± 0.03** |
| Yeast         | 1484 | 8   | 10  | 0.57 ± 0.02            | 0.57 ± 0.02       | 0.46 ± 0.02            | **0.58 ± 0.02**     | 0.57 ± 0.02    |

6 Conclusion and Future Works

In this paper, we proposed multiscale $k$-NN (20), that extrapolates $k$-NN estimators from $k \geq 1$ to $k = 0$ via regression. MS-$k$-NN corresponds to finding favorable real-valued weights (22) for weighted $k$-NN, and it attains the convergence rate $O(n^{-(1+\alpha)(\beta/(2\beta+d))})$ shown in Theorem 2. It coincides with the optimal rate shown in Samworth (2012) in the case $\alpha = 1$, $\beta = 2u$ ($u \in \mathbb{N}$). For future work, it would be worthwhile to relax assumptions in theorems, especially the $\beta$-Hölder condition on $\mu$ and the limitation on the distance to Euclidean (4). Adaptation to small samples and high-dimensional settings are also appreciated.

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A  Related works

For choosing adaptive \( k = k(X_*) \) with non-negative weights \( w_i = 1/k \), i.e., \( k \) depending on the query \( X_* \), Balsubramani et al. (2019) considers the confidence interval of the \( k \)-NN estimator from the decision boundary, and Cannings et al. (2017) considers the asymptotic expansion used in Samworth (2012) and obtains the rate of \( O(n^{-4/(4+d)}) \), same rate as unweighted \( k \)-NN up to constant factor. Anava & Levy (2016) considers adaptive non-negative weights and \( k = k(X_*) \) but the approach is rather heuristic.

B  Using \( \log k \) as the predictor

The standard MS-\( k \)-NN predicts unweighted \( k \)-NN estimators through the radius \( r = r(k) \), that is computed via sample \( D_n \). As an alternative approach, we instead consider predicting the estimators directly from \( k \).

For clarifying the relation between the radius \( r_v := \|X_{(k_v)} - X_*\|_2 \) used in (18) is roughly proportional to \( k_v^{1/d} \) since the volume of the ball of radius \( r_v \) is proportional to \( r_v^d \).

Then, for sufficiently large \( d \),
\[
 r_v^2 \propto k_v^{2/d} = \exp \left( \frac{2}{d} \log k_v \right) = 1 + \frac{2}{d} \log k_v + O(d^{-2}). \tag{23}
\]

Thus, (18) can be expressed as a polynomial with respect to \( \log k_v \) instead of \( r_v^2 \). In numerical experiments, we then extrapolate unweighted \( k \)-NN to \( k = 1 \).

C  A Note on Proposition 2

Regarding the symbols, \((\alpha, \beta)\) in Chaudhuri & Dasgupta (2014) correspond to \((\bar{\gamma}, \alpha)\) in this paper, where \( \bar{\gamma} := \gamma/d \) is formally defined in the following. Chaudhuri & Dasgupta (2014) in fact employs “\((\alpha, L)\)-smooth” condition
\[
 |\eta(X_*) - \eta(\infty)(B(X_*; r))| \leq L \left( \int_{B(X_*; r)} \mu(X) dX \right)^{\bar{\gamma}}, \tag{24}
\]
which is different from our definition of the \( \gamma \)-neighbour average smoothness, i.e.,
\[
 |\eta(X_*) - \eta(\infty)(B(X_*; r))| \leq L_\gamma r^\gamma. \tag{25}
\]

However, their definition (24) can be obtained from our definition (25), by imposing an additional assumption \( \mu(X) \geq \mu_{\min} \) for all \( X \in X \). The proof is straightforward: the integrant in (24) is lower-bounded by
\[
 \int_{B(X_*; r)} \mu(X) dX \geq \mu_{\min} \frac{\pi^{d/2}}{\Gamma(1 + d/2)} r^d =: D r^d,
\]
then
\[
 |\eta(X_*) - \eta(\infty)(B(X_*; r))| \leq L_\gamma r^\gamma \leq L_\gamma \left( \frac{1}{D} \int_{B(X_*; r)} \mu(X) dX \right)^{\gamma/d} = L \left( \int_{B(X_*; r)} \mu(X) dX \right)^{\bar{\gamma}} \tag{25}
\]
by specifying \( L := L_\gamma / D^{\gamma/d} \), \( \tilde{\gamma} = \gamma / d \). Therefore, Chaudhuri & Dasgupta (2014) Theorem 4(b) proves Proposition 2, by considering the above correspondence of the symbols and the assumption.

D Samworth (2012) Theorem 6

For each \( s \in (0, 1/2) \), \( \mathcal{W}_{n,s} \) denotes the set of all sequences of real-valued weight vectors \( \mathbf{w}_n := (w_1, w_2, \ldots, w_n) \in \mathbb{R}^n \) satisfying

\[
\sum_{i=1}^{n} w_i = 1, \quad \frac{n^{2u/d}}{n^{2u/d}} \sum_{i=1}^{n} \delta_i^{(t)} u_i \leq \frac{1}{\log n} \quad (\forall t \in [u - 1]),
\]

\[
\sum_{i=1}^{n} u_i^2 \leq n^{-s},
\]

\[
n^{-4u/d} \sum_{i=1}^{n} \delta_i^{(u)} u_i^2 \leq n^{-s},
\]

\[
\exists k_2 \leq [n^{1-s}] \text{ s.t. } \frac{n^{2u/d}}{n^{2u/d}} \sum_{i=k_2+1}^{n} \sum_{i=1}^{n} \delta_i^{(u)} u_i^2 \leq \frac{1}{\log n} \quad \text{and } \sum_{i=1}^{k_2} \delta_i^{(u)} u_i \geq \beta k_2^{2u/d},
\]

where \( \delta_i^{(u)} = i^{1+2d/d} - (i-1)^{1+2d/d} \) for all \( t \in [u - 1] \).

For the rigorous proof, Samworth (2012) considers the following assumptions.

(i) \( \mathcal{X} \subset \mathbb{R}^d \) is a compact \( d \)-dimensional manifold with boundary \( \partial \mathcal{X} \),

(ii) \( \mathcal{S} := \{ x \in \mathcal{X} \mid \eta(x) = 1/2 \} \) is nonempty. There exists an open subset \( U_0 \subset \mathbb{R}^d \) that contains \( \mathcal{S} \) and such that the following properties hold: (1) \( \eta \) is continuous on \( U \setminus U_0 \), where \( U \) is an open set containing \( \mathcal{X} \), and (2) restrictions of \( P_0(X) := \mathbb{P}(X \mid Y = 0) \), \( P_1(X) := \mathbb{P}(X \mid Y = 1) \) to \( U_0 \) are absolutely continuous w.r.t. Lebesgue measure, with \( 2u \)-times continuously differentiable \((C^{2u}) \) Radon-Nikodym derivatives \( f_0, f_1 \), respectively. Since \( f_0, f_1 \in C^{2u} \), we also have \( \eta(x) = \mathbb{P}(Y = 1)f_1(x)/\{\mathbb{P}(Y = 0)f_0(x) + \mathbb{P}(Y = 1)f_1(x)\} \) is \( C^{2u} \).

(iii) There exists \( \rho > 0 \) such that \( \int_{\mathbb{R}^d} \|x^r\|^2 d\mathbb{P}(x) < \infty \). Moreover, for sufficiently small \( r > 0 \), the ratio \( \mathbb{P}(B(x; r))/(a dr^d) \) is bounded away from zero, uniformly for \( x \in \mathcal{X} \).

(iv) \( \partial \eta(x)/\partial x \neq 0 \) for all \( x \in \mathcal{X} \) and its restriction to \( \mathcal{S} \) is also nonzero for all \( x \in \mathcal{S} \cap \partial \mathcal{X} \).

Proposition 4 (Samworth (2012) Theorem 6). Assuming that (i)–(iv), it holds for each \( s \in (0, 1/2) \) that

\[
\mathcal{E}(\tilde{g}_{n,k,w}) = \left( B_1 \sum_{i=1}^{n} w_i^2 + B_2 \left( \sum_{i=1}^{n} \frac{\delta_i^{(u)} u_i}{\gamma^{2u/d}} \right)^2 \right) \{1 + o(1)\}
\]

for some constants \( B_1, B_2 > 0 \), as \( n \to \infty \), uniformly for \( \mathbf{w} \in \mathcal{W}_{n,s} \), and \( \delta_i^{(u)} := i^{1+2d/d} - (i-1)^{1+2d/d}, \ell \in [u - 1] \).

Whereas the weights are constrained as

\[
\sum_{i=1}^{n} w_i = 1, \quad \sum_{i=1}^{n} \delta_i^{(u)} w_i = 0 \quad (\forall \ell \in [u - 1]),
\]

(26)
and \( w_i = 0 \) for \( i = k^* + 1, \ldots, n \) with \( k^* \asymp n^{2\beta/(2\beta + d)} \). Samworth (2012) eq. (4.3) shows that the optimal weight should be in the form

\[
 w_i^* := \begin{cases} (a_0 + a_1 \delta_i^{(u)} + \cdots + a_n \delta_i^{(n)}) / k^* & (i \in [k^*]) \\ 0 & \text{(otherwise.)} \end{cases}.
\]  

(27)

Coefficients \( a = (a_0, a_1, \ldots, a_n) \) are determined by solving the equations (26) and (27) simultaneously; then the optimal weights are obtained by substituting it to (27).

