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mean squared error

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1 Introduction

Let the label Y be a real valued random variable and let the feature vector $\mathbf{X} = (X_1, \dots, X_d)$ be a d -dimensional random vector. The regression function m is defined by

$$m(\mathbf{x}) = \mathbf{E}\{Y \mid \mathbf{X} = \mathbf{x}\}.$$

The minimum mean squared error, called also variance of the residual $Y - m(\mathbf{X})$, is denoted by

$$L^* := \mathbf{E}\{(Y - m(\mathbf{X}))^2\} = \min_f \mathbf{E}\{(Y - f(\mathbf{X}))^2\}.$$

The regression function m and the minimum mean squared error L^* cannot be calculated when the distribution of (\mathbf{X}, Y) is unknown. Assume, however, that we observe data $D_n = \{(\mathbf{X}_1, Y_1), \dots, (\mathbf{X}_n, Y_n)\}$ consisting of independent and identically distributed copies of (\mathbf{X}, Y) . D_n can be used to produce an estimate of L^* .

For nonparametric estimates of the minimum mean squared error $L^* = \mathbf{E}\{(Y - m(\mathbf{X}))^2\}$ see, e.g., Dudoit and van der Laan [4], Liitiäinen et al. [9], [10], Liitiäinen et al. [11], Müller and Stadtmüller [12], Neumann [14], Stadtmüller and Tsybakov [15], Müller, Schick and Wefelmeyer [13] and the literature cited there.

Devroye et al. [3] proved that without any tail and smoothness condition, L^* cannot be estimated with guaranteed rate of convergence. They introduced a modified nearest neighbor cross-validation estimate

$$\hat{L}_n = \frac{1}{2n} \sum_{i=1}^n (Y_i - Y_{j(i)})^2, \quad n \geq 2,$$

where $Y_{j(i)}$ is the label of the modified first nearest neighbor of \mathbf{X}_i among $\mathbf{X}_1, \dots, \mathbf{X}_{i-1}, \mathbf{X}_{i+1}, \dots, \mathbf{X}_n$. If Y and \mathbf{X} are bounded, and m is Lipschitz continuous

$$|m(\mathbf{x}) - m(\mathbf{z})| \leq C\|\mathbf{x} - \mathbf{z}\|, \quad (1)$$

then for $d \geq 3$, they proved that

$$\mathbf{E}\{|\hat{L}_n - L^*|\} \leq c_1 n^{-1/2} + c_2 n^{-2/d}. \quad (2)$$

Liitiäinen et al. ([9], [10]) introduced another estimate of the minimum mean squared error L^* by the first and second nearest neighbor cross-validation

$$L_n = \frac{1}{n} \sum_{i=1}^n (Y_i - Y_{n,i,1})(Y_i - Y_{n,i,2}), \quad n \geq 3,$$

where $Y_{n,i,1}$ and $Y_{n,i,2}$ are the labels of the first and second nearest neighbors $\mathbf{X}_{n,i,1}$ and $\mathbf{X}_{n,i,2}$ of \mathbf{X}_i among $\mathbf{X}_1, \dots, \mathbf{X}_{i-1}, \mathbf{X}_{i+1}, \dots, \mathbf{X}_n$, resp. (In the sequel, assume that for calculating the first and second nearest neighbors, ties occur with probability zero. When \mathbf{X} has a density, the case of ties among nearest neighbor distances occurs with probability zero.) If Y and \mathbf{X} are bounded and m is Lipschitz continuous, then for $d \geq 2$, they proved the rate of convergence of order in the inequality (2).

In this paper we introduce a non-recursive and a recursive estimator of the minimum mean squared error L^* , and prove their distribution-free strong consistencies. Under some mild conditions on the regression function m and on the distribution of (\mathbf{X}, Y) , we bound the rate of convergence of the non-recursive estimate.

2 Strong universal consistency

One can derive a new and simple estimator of L^* , considering the definition

$$L^* = \mathbf{E}\{(Y - m(\mathbf{X}))^2\} = \mathbf{E}\{Y^2\} - \mathbf{E}\{m(\mathbf{X})^2\}.$$

Obviously, $\mathbf{E}\{Y^2\}$ can be estimated by $\frac{1}{n} \sum_{i=1}^n Y_i^2$, while we estimate the term $\mathbf{E}\{m(\mathbf{X})^2\}$ by $\frac{1}{n} \sum_{i=1}^n Y_i Y_{n,i,1}$. Thus estimate L^* by

$$\tilde{L}_n := \frac{1}{n} \sum_{i=1}^n Y_i^2 - \frac{1}{n} \sum_{i=1}^n Y_i Y_{n,i,1}.$$