They also show the asymptotic solution of the above equations, in the case of \( u = 2 \); the solution is

\[
 a_1 = \frac{1}{(k^*)^{2/d}} \left\{ \frac{(d + 4)^2}{4} - \frac{2(d + 4)}{d + 2} a_0 \right\}, \quad a_2 = \frac{1 - a_0 - (k^*)^{2/d} a_1}{(k^*)^{4/d}}.
\]

E Real-valued Weights Obtained via MS-k-NN

Let \( X_* \in \mathcal{X} \) any given query, and let denote \( k \)-NN estimator by \( \hat{\varphi}_{n,k} := \hat{\eta}_{n,k}^{(kNN)}(X_*) \). Considering

\[
 \hat{\varphi}_{n,k} = \varphi_{n,k}(X_*):= (\varphi_{n,k1}, \varphi_{n,k2}, \ldots, \varphi_{n,kV}) \in \mathbb{R}^V,
\]

(28)

\[
 R = R(X_*):= \begin{pmatrix} r^2_1 & r^4_1 & \cdots & r^{2C}_1 \\ r^2_2 & r^4_2 & \cdots & r^{2C}_2 \\ \vdots & \vdots & \ddots & \vdots \\ r^2_V & r^4_V & \cdots & r^{2C}_V \end{pmatrix} \in \mathbb{R}^{V \times C},
\]

(29)

\[
 A = A(X_*):= (1 R) \in \mathbb{R}^{V \times (C+1)},
\]

(30)

\[
 b = b(X_*):= (b_0, b_1, b_2, \ldots, b_C) \in \mathbb{R}^{C+1},
\]

(31)

the minimization problem (19) becomes

\[
 \hat{b} = \arg\min_{b \in \mathbb{R}^{C+1}} \sum_{v=1}^V \left( \hat{\eta}_{n,k}^{(kNN)}(X_*) - \sum_{c=0}^C b_c r^c_v \right) = \arg\min_{b \in \mathbb{R}^{C+1}} \| \varphi_{k,n} - A b \|^2 = \left( A^T A \right)^{-1} A^T \varphi_{k,n},
\]

Therefore, denoting the first row of the matrix (\( \bullet \)) by the vector \( z^T = (z_1, z_2, \ldots, z_V)^T \in \mathbb{R}^V \), MS-k-NN estimator is \( \hat{\eta}_{k,n}^{MS-kNN}(X_*) = b_0 = z^T \varphi_{k,n} \). To obtain the explicit form of \( z \), we hereinafter expand the matrix (\( \bullet \)).

Considering the inverse of block matrix

\[
 \begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} (A - BD^{-1}C)^{-1} & -(A - BD^{-1}C)^{-1}BD^{-1} \\ -D^{-1}C(A - BD^{-1}C)^{-1} & D^{-1} + D^{-1}C(A - BD^{-1}C)^{-1}BD^{-1} \end{pmatrix}
\]

(see, e.g., Petersen & Pedersen (2012) Section 9.1.3.), we have

\[
 \left( \begin{pmatrix} V \\ R^T 1 \end{pmatrix} 1^{T} R^{R^T} R \right)^{-1} = \left( \begin{pmatrix} V \\ R^T 1 \end{pmatrix} 1^{T} R^{R^T} R \right)^{-1} (1 R)^T 
\]

\[
 = \left( -\frac{1}{e^{(R^T R)^{-1} - 1} R^T 1} \left( \frac{1}{e} R^T R^{(R^T R)^{-1} - 1} R^T R \right)^{-1} \right) (1 R)^T, \quad \text{where}
\]

\[
 e := A - BD^{-1}C = V - 1^{T} R(R^T R)^{-1} R^T 1 \in \mathbb{R}.
\]

Therefore, its first column is,

\[
 z = \frac{1}{e} \left\{ I - R(R^T R)^{-1} R^T \right\} 1 = \frac{1}{V - 1^{T} R(R^T R)^{-1} R^T 1} \left\{ I - R(R^T R)^{-1} R^T \right\} 1 = \frac{(I - PR) 1}{V - 1^{T} PR 1}.
\]
where $P := R(R^T R)^{-1} R^T$ represents a projection matrix; the equation (21) is proved.

In addition, using the vector $z$,

$$
\hat{\eta}_{k,n}^{MS-kNN}(X) = z^T \phi_{k,n} = \sum_{v=1}^{V} z_v \hat{\eta}_{k,n}^{(kNN)} = \sum_{v=1}^{V} \frac{1}{k_v} \sum_{i=1}^{k_v} Y(i) = \sum_{i=1}^{k_v} w_i^* Y(i) = \eta_{n,k_v,w}(X),
$$

where

$$
w_i^* := \sum_{e=1 \leq k_v} \frac{z_v}{k_v} \in \mathbb{R}, \quad (\forall i \in [k_v]),
$$

is the real-valued weight obtained via MS-$k$-NN. Thus (22) is proved.

## F Proof of Theorem 1

We first prove Proposition 6 and its Corollary in the following Section F.1; subsequently, applying the Corollary proves Theorem 1.

### F.1 Preliminaries

In this section, we first formally define Taylor expansion of the multivariate function in the following Definition 9; Taylor expansion can approximate the function as shown in the following Proposition 5. Subsequently, we consider integrals of functions over a ball, in Proposition 6 and Corollary 2, for proving Theorem 1 in Section F.2.

**Definition 9** (Taylor expansion). Let $d \in \mathbb{N}$ and $q \in \mathbb{N} \cup \{0\}$. For $q$-times differentiable function $f : \mathcal{X} \to \mathbb{R}$, the Taylor polynomial of degree $q \in \mathbb{N} \cup \{0\}$ at point $X^* = (x_{1}^*, x_{2}^*, \ldots, x_{d}^*) \in \mathcal{X}$ is defined as

$$
T_q, X^*[f](X) := \sum_{s=0}^{q} \sum_{|i| = s} \frac{(X - X^*)^i}{i!} D^i f(X^*),
$$

where $i = (i_1, i_2, \ldots, i_d) \in (\mathbb{N} \cup \{0\})^d$ represents multi-index, $|i| = i_1 + i_2 + \cdots + i_d$, $X^i = x_1^{i_1} x_2^{i_2} \cdots x_d^{i_d}$, $i! = i_1! i_2! \cdots i_d!$ and $D^i = \frac{\partial^{|i|}}{\partial x_1^{i_1} \partial x_2^{i_2} \cdots \partial x_d^{i_d}}$.

**Proposition 5.** Let $d \in \mathbb{N}, \beta > 0$. If $f : \mathcal{X} \to \mathbb{R}$ is $\beta$-Hölder, there exists a function $\varepsilon_{\beta,X^*} : \mathcal{X} \to \mathbb{R}$ such that

$$
f(X) = T_{[\beta],X^*}[f](X) + \varepsilon_{\beta,X^*}(X),
$$

and $|\varepsilon_{\beta,X^*}(X)| \leq L_\beta \|X - X^*\|^\beta_2 \leq L_\beta r^\beta, \quad \forall X \in B(X^*; r)$, where $L_\beta$ is a constant for $\beta$-Hölder condition described in Definition 2.

**Proof of Proposition 5.** This Proposition 5 immediately follows from the definition of $\beta$-Hölder condition (Definition 2). \hfill $\square$

**Proposition 6.** Let $d \in \mathbb{N}, \beta > 0$ and let $f : \mathcal{X} \to \mathbb{R}$ be a $\beta$-Hölder function. Then, for any query
We first evaluate the term \( \int_{B(X_*,r)} f(X) dX = \sum_{u \in \{0\}^d} \frac{D^2 u f(X_*)}{(2u)!} \frac{g(u)}{|u| + d} r^{2|u| + d} + \bar{\epsilon}_\beta, \quad |\bar{\epsilon}_\beta| \leq L_{\beta} r^\beta + d \int_{B(0,1)} d\sigma \\
\) where \( g(u) := \frac{2\Gamma(u_1+1/2)\Gamma(u_2+1/2)\cdots\Gamma(u_d+1/2)}{\Gamma(u_1+u_2+\cdots+u_d+d/2)} \) and \( \Gamma(u) \) is Gamma function.

**Proof of Proposition 6.** Let \( q := \lfloor \beta \rfloor \). In this proof, we first calculate the Taylor expansion \( T_{q,X_*}[\eta](X) \). Then we integrate it over the ball \( B(X_*,r) \), by referring to Folland (2001).

Proposition 5 indicates that, there exists a function \( \epsilon_{\beta,X_*}(X) \) such that

\[
 f(X) = T_{q,X_*}[f](X) + \epsilon_{q,X_*}(X) = \sum_{i=0}^{q} \sum_{|i|=s} \frac{(X - X_*)^i}{i!} D^i f(X_*) + \epsilon_{\beta,X_*}(X)
\]

and \( |\epsilon_{\beta,X_*}(X)| \leq L_{\beta} r^\beta \), for all \( X \in B(X_*,r) \). Therefore, we have

\[
 \int_{B(X_*,r)} f(X) dX = \sum_{i=0}^{q} \sum_{|i|=s} \frac{D^i f(X_*)}{i!} \int_{B(X_*,r)} (X - X_*)^i dX = \int_{B(X_*,r)} \epsilon_{\beta,X_*}(X) dX.
\]

We first evaluate the term \( (*) \) in the following.

(a) If at least one entry of \( i = (i_1, i_2, \ldots, i_d) \) is odd number, i.e., there exists \( j \in [d], u \in \mathbb{N} \cup \{0\} \) such that \( i_j = 2u + 1 \), it holds that

\[
(*) = \int_{B(X_*,r)} (X - X_*)^i dX = \int_{B(0,r)} X^i dX = \int_{B(0,r')} X^{i_j - j} \left\{ \int_{\sqrt{r^2 - r'^2}} x_j^i d\sigma(x) \right\} d\sigma(x) = 0,
\]

where \( X^{-j} := (x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_d) \in \mathbb{R}^{d-1}, i^{-j} = (i_1, \ldots, i_{j-1}, i_{j+1}, \ldots, i_d) \in \{0\}^{d-1} \).

(b) Therefore, in the remaining, we consider the case that all of entries in \( i = (i_1, i_2, \ldots, i_d) \) are even numbers, i.e., there exist \( u_j \in \mathbb{N} \cup \{0\} \) such that \( i_j = 2u_j \) for all \( j \in [d] \). It holds that

\[
(*) = \int_{B(X_*,r)} (X - X_*)^i dX = \int_{B(0,r)} X^i dX
\]

\[
= \int_0^r \frac{1}{i^{|i|+d-1}} \int_{\partial B(0,r')} X^i d\sigma(\hat{x}) d\hat{r}, \quad (\text{: polar coordinate})
\]

\[
= g(u) \int_0^r \frac{1}{i^{|i|+d-1}} d\hat{r} = \frac{1}{|i| + d} g(u)
\]

where \( \partial B(X; \hat{r}) \) denotes a surface of the ball \( B(X; \hat{r}) \), \( \sigma \) represents \( (d-1) \)-dimensional surface measure, \( g(u) := \frac{2\Gamma(u_1+1/2)\Gamma(u_2+1/2)\cdots\Gamma(u_d+1/2)}{\Gamma(u_1+u_2+\cdots+u_d+d/2)} \) and \( \Gamma(u) \) is Gamma function.

Considering above (a) and (b), we have

\[
\int_{B(X_*,r)} f(X) dX = \sum_{|i| \leq q} \frac{D^i f(X_*)}{i!} \frac{g(u)}{|i| + d} r^{|i|+d} + \bar{\epsilon}_\beta
\]
Therefore, the assertion is proved.

\[
\text{Proof of Corollary 2.} \text{ Proposition 6 immediately proves the assertion.}
\]

\textbf{F.2 Main body of the proof}

For the function

\[
\eta^{(\infty)}(B(X_\ast; r)) = \frac{\int_{B(X_\ast; r)} \eta(x) \mu(x) dx}{\int_{B(X_\ast; r)} \mu(x) dx},
\]

(32)

Corollary 2 indicates that there exist

\[
a_1 = b_1(\eta \mu, X_\ast), a_2 = b_2(\eta \mu, X_\ast), \ldots, a_{\lfloor \beta/2 \rfloor} = b_{\lfloor \beta/2 \rfloor}(\eta \mu, X_\ast) \in \mathbb{R},
b_1 = b_1(\mu, X_\ast), b_2 = b_2(\mu, X_\ast), \ldots, b_{\lfloor \beta/2 \rfloor} = b_{\lfloor \beta/2 \rfloor}(\mu, X_\ast) \in \mathbb{R}
\]

(33)

and \(\varepsilon^{(1)}_\beta, \varepsilon^{(2)}_\beta \in \mathbb{R}\) such that

\[
(32) = \frac{\frac{g(0)r^d}{d} \eta(X_\ast) \mu(X_\ast) + \sum_{c=1}^{\lfloor \beta/2 \rfloor} a_c r^{2c+d} + \varepsilon^{(1)}_\beta}{\frac{g(0)r^d}{d} \mu(X_\ast) + \sum_{c=1}^{\lfloor \beta/2 \rfloor} b_c r^{2c+d} + \varepsilon^{(2)}_\beta}, \quad |\varepsilon^{(1)}_\beta|, |\varepsilon^{(2)}_\beta| \leq L_\beta r^{\beta+d} \int_{B(0;1)} dx,
\]

(34)

since \(\mu\) and \(\eta \mu\) are \(\beta\)-Hölder. Both the numerator and denominator are divided by \(r^d\), then for sufficiently small \(r > 0\), the asymptotic expansion is of the form

\[
(34) = \eta(X_\ast) + \sum_{c=1}^{\lfloor \beta/2 \rfloor} b_c^* r^{2c} + \delta_{\beta, r}(X_\ast),
\]

(35)

where \(\delta_{\beta, r}(X_\ast) = O(r^{2\lfloor \beta/2 \rfloor + 2}) + O(r^\beta)\). The two error terms are in fact combined as \(\delta_{\beta, r}(X_\ast) = O(r^\beta)\), because \(2\lfloor \beta/2 \rfloor + 2 \geq \beta\). Thus, by specifying a sufficiently small \(\tilde{r} > 0\), the error term is bounded as \(\delta_{\beta, \tilde{r}}(X_\ast) < L_{\beta}^* r^{\beta}\) for \(r \in (0, \tilde{r}]\) with a continuous function \(L_{\beta}^*(X_\ast)\). For \(L_{\beta}^* = \sup_{X \in S(\mu)} L_{\beta}^*(X_\ast) < \infty\), we have

\[
(35) = \eta(X_\ast) + \sum_{c=1}^{\lfloor \beta/2 \rfloor} b_c^* r^{2c} + \delta_{\beta, \tilde{r}}(X_\ast), \quad |\delta_{\beta, r}(X_\ast)| < L_{\beta}^* r^{\beta}, \quad (\forall r \in (0, \tilde{r}], X_\ast \in S(\mu)).
\]
Thus proving the assertion. Note that, by rearranging the terms of order $r^{2+d}$, we obtain the equation

$$g(0) \frac{d}{d} \mu(X_*) b^*_1 + \eta(X_*) b_1 = a_1,$$

where $a_1 := \frac{1}{2 + d} \sum_{u=1} D^2 u (\eta(X_*) \mu(X_*)) g(u), b_1 := \frac{1}{2 + d} \sum_{u=1} D^2 u (\mu(X_*)) g(u)$; subsequently, solving the equation yields

$$b^*_1 = \frac{1}{2 + d} \mu(X_*) \sum_{u=1} \left\{ \frac{D^2 u (\eta(X_*) \mu(X_*))}{(2u)!} - \eta(X_*) D^2 u (\mu(X_*)) \right\} \frac{g(u)}{g(0)}$$

$$= \frac{1}{2 + d} \mu(X_*) \left\{ \frac{\Delta \eta(X_*) \mu(X_*) - \eta(X_*) \Delta \mu(X_*)}{2 \Gamma(1/2)^d \Gamma(3/2)/\Gamma(1 + d/2)} \right\}$$

$$= \frac{1}{2 + d} \mu(X_*) \left\{ \frac{\Delta \eta(X_*) \mu(X_*) - \eta(X_*) \Delta \mu(X_*)}{2 \Gamma(1/2)^d \Gamma(3/2)/\Gamma(1 + d/2)} \right\}$$

In general, $b^*_1 \neq 0$, thus $\gamma = 2$ for $\beta > 2$. For the case of $\beta = 2$, we have $|\beta/2| = 0$, thus (34) = $\gamma(X_*) + O(r^\beta)$, meaning $\gamma = 2$.

\section{Proof of Theorem 2}

We basically follow the proof of Chaudhuri & Dasgupta (2014) Theorem 4(b). In Section G.1, we first define symbols used in this proof. In Section G.2, we describe the sketch of the proof and main differences between our proof and that of Chaudhuri & Dasgupta (2014) 4(b). Section G.3 shows the main body of the Proof, by utilizing several Lemmas listed in Section G.4.

\subsection*{G.1 Definitions of symbols}

- **$k$ and radius $r$:** We first specify a real-valued vector $\ell = (\ell_1, \ell_2, \ldots, \ell_V) \in \mathbb{R}^V$ satisfying $\ell_1 = 1 < \ell_2 < \cdots < \ell_V$. $k_{1,n} \succ n^{-2\beta/(2\beta+d)}$ is assumed in (C-1), and in (C-2), $\{k_{v,n}\}$ are specified so that

$$k_{v,n} = \min\{k \in [n] | \|X(k) - X_*\|_2 \geq r_{v,n}\}, \quad \forall v \in \{2, 3, \ldots, V\}$$

from $r_{1,n} := \|X(k_{1,n}) - X_*\|_2$. Then, for $r_{v,n} := \|X(k_{v,n}) - X_*\|_2$, $v = 2, \ldots, V$, we have $r_{v,n}/r_{1,n} \to \ell_v$.

- **Estimators:** Similarly to Supplement E, we denote the $k$-NN estimators and MS-$k$-NN estimator by

\begin{align*}
\varphi_{n,k} &= \varphi_{n,k}(X_*) := \frac{1}{k} \sum_{i=1}^k Y(i,X_*) \in \mathbb{R} \\
\varphi_{n,k} &= \varphi_{n,k}(X_*) := (\varphi_{n,k_1}(X_*), \varphi_{n,k_2}(X_*), \ldots, \varphi_{n,k_V}(X_*)) \in \mathbb{R}^V, \\
\rho_{n,k} &= \rho_{n,k}(X_*) := z_{n,k}(X_*)^\top \varphi_{n,k}(X_*) \in \mathbb{R},
\end{align*}

where $z_{n,k}(X_*) \in \mathbb{R}^V$ denotes vector $z$ considered in Supplement E, i.e.,

$$z_{n,k}(X_*) := \frac{(I - \mathcal{P}_{R_{n,k}(X_*)}) \mathbf{1}}{V - \mathbf{1}^\top \mathcal{P}_{R_{n,k}(X_*)} \mathbf{1}}$$

where $\mathcal{P}_R := R(R^\top R)^{-1}R^\top$ and the $(i,j)$-th entry of the matrix $R_{n,k}(X_*)$ is $r_{i,j} = \|X(k_i) - X_*\|_2^2$. Whereas the vector $z_{n,k}(X_*)$ is simply denoted by $z$ in the above discussion, here we emphasize the dependence to the sample $D_n$, parameters $k = (k_1, k_2, \ldots, k_V)$ and the query $X_*$. 

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We here define the asymptotic variants of the estimators by
\[
\begin{align*}
\varphi^{(\infty)}_r &= \varphi^{(\infty)}_r(X) := \eta^{(\infty)}(B(X; r)) \in \mathbb{R}, \\
\varphi^{(\infty)}_r(X) &= \varphi^{(\infty)}_r(X) := (\varphi^{(\infty)}_1(X), \varphi^{(\infty)}_2(X), \ldots, \varphi^{(\infty)}_{r_V}(X)) \in \mathbb{R}^V, \\
\rho^{(\infty)}_r(X) &= \rho^{(\infty)}_r(X) := x^T \varphi^{(\infty)}_r(X) \in \mathbb{R},
\end{align*}
\]
where \( r = (r_1, r_2, \ldots, r_V) \),
\[
z_r = \frac{(I - P_R)1}{V - 1}' P_R 1,
\]
and the \((i, j)\)-th entry of the matrix \( R \) is \( r_i^j \).

- **Point-wise errors** for \((X_s, Y_s) \in \mathcal{X} \times \{0, 1\}\) are defined as
\[
R_{n,k}(X_s, Y_s) := \mathbb{I}(\rho_{n,k}(X_s) \neq Y_s), \quad R_s(X_s, Y_s) := \mathbb{I}(g_s(X_s) \neq Y_s),
\]
where \( g_s(X) := \mathbb{I}(\eta(X) \geq 1/2) \) is the Bayes-optimal classifier equipped with \( \eta(X) := \mathbb{E}(Y | X) \).

- **A minimum radius** whose measure of the ball is larger than \( t > 0 \), i.e.,
\[
\hat{r}_t(X) := \inf \left\{ r > 0 \left| \int_{B(X; r)} \mu(X) dX \geq t \right. \right\}.
\]

- **Sets for the decision boundary with margins** are defined as
\[
\begin{align*}
\mathcal{X}^{+}_{t,\Delta} &= \left\{ X \in S(\mu) \mid \eta(X) > \frac{1}{2}, \quad \varphi^{(\infty)}_r(X) \geq \frac{1}{2} + \Delta, \quad \forall r \leq \hat{r}_t(X) \right\}, \\
\mathcal{X}^{-}_{t,\Delta} &= \left\{ X \in S(\mu) \mid \eta(X) < \frac{1}{2}, \quad \varphi^{(\infty)}_r(X) \leq \frac{1}{2} - \Delta, \quad \forall r \leq \hat{r}_t(X) \right\}, \\
\partial_{t,\Delta} &= \mathcal{X} \setminus (\mathcal{X}^{+}_{t,\Delta} \cup \mathcal{X}^{-}_{t,\Delta}),
\end{align*}
\]
where \( S(\mu) \) is defined in (9), and \( r \) is meant for \( r_1 \).

**G.2 Sketch of the proof**

**Sketch of the proof:** We mainly follow the proof of Chaudhuri & Dasgupta (2014) Theorem 4(b), that proves the convergence rate for the unweighted \( k \)-NN estimator. Similarly to Chaudhuri & Dasgupta (2014) Lemma 7, we first consider decomposing the difference between point-wise errors \( R_{n,k}(X_s, Y_s) - R_s(X_s, Y_s) \) as shown in the following Lemma 1; this Lemma plays an essential role for proving Theorem 1.

Subsequently, we consider the following two steps using Lemma 1–7:
\begin{enumerate}
\item taking expectation of the decomposition w.r.t. sample \( \mathcal{D}_n \) for showing point-wise excess risk, (cf. Chaudhuri & Dasgupta (2014) Lemma 20)
\item further taking expectation w.r.t. the query \((X_s, Y_s)\), and evaluate the convergence rate. (cf. Chaudhuri & Dasgupta (2014) Lemma 21)
\end{enumerate}

Then, the assertion is proved.

**Main difference** between the Proof of Chaudhuri & Dasgupta (2014) and ours is bias evaluation. Chaudhuri & Dasgupta (2014) leverages the \( \gamma \)-neighbour average smoothness condition
\[
(\text{asymptotic bias of } k\text{-NN}) \quad | \frac{\varphi^{(\infty)}_r(X_s)}{\varphi^{(\infty)}_r(X_s)} - \eta(X_s)| \leq L_\gamma r^\gamma,
\]

(\text{asymptotic) } k\text{-NN}
that represents the asymptotic bias of the \( k \)-NN, where \( \gamma \) is upper-bounded by 2 even if highly-smooth function is employed (\( \beta \gg 2 \); Theorem 1). However, MS-\( k \)-NN asymptotically satisfies an inequality

\[
\text{(asymptotic bias of MS-}\ k\text{-NN) \quad | \hat{\mu}_{\ell}^{(\infty)}(X_i) - \eta(X_i)| \leq L_{\beta}^{**} r^\beta
\]

for any \( \beta > 0 \), as formally described in Lemma 2. By virtue of the smaller asymptotic bias, Lemma 4 proves that smaller margin is required for the decision boundary, in order to evaluate the convergence rate; it results in the faster convergence rate.

Although the the bias evaluation is different, variance evaluation for MS-\( k \)-NN is consequently almost similar to the \( k \)-NN, as MS-\( k \)-NN can be regarded as a linear combination of several \( k \)-NN estimators, i.e.,

\[
\rho_{n,k}(X_s) = z_{n,k}(X_s)^T \varphi_{n,k}(X_s); \quad \text{MS-\( k \)-NN estimator}
\]

\[
\Delta(X_s) \quad \text{\( k \)-NN estimators}
\]

we adapt several Lemmas in Chaudhuri & Dasgupta (2014) to our setting, for proving our Theorem 2.

G.3 Main body of the proof

See the following Section G.4 for Lemma 1–7 used in this proof. Throughout this proof, we assume that \( X_s \in \mathcal{S}(\mu) \), as Cover & Hart (1967) proves that \( P(X_s \in \mathcal{S}(\mu)) = 1 \); the remaining \( X_s \notin \mathcal{S}(\mu) \) can be ignored.

Let \( n \in \mathbb{N}, k_{1,n} \geq n^{2\beta/(2\beta + d)}, t_n := 2k_{1,n}/n, \Delta_\circ := L_{\beta}^{**} n^{\beta/d} \) where \( L_{\beta}^{**} \in (0, \infty) \) is a constant defined in Lemma 4, and let \( \Delta(X) := |\eta(X) - 1/2| \) denotes the difference between the underlying conditional expectation \( \eta(X) \) from the decision boundary \( 1/2 \).

By specifying arbitrary \( i_o \in \mathbb{N} \) and \( \Delta_{i_o} := 2t_n \Delta_\circ \), we consider the following two steps (i) and (ii) for proving Theorem 2. In step (i), queries are first classified into two different cases, i.e., \( \Delta(X_s) \leq \Delta_{i_o} \) and \( \Delta(X_s) > \Delta_{i_o} \). Thus \( i_o \) regulates the margin near the decision boundary, and it will be specified as \( i_o = \max\{1, \lfloor \log_2 \left( \frac{\sqrt{2(\alpha + 2)}}{k_{1,n} \Delta_\circ} \right) \} \). For each case, we take expectation of the difference between point-wise errors \( R_{n,k}(X_s, Y_s) - \rho_s(X_s, Y_s) \) with respect to the sample \( D_n \). Subsequently, (ii) we further take its expectation with respect to the query \( (X_s, Y_s) \); the assertion is then proved. Note that these steps (i) and (ii) correspond to Chaudhuri & Dasgupta (2014) Lemma 20 and 21, respectively.

(i) We first consider the case \( \Delta(X_s) \leq \Delta_{i_o} \). Then, we have

\[
\mathbb{E}_{D_n}(R_{n,k}(X_s, Y_s) - \rho_s(X_s, Y_s)) \leq |1 - 2\eta(X_s)| \mathbb{E}_{D_n} \{ \mathbb{1}(\rho_{n,k}(X_s) \neq g_s(X_s)) \}
\]

\[(\therefore \text{Devroye et al. (1996) Theorem 2.2)} \]

\[
\leq |1 - 2\eta(X_s)| \leq 2\Delta(X_s) \leq 2\Delta_{i_o}.
\]

(ii) We second consider the case \( \Delta(X_s) > \Delta_{i_o} \). Assuming that \( \eta(X_s) > 1/2 \) without loss of generality, it holds for \( r = r_{1,n} := \|X_{(k_{1,n})} - X_s\|_2 \) that

\[
\mathbb{E}_{D_n} \{ R_{n,k}(X_s, Y_s) - \rho_s(X_s, Y_s) \}
\]

\[
\leq |1 - 2\eta(X_s)| \mathbb{E}_{D_n} \{ \mathbb{1}(\rho_{n,k}(X_s) \neq g_s(X_s)) \}
\]

\[(\therefore \text{Devroye et al. (1996) Theorem 2.2)} \]

\[
\leq 2\Delta(X_s) \mathbb{E}_{D_n} \{ \mathbb{1}(\rho_{n,k}(X_s) \neq g_s(X_s)) \}
\]

\[
\leq 2\Delta(X_s) \mathbb{E}_{D_n} \{ \mathbb{1}(X_s \in \partial_{i_o, \Delta(X_s) - \Delta_{i_o}}) \}
\]

\[
\leq 2\Delta(X_s) \mathbb{E}_{D_n} \{ \mathbb{1}(X_s \in \partial_{i_o, \Delta(X_s) - \Delta_{i_o}}) \}
\]
\[
\begin{align*}
&+ 1 \left( |\rho_{n,k}(X_s) - \rho_{\tilde{r},\ell}(X_s)| \geq \frac{\Delta(X_s) - \Delta_{i_0}}{2} \right) \\
&+ 1 \left( |\rho_{n,k}(X_s) - \eta(X_s)| \geq \frac{\Delta(X_s) - \Delta_{i_0}}{2} \right) \\
&+ 1 \left( \|X(k_{1,n}) - X_s\|_2 > \tilde{r}_{i_0}(X_s) \right) \\
\end{align*}
\]

\(\vdash\) Lemma 1 with \(\Delta := \Delta(X_s) - \Delta_{i_0} \in [0,1/2]\)

\[
\leq 2\Delta(X_s)E_{D_n} \left\{ 1 \left( |\rho_{n,k}(X_s) - \rho_{\tilde{r},\ell}(X_s)| \geq \frac{\Delta(X_s) - \Delta_{i_0}}{2} \right) \\
+ 1 \left( |\rho_{n,k}(X_s) - \eta(X_s)| \geq \frac{\Delta(X_s) - \Delta_{i_0}}{2} \right) \\
+ 1 \left( \|X(k_{1,n}) - X_s\|_2 > \tilde{r}_{i_0}(X_s) \right) \right\} \\
\leq 2\Delta(X_s) \left\{ P_{D_n} \left( |\rho_{n,k}(X_s) - \rho_{\tilde{r},\ell}(X_s)| \geq \frac{\Delta(X_s) - \Delta_{i_0}}{2} \right) \\
+ P_{D_n} \left( |\rho_{n,k}(X_s) - \eta(X_s)| \geq \frac{\Delta(X_s) - \Delta_{i_0}}{2} \right) \\
+ P_{D_n} \left( \|X(k_{1,n}) - X_s\|_2 > \tilde{r}_{i_0}(X_s) \right) \right\} \\
\vdash\) Lemma 4, i.e., \(X_s \notin \partial_{i_0,\Delta(X_s) - \Delta_{i_0}} \)

\[
\leq \Delta(X_s) \left\{ \exp \left( -C_1k_{1,n}(\Delta(X_s) - \Delta_{i_0})^2 \right) + \exp \left( -C_2k_{1,n}(\Delta(X_s) - \Delta_{i_0})^2 \right) \\
+ \exp(-Ln \exp^{-\frac{d}{2}(\beta+d)}(\Delta(X_s) - \Delta_{i_0})) + \exp(-3k_{1,n}/2)(1 + o(1)) \\
+ \exp(-n) + \exp \left( -\frac{k_{1,n}}{2} \left( 1 - \frac{k_{1,n}}{nt_n} \right)^2 \right) \right\} \\
\vdash\) Lemma 5, 6 and 7 with \(\delta = k_{1,n}/nt\)

\[
\leq \Delta(X_s) \exp \left( -C_2k_{1,n}(\Delta(X_s) - \Delta_{i_0})^2 \right) + \exp(-3k_{1,n}/2)(1 + o(1)) + \exp(-k_{1,n}/8) \\
\vdash\) \(t_n = 2(k_{1,n}/n)\) indicates that \(\frac{k_{1,n}}{2} \left( 1 - \frac{k_{1,n}}{nt_n} \right)^2 = \frac{k_{1,n}}{2} \left( 1 - \frac{1}{2} \right)^2 = \frac{k_{1,n}}{8} \)

where \(C_2 = C/2 = 1/16V^2L^2\) is defined in Lemma 6.

(ii) Excess risk of the misclassification error rate is then evaluated by

\[
\varepsilon(\rho_{n,k}) = E_{X,Y} \{ E_{D_n}(R_{n,k}(X_s, Y_s) - R_s(X_s, Y_s)) \} \\
= E_{X,Y} \{ E_{D_n}(R_{n,k}(X_s, Y_s) - R_s(X_s, Y_s)) \} \mid \Delta(X_s) \leq \Delta_{i_0} \\
\leq \Delta_{i_0} \Delta_{R}^2 \quad \text{\(\vdash\ \text{Lemma 9, \'\alpha\'-margin cond.)} \leq 2\Delta_{i_0} \quad \text{\(\vdash\ \text{ineq. (36)}\)} \\
+ P_{X,Y} \{ (\Delta(X_s) > \Delta_{i_0}) \} E_{X,Y} \{ E_{D_n}(R_{n,k}(X_s, Y_s) - R_s(X_s, Y_s)) \} \mid \Delta(X_s) > \Delta_{i_0} \\
\leq \Delta_{i_0} + P_{X,Y} \{ (\Delta(X_s) > \Delta_{i_0}) \} E_{D_n}(R_{n,k}(X_s, Y_s) - R_s(X_s, Y_s)) \mid \Delta(X_s) > \Delta_{i_0} \\
\leq \Delta_{i_0} + \frac{1}{\Delta_{i_0} + \exp(-C_2k_{1,n}(\Delta(X_s) - \Delta_{i_0})^2) \exp(-3k_{1,n}/2)(1 + o(1))} \leq \Delta_{i_0} \quad \text{\(\vdash\ \text{similarly to Proof of Lemma 20 in Chaudhuri & Dasgupta (2014)}\)} \\
\leq \Delta_{i_0} + \exp(-3k_{1,n}/2)(1 + o(1)).
\]
If we set \( i_0 = \max\{1, \lceil \log_2 \sqrt{\frac{2(\alpha+2)}{k_1,n\Delta_o}} \rceil \} \),

\[
\varepsilon(\hat{\eta}_{n,k}^{(\text{MS-KNN})}) = \varepsilon(\hat{\rho}_{n,k}) \\
\lesssim \Delta_o^{1+\alpha} + \exp(-3k_{1,n}/2)(1 + o(1)) \\
\lesssim (2^i_o)^{1+\alpha} \Delta_o^{1+\alpha} + \exp(-3k_{1,n}/2)(1 + o(1)) \\
\lesssim \left(\max\left\{1, \sqrt{\frac{2(\alpha+2)}{k_1,n\Delta_o}}\right\}\right)^{1+\alpha} \Delta_o^{1+\alpha} + \exp(-3k_{1,n}/2)(1 + o(1)) \\
\lesssim \max\left\{\Delta_o, \sqrt{\frac{1}{k_1,n}}\right\}^{1+\alpha} + \exp(-3k_{1,n}/2)(1 + o(1)) \\
\lesssim \max\left\{t_n^{\beta/d}, \sqrt{\frac{1}{k_1,n}}\right\}^{1+\alpha} + \exp(-3k_{1,n}/2)(1 + o(1)) \quad (\Delta_o \approx t_n^{\beta/d}) \\
\lesssim \max\left\{\left(\frac{k_{1,n}}{n}\right)^{\beta/d}, \sqrt{\frac{1}{k_1,n}}\right\}^{1+\alpha} + \exp(-3k_{1,n}/2)(1 + o(1)) \quad (: t_n \approx k_{1,n}/n).}

Recalling that \( k_{1,n} \approx n^{2\beta/(2\beta+d)} \), the assertion is proved as

\[
\varepsilon(\hat{\eta}_{n,k}^{(\text{MS-KNN})}) \lesssim n^{-1+(\alpha)\beta/(2\beta+d)}.
\]

\[\blacksquare\]

### G.4 Lemmas

We here list Lemma 1–7 used in the proof for Theorem 2. Roughly speaking,

- **Lemma 1** indicates the decomposition of the point-wise error.
  (cf. Chaudhuri & Dasgupta (2014) Lemma 7)
- **Lemma 2** indicates the bias evaluation of MS-\(k\)-NN.
- **Lemma 3** indicates the convergence rate of \( \|z_{n,k}(X_*) - z_{r,\ell}\|_\infty \).
- **Lemma 4** adapts the first part of Chaudhuri & Dasgupta (2014) Lemma 20 from unweighted \(k\)-NN to MS-\(k\)-NN.
- **Lemma 5** and 6 indicate the convergence rates related to the bias and variance evaluation of the MS-\(k\)-NN.
  (cf. Chaudhuri & Dasgupta (2014) Lemma 9)
- **Lemma 7** indicates how fast the radius \( r > 0 \) decreases to 0 as \( k \) increases.
  (cf. Chaudhuri & Dasgupta (2014) Lemma 8)

Similarly to Chaudhuri & Dasgupta (2014) Lemma 7, we prove the following Lemma 1, that decomposes the point-wise error into four different parts.

**Lemma 1.** Let \( g_{n,k} \) be the MS-\(k\)-NN classifier based on sample \( D_n \), and let \( X_* \in S(\mu), t \in [0,1], \Delta \in [0,1/2] \). Then, it holds for \( r = r_{1,n} := \|X(k_{1,n}) - X_*\|_2 \) that

\[
\mathbb{I}(g_{n,k}(X_*) \neq g_*(X_*)) \leq \mathbb{I}(X_* \in \partial_{r,\Delta}) \\
+ \mathbb{I}(\|\hat{\rho}_{n,k}(X_*) - \rho^{(\infty)}_{r,\ell}(X_*)\| \geq \Delta/2)
\]

(38) (39)
\[ \mathbb{I}(|\rho_{n,k}(X_s) - \eta(X_s)| \geq \Delta/2) + \mathbb{I}(r > \hat{r}_1(X_s)). \]

**Proof of Lemma 1.** Let \( A \) be an event that \( g_{n,k}(X_s) \neq g_s(X_s) \), and let \( B_1, B_2, B_3, B_4 \) be events defined by the indicator functions (38)–(41), respectively. Then, it suffices to prove \( A \Rightarrow [B_1 \lor B_2 \lor B_3 \lor B_4] \) or its contrapositive \( [\neg B_1 \land \neg B_2 \land \neg B_3 \land \neg B_4] \Rightarrow \neg A \), where \( \neg \) represents the negation. Here, we prove the contrapositive.

\( \neg B_1 \) indicates that \( X_s \in \mathcal{X}^+_{\ell_1,\Delta} \) or \( X_s \in \cup \mathcal{X}^-_{l,\Delta} \).

- We here consider the former case \( X_s \in \mathcal{X}^+_{\ell_1,\Delta} \); then, \( \neg B_4 \), i.e., \( r \leq \hat{r}_1(X) \), indicates that

\[ \rho^{(\infty)}_{r_1}(X_s) \geq \frac{1}{2} + \Delta (> 1/2). \]

\( \neg B_2 \) and \( \neg B_3 \) represent

\[ |\rho_{n,k} - \rho^{(\infty)}_{r_1}(X_s)| < \Delta/2, \quad |\rho_{n,k} - \eta(X)| < \Delta/2, \]

respectively; above inequalities (42) and (43) indicate

\[ \eta(X_s) \geq \rho^{(\infty)}_{r_1}(X_s) - |\rho_{n,k} - \rho^{(\infty)}_{r_1}(X_s)| - |\rho_{n,k} - \eta(X)| > \frac{1}{2} + \Delta - \Delta/2 - \Delta/2 = 1/2. \]

(42) and (44) prove that both of corresponding classifiers output the same label 1, whereupon \( \neg A \).

- Similarly, for the latter case \( X_s \in \mathcal{X}_{l,\Delta}^- \), both classifiers output 0 and thus \( \neg A \).

Therefore, the assertion is proved. \( \square \)

**Lemma 2.** Assuming the assumption (C-3), i.e., there exists \( L_z \in (0, \infty) \) such that \( \|z\|_\infty < L_z \). Then, there exist \( \tilde{r}, L^*_{\beta} \in (0, \infty) \) such that

\[ |\rho^{(\infty)}_{r_1}(X_s) - \eta(X_s)| \leq L^*_{\beta} r^3, \quad (\forall X_s \in \mathcal{X}, r \in (0, \tilde{r}]). \]

**Proof of Lemma 2.** Theorem 1 proves

\[ \varphi^{(\infty)}_{r}(X_s) = \varphi^{(\infty)}_{r_1}(X_s) = \eta(X_s) + \sum_{c=1}^{[\beta/2]} b^*_{c} r^{2c} + \delta_{r}(X_s), \quad |\delta_{r}(X_s)| \leq L^*_{\beta} r^3, \]

for all \( X_s \in \mathcal{S}(\mu), r \in (0, \tilde{r}) \), for some \( \tilde{r} \in (0, \infty) \); we have a simultaneous equation

\[ \varphi^{(\infty)}_{r_1}(X_s) = A_{r_1}(X_s) b_s(X_s) + \delta_{r}(X_s), \quad |\delta_{r}(X_s)| \leq L^*_{\beta} r^3, \quad (\forall X_s \in \mathcal{X}, r \in (0, \tilde{r}]), \]

where \( A_{r_1} = A_{r}(X_s) = (\mathbf{1} \mathbf{R}(X_s)) \in \mathbb{R}^{V \times (C+1)} \) is defined as same as \( A \) in (30) with the radius vector \( r = (r_1, r_2, \ldots, r_V) = r \ell \), and the entries in \( b_s(X_s) = (\eta(X_s), b_{1}^*, b_{2}^*, \ldots, b_{[\beta/2]}^*) \) are specified in Theorem 1. Denoting the first entry of the vector \( b \) by \( [b]_1 \),

\[ |\rho^{(\infty)}_{r_1}(X_s) - \eta(X_s)| \leq \left| [\{(A^T A)^{-1} A^T \varphi^{(\infty)}_{r_1}\}]_1 - \eta(X_s) \right| \]

\[ \leq \left| [(A^T A)^{-1} A^T (A(X_s) b_s(X_s) + \delta_{r}(X_s))]_1 - \eta(X_s) \right| \]
by leveraging (45).

In this proof, (i) we first evaluate the probability

\[
\left| \mathcal{L}(X) \right| = |\mathcal{L}(X)| = |z_\ell^\top \delta_r(X)|
\leq \|z_\ell\|_\infty \|\delta_r(X)\|_\infty
\leq L_\ell \leq L_\ell^* r_\beta^3.
\]

Specifying \(L_\beta^* := L_\ell L_\beta^3\) leads to the assertion. \(\square\)

**Lemma 3.** Assuming that \(X_* \in \mathcal{S}(\mu)\), (C-1) \(k_{1,n} \asymp n^{2\beta/(2\beta+d)}\) and (C-2) \(k_{n,v} = \min\{k \in [n] | \|X(k) - X_*\|_2 \geq \ell_v r_{1,n}\}\) where \(r = r_{1,n} := \|X(k_{1,n}) - X_*\|_2\). Then, for sufficiently large \(n \in \mathbb{N}\), there exists \(L_\ell > 0\) such that

\[
\mathbb{P}(\|z_{n,k}(X_*) - z_\ell\|_\infty > \Delta) \leq \exp(-L_\ell n^{2\beta/(\beta+d)} \Delta) + \exp(-3k_{1,n}/2) (1 + o(1)).
\]

**Proof of Lemma 3.** In this proof, (i) we first evaluate the probability

\[
\mathbb{P}_{D_n}\left(\frac{r_{v,n}}{r_{1,n}} - \ell_v \geq \Delta\right)
\]

Subsequently, (ii) evaluate

\[
\mathbb{P}_{D_n}(\|z_{n,k}(X_*) - z_\ell\|_\infty > \Delta)
\]

by leveraging (45).

(i) For any positive sequence \(\{b_n\}_{n \geq 1} \subset \mathbb{R}_{>0}\), we define \(k'_{v,n} := \min\{k \in [n] | \|X(k) - X_*\|_2 \geq \ell_v b_n\}\).

Although the corresponding radius \(r'_{v,n} := \|X(k_{v,n}) - X_*\|_2\) is computed through the sequence \(\{b_n\}\), it coincides with \(r_{v,n} := \|X_{k_{v,n}} - X_*\|_2\) as \(b_n = r_{1,n}\) will be specified later.

For any \(v \in \{2, 3, \ldots, V\}\), it holds that

\[
\mathbb{P}_{D_n}\left(\frac{r'_{v,n}}{b_n} - \ell_v \geq \Delta\right) = \mathbb{P}_{D_n}\left(r'_{v,n} - b_n \ell_v \geq b_n \Delta\right)
\]

\[
= \mathbb{P}_{D_n}\left(r'_{v,n} \geq b_n (\ell_v + \Delta)\right)
\]

\[
= \mathbb{P}_{D_n}(\forall i \in [n], X_i \notin B(X_*; r'_{v,n}) \setminus B(X_*; b_n \ell_v))
\]

\[
\leq \mathbb{P}_{D_n}(\forall i \in [n], X_i \notin B(X_*; b_n (\ell_v + \Delta)) \setminus B(X_*; b_n \ell_v)).
\]

(47)

Considering a random variable \(Z_i := 1(X_i \notin B(X_*; b_n (\ell_v + \varepsilon)) \setminus B(X_*; b_n \ell_v))\), that i.i.d. follows a Bernoulli distribution whose expectation is

\[
q_n = 1 - \int_{B(X_*; b_n (\ell_v + \varepsilon)) \setminus B(X_*; b_n \ell_v)} \mu(X) dX
\]

\[
\leq 1 - \mu_{\min} \int_{B(X_*; b_n (\ell_v + \Delta)) \setminus B(X_*; b_n \ell_v)} dX
\]

\[
\leq 1 - \mu_{\min} \frac{\pi^{d/2}}{\Gamma(d/2 + 1)} b_n^d ((\ell_v + \Delta) - \ell_v^d)
\]

\[
\leq 1 - \mu_{\min} \frac{\pi^{d/2}}{\Gamma(d/2 + 1)} d\ell_v \cdot b_n \Delta,
\]

\[
=: L_v
\]

26
(47) can be evaluated as
\begin{equation}
(47) = \mathbb{P}(Z_i = 1, \forall i \in [n]) = \mathbb{P}(Z_i = 1)^n = q_n^n \leq (1 - L_v b_n^d \Delta)^n.
\end{equation}

By leveraging (48) and specifying \( b_n = r_{1,n} \), we hereinafter evaluate (45). For any sequence \( \{a_n\}_{n \geq 1} \subset \mathbb{R}_{> 0} \),
\begin{align*}
P_{D_n} \left( \frac{r_{v,n}}{r_{1,n}} - \ell_v \geq \Delta \right) &= \int_0^\infty P_{D_n} \left( \left| \frac{r_{v,n}}{b_n} - \ell_v \right| \geq \Delta \right) P_{D_n}(r_{1,n} = b_n) \, db_n \\
&\leq \left\{ \int_0^{a_n} + \int_0^{\infty} \right\} P_{D_n} \left( \left| \frac{r_{v,n}}{b_n} - \ell_v \right| \geq \Delta \right) P_{D_n}(r_{1,n} = b_n) \, db_n \\
&\leq P_{D_n} \left( \left| \frac{r_{v,n}}{b_n} - \ell_v \right| \geq \Delta \mid b_n > a_n \right) P_{D_n}(r_{1,n} > a_n) \\
&\quad \leq (1 - L_v a_n^d \Delta)^n
\end{align*}

By specifying \( a_n := n^{-1/(\beta + d)} \), the terms \((\star 1), (\star 2)\) are evaluated as follows.

(a) Regarding \((\star 1)\), it holds that
\begin{equation}
(\star 1) = (1 - L_1 n^{-d/(\beta + d)} \Delta)^n \leq \exp \left( -n^{\beta/(\beta + d)} L_1 \Delta \right),
\end{equation}
as \( (1 - 1/a)^b \leq ((1 - 1/a)^a)^{b/a} \leq \exp(-1)^{b/a} = \exp(-b/a) \) for all \( a, b > 0 \).

(b) Here we evaluate the second term \((\star 2)\): considering a random variable \( Z_i := I(X_i \in B(X_0; a_n)) \) that i.i.d. follows a Bernoulli distribution whose expectation is
\begin{equation}
q'_{n} := \int_{B(X_0; a_n)} \mu(X) \, dX \leq \mu_{\min} \int_{B(X_0; a_n)} \, dX \leq \mu_{\min} \frac{\pi^d}{2(d/2 + 1)} a_n^d \lesssim n^{-d/(\beta + d)},
\end{equation}
we have an inequality
\begin{align*}
P(r_{1,n} \leq a_n) &= \mathbb{P} \left( \sum_{i=1}^n Z_i \geq k_{1,n} \right) = \mathbb{P} \left( \sum_{i=1}^n Z_i \geq n q'_{n} + \lambda \right) \quad (\text{where } \lambda := k_{1,n} - n q'_{n}) \\
&\leq \exp \left( -\frac{\lambda^2}{2(n q'_{n} + \lambda/3)} \right) \\
&\leq \exp \left( -\frac{(k_{1,n} - n q'_{n})^2}{2(n q'_{n} + (k_{1,n} - n q'_{n})/3)} \right) \\
&\lesssim \exp(-3k_{1,n}/2)(1 + o(1)) \quad (\because n q'_{n} = o(k_{1,n}))
\end{align*}
by referring to a Chernoff bound \((\text{Chung} \& \text{Lu, 2006, Theorem 2.4})\) with \( E_{D_n} (\sum_{i=1}^n Z_i) = n q'_{n} \).

Therefore, above (a) and (b) yield
\begin{equation}
P_{D_n} \left( \left| \frac{r_{v,n}}{r_{1,n}} - \ell_v \right| \geq \Delta \right) \lesssim \exp \left( -n^{\beta/(\beta + d)} L_1 \Delta \right) + \exp (-3k_{1,n}/2)(1 + o(1)).
\end{equation}
(ii) We second evaluate (46). As it holds that

\[
(1^\top (I - \mathcal{P}_{n,k})1)(1^\top (I - \mathcal{P}_R)1)\|z_{n,k} - z_{r_1,n}\|
\]

\[
= (1^\top (I - \mathcal{P}_{n,k})1)(1^\top (I - \mathcal{P}_R)1)\|I - \mathcal{P}_{n,k} - \mathcal{P}_R\|_\infty
\]

\[
\leq \|(1^\top (I - \mathcal{P}_{n,k})1)(I - \mathcal{P}_R) - (1^\top (I - \mathcal{P}_R)1)(I - \mathcal{P}_{n,k})\|_\infty
\]

there exist constants \(L^{(1)}, L^{(2)} > 0\) such that

\[
\|z_{n,k}(X_s) - z_{r_\ell}\|_\infty \leq L^{(1)}\|\mathcal{P}_{n,k} - \mathcal{P}_R\|_\infty \leq L^{(2)}\|r_n/r_{1,n} - \ell\|_\infty,
\]

where \(r_n = (r_{1,n}, r_{2,n}, \ldots, r_{V,n})\) ∈ \(\mathbb{R}^V\).

Consequently, above (i) and (ii) yield

\[
\mathbb{P}(\|z_{n,k}(X_s) - z_{r_\ell}\|_\infty > \Delta) \leq \mathbb{P}(L^{(2)}\|r_n/r_{1,n}\|_\infty > \Delta)
\]

\[
\leq \exp(-L_\ell \eta^{\beta/(\beta + d)} \Delta) + \exp(-3k_n/2)(1 + o(1)).
\]

for some constant \(L_\ell > 0\). \(\square\)

**Lemma 4 (Evaluation for (38)).** Let

- \(X_s \in S(\mu), \beta > 0, t \in [0, 1], i_o \in \mathbb{N},\)
- \(L^{*\ast}_\beta := L^{\ast}_\beta L^{-\beta/d}, \text{ where } \hat{L} := (\sup_{X \in \chi} \mu(X))^{\pi^{d/2}/(d/2 + 1)}\) and \(L^{*\ast}_\beta\) is defined in Lemma 2.
- \(\Delta_o := L^{*\ast}_\beta t^{\beta/d}, \Delta_{i_o} := 2^{i_o} \Delta_o.\)

If \(\Delta(X_s) > \Delta_{i_o}\), it holds that \(X_s \notin \partial_{t,\Delta(X_s) - \Delta_{i_o}}.\)

**Proof of Lemma 4.** For any \(r \in (0, \hat{r}_t(X_s)],\)

\[
t \leq \int_{B(X_s,r)} \mu(X)dX \leq \left(\sup_{X \in \chi} \mu(X)\right) \int_{B(X_s,r)} dX = \left(\sup_{X \in \chi} \mu(X)\right) \frac{\pi^{d/2}}{\Gamma(d/2 + 1)} r^d = \hat{L} r^d.
\]

Assuming that \(\eta(X_s) > 1/2\) without loss of generality, we have

\[
\rho_{r_\ell}(X_s) \geq \eta(X_s) - L^{*\ast}_\beta r^{\beta} \geq \eta(X_s) - L^{\ast}_\beta (\hat{L}^{-1/d} t^{1/d})^{\beta} \geq \eta(X_s) - (L^{*\ast}_\beta \hat{L}^{-\beta/d}) t^{\beta/d} = \eta(X_s) - \Delta_o \geq \eta(X_s) - 2^{-i_o} \Delta_{i_o} \geq \frac{1}{2} + (\Delta(X_s) - 2^{-i_o} \Delta_{i_o})
\]

(\(\cdot \cdot \) Lemma 2)

(\(\cdot \cdot \) ineq. (50))

(\(\cdot \cdot \) \(\cdot \cdot \) \(\cdot \cdot \) \(\cdot \cdot \))

(\(\cdot \cdot \) \(\cdot \cdot \) \(\cdot \cdot \))

(\(\cdot \cdot \))

(\(\cdot \cdot \) \(\cdot \cdot \) \(\cdot \cdot \))
where the terms (51), (52) are evaluated as follows.

By simply decomposing the terms, we have

$$\eta$$

for any $r \in (0, r_t(X_s)]$; it means that $X_s \in X_t^r \Delta(X_s) - \Delta_{io}$, whereupon $X_s \notin \partial_t \Delta(X_s) - \Delta_{io}$. Similar holds for the case $\eta(X_s) < 1/2$. Thus we have proved $X_s \notin \partial_t \Delta(X_s) - \Delta_{io}$.

Lemma 5 (Evaluation for (39)). Let $X_s \in \mathcal{X}$, $\Delta \in [0, 1/2]$ and $r_{1,n} := \|X_{(k_{1,n})} - X_s\|_2$. Then, it holds for $C_1 = 1/8V^2L_z^2$ that

$$\mathbb{P}_{\mathcal{D}_n}\left(\left|\rho_{n,k}(X_s) - \rho_{r_{1,n},L}^{(\infty)}(X_s)\right| \geq \Delta/2\right) \lesssim \exp(-C_1 k_{1,n} \Delta^2) + \exp(-L \ell \gamma^{(\beta+d)} \Delta) + \exp(-3k_{1,n}/2)(1 + o(1)).$$

Proof of Lemma 5. By simply decomposing the terms, we have

$$|\rho_{n,k}(X_s) - \rho_{r_{1,n},L}^{(\infty)}(X_s)| = \left|z_{n,k}(X_s)\right|_{\rho_{n,k}(X_s)} + \left|z_{r_{1,n},L}^{(\infty)}(X_s)\right|_{\rho_{r_{1,n},L}^{(\infty)}(X_s)}$$

where the terms (51), (52) are evaluated as follows.

(i) Regarding the first term (51),

$$(51) = \left|\{z_{n,k}(X_s) - z_{r_{1,n},L}\} \varphi_{n,k}(X_s)\right| \leq \|z_{n,k}(X_s) - z_{r_{1,n},L}\| \|\varphi_{n,k}(X_s)\|_{\infty} \leq 1.$$ 

Therefore, Lemma 3 leads to

$$\mathbb{P}(51) \geq \Delta/4 \leq \mathbb{P}(\|z_{n,k}(X_s) - z_{r_{1,n},L}\| \geq \Delta/4) \lesssim \exp(-L \ell \gamma^{(\beta+d)} \Delta) + \exp(-3k_{1,n}/2)(1 + o(1)),$$

for some constant $L \ell > 0$.

(ii) Regarding the second term (52),

$$(52) = \left|z_{r_{1,n},L}^{(\infty)}(X_s)\right| \leq \sum_{v=1}^{V} \|\varphi_v(X_s)\|_{\infty} \|\varphi_{n,k}(X_s) - \varphi_{r_{1,n},L}^{(\infty)}(X_s)\|.$$ 

and Chaudhuri & Dasgupta (2014) Lemma 9 proves that

$$\mathbb{P}\left(\|\varphi_v(X_s) - \varphi_{r_{1,n},L}^{(\infty)}(X_s)\| \geq \Delta/4V L_z\right) \lesssim \exp(-2k_{1,n}(\Delta/4VL_z)^2).$$

Therefore, we have

$$\mathbb{P}(52) \geq \Delta/4 \lesssim \mathbb{P}\left(L_z \sum_{v=1}^{V} \|\varphi_v(X_s) - \varphi_{r_{1,n},L}^{(\infty)}(X_s)\| \geq \Delta/4\right) \leq \sum_{v=1}^{V} \mathbb{P}(\|\varphi_v(X_s) - \varphi_{r_{1,n},L}^{(\infty)}(X_s)\| \geq \Delta/4V L_z) \lesssim \exp(-2k_{1,n}(\Delta/4VL_z)^2) = \exp(-k_{1,n} C_1 \Delta^2),$$

with $C_1 := 1/8V^2L_z^2$. 29
By simply decomposing the terms, we have
\[ \Pr(|\rho_{n,k}(X_*) - \eta(X_*)| \geq \Delta/2) \leq \Pr((51) \geq \Delta/4) + \Pr((52) \geq \Delta/4) \lesssim \exp(-C_1 k_1 \Delta^2) + \exp(-L \kappa \beta(\beta+d) \Delta) + \exp(-3k_2/2)(1+o(1)). \]
The assertion is proved. \( \square \)

**Lemma 6** (Evaluation for (40)). Let \( X_* \in \mathcal{X} \) and \( \Delta \in [0,1/2] \). Then, it holds for \( C_2 = 1/(2V L^2) \) that
\[ \Pr_{D_n}(|\rho_{n,k}(X_*) - \eta(X_*)| \geq \Delta/2) \lesssim \exp(-C_2 k_1 \Delta^2) + \exp(-n). \]

**Proof of Lemma 6.** By simply decomposing the terms, we have
\[
|\rho_{n,k}(X_*) - \eta(X_*)| \leq |\rho_{n,k}(X_*) - \rho^{(\infty)}_{t_1,n}(X_*)| + |\rho^{(\infty)}_{t_1,n}(X_*) - \eta(X_*)|. \tag{53}
\]

- Regarding the first term (\( \ast1 \)), applying Lemma 5 immediately leads to
\[ \Pr((\ast1) \geq \Delta/4) \lesssim \exp(-C_2 k_1 \Delta^2), \]
where \( C_2 := C_1/2 = 1/16 V^2 L^2 \).

- Here, we consider the second term (\( \ast2 \)). As Lemma 2 shows that \( |\rho^{(\infty)}_{t_1,n}(X_*) - \eta(X_*)| \leq L^* r_1 \), we have
\[ \Pr(|\rho^{(\infty)}_{t_1,n}(X_*) - \eta(X_*)| \geq \Delta/2) \leq \Pr(\Delta/2 L^* r_1 \geq \Delta/2) = \Pr(r_1 \geq (\Delta/2 L^*)^{1/2}). \tag{54} \]

(54) represents the probability that less than \( k_1 \) out of \( n \) feature vectors lie in a region \( B(X_*; \Delta_x) \) with \( \Delta_x := (\Delta/2 L^*)^{1/2} \); considering a random variable \( Z_i := \mathbb{I}(X_i \in B(X_*; \Delta_x)) \), that i.i.d. follows a Bernoulli distribution whose expectation is \( q_* := \int_{B(X_*; \Delta_x)} \mu(X) dX > 0 \),
\[ (54) = \Pr\left( \bar{Z}_n < \frac{k_1}{n} \right) \leq \Pr\left( |\bar{Z}_n - q_*| \geq \frac{q_* - \frac{k_1}{n}}{\sqrt{n}} \right) \leq 2 \exp\left( -2n \left( q_* - \frac{k_1}{n} \right)^2 \right) \]
by Hoeffding’s inequality. As \( \frac{k_1}{n} \approx n^{-d/(2\beta + d)} \leq q_*/2 \) for sufficiently large \( n \), we have \( (54) \lesssim \exp(-n) \).

Considering above (\( \ast1 \)) and (\( \ast2 \))
\[ \Pr(|\rho_{n,k}(X_*) - \eta(X_*)| \geq \Delta) \leq \Pr((\ast1) \geq \Delta/2) + \Pr((\ast2) \geq \Delta/2) \lesssim \exp(-C_2 k_1 \Delta^2) + \exp(-n) \]
for some \( C_2 > 0 \); the assertion is then proved. \( \square \)

**Lemma 7** (Evaluation for (41)). Let \( X_* \in \mathcal{X}, t, \delta \in [0,1] \) and \( k \in [(1-\delta)nt] \). Then,
\[ \Pr_{D_n}\left( \|X(k) - X_*\|_2 > \bar{r}_1(X_*) \right) \lesssim \exp(-k\delta^2/2). \]

**Proof of Lemma 7.** The assertion is obtained by Chaudhuri & Dasgupta (2014) Lemma 8. \( \square \)
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