Theorem 1. Assume that ties occur with probability zero. If $|Y|$ is bounded then

$$\tilde{L}_n \rightarrow L^* \quad a.s.$$

If $\mathbf{E}\{Y^2\} < \infty$ then

$$\bar{L}_n := \frac{1}{n} \sum_{k=1}^n \tilde{L}_k \rightarrow L^* \quad a.s.$$

Proof. This theorem says that, for bounded $|Y|$, the estimate \tilde{L}_n is strongly consistent, while the estimate \bar{L}_n is strongly universally consistent. The theorem is an easy consequence of Ferrario and Walk [6] (Theorems 2.1 and 2.5), who proved that, for bounded Y ,

$$L_n \rightarrow L^* \tag{3}$$

a.s., and moreover, under the only condition $\mathbf{E}\{Y^2\} < \infty$

$$\frac{1}{n} \sum_{k=1}^n L_k \rightarrow L^* \tag{4}$$

a.s. We simply use the decomposition

$$L_n = \tilde{L}_n - \frac{1}{n} \sum_{i=1}^n Y_i Y_{n,i,2} + \frac{1}{n} \sum_{i=1}^n Y_{n,i,1} Y_{n,i,2}.$$

Then, as in the proof of Theorem 2.1 in Ferrario and Walk [6], on the basis of (21)-(25) in [9], one can show that, for bounded Y ,

$$\frac{1}{n} \sum_{i=1}^n Y_i Y_{n,i,2} \rightarrow \mathbf{E}\{m(\mathbf{X})^2\} \tag{5}$$

a.s. and

$$\frac{1}{n} \sum_{i=1}^n Y_{n,i,1} Y_{n,i,2} \rightarrow \mathbf{E}\{m(\mathbf{X})^2\} \tag{6}$$

a.s. Similarly, as in the proof of Theorem 2.5 in [6], for $\mathbf{E}\{Y^2\} < \infty$, one can show that

$$\frac{1}{n} \sum_{k=1}^n \frac{1}{k} \sum_{i=1}^k Y_i Y_{k,i,2} \rightarrow L^* \tag{7}$$

a.s. and

$$\frac{1}{n} \sum_{k=1}^n \frac{1}{k} \sum_{i=1}^k Y_{k,i,1} Y_{k,i,2} \rightarrow L^* \tag{8}$$

a.s. Now the statements of the theorem follow from (3), (5), (6), and from (4), (7) and (8), respectively. \square

Next we consider a recursive estimate

$$L'_n := \frac{1}{n} \sum_{i=1}^n Y_i^2 - \frac{1}{n} \sum_{i=1}^n Y_i Y_{i,i,1}, \quad n \geq 2,$$

where $Y_{1,1,1} := 0$. It is really recursive since

$$L'_n = \left(1 - \frac{1}{n}\right) L'_{n-1} + \frac{1}{n} (Y_n^2 - Y_n Y_{n,n,1}).$$

Theorem 2. Assume that ties occur with probability zero. If $\mathbf{E}\{Y^2\} < \infty$ then

$$L'_n \rightarrow L^* \quad a.s.$$

Proof. We have to show that

$$\frac{1}{n} \sum_{i=1}^n Y_i Y_{i,i,1} \rightarrow \mathbf{E}\{m(\mathbf{X})^2\} \quad a.s. \quad (9)$$

For $a > 0$, introduce the truncation function

$$T_a(z) = \begin{cases} a & \text{if } z > a; \\ z & \text{if } |z| < a; \\ -a & \text{if } z < -a. \end{cases}$$

Similarly to the proof of Theorem 2.5 in Ferrario and Walk [6] one can check that in order to show (9), it suffices to prove that

$$\frac{1}{n} \sum_{i=1}^n T_{\sqrt{i}}(Y_i) T_{\sqrt{i}}(Y_{i,i,1}) \rightarrow \mathbf{E}\{m(\mathbf{X})^2\} \quad (10)$$

a.s. Let \mathcal{F}_{i-1} be the σ -algebra generated by $(\mathbf{X}_1, Y_1), \dots, (\mathbf{X}_{i-1}, Y_{i-1})$. Introduce the decomposition

$$\frac{1}{n} \sum_{i=1}^n T_{\sqrt{i}}(Y_i) T_{\sqrt{i}}(Y_{i,i,1}) = I_n + J_n,$$

where

$$I_n = \frac{1}{n} \sum_{i=1}^n (T_{\sqrt{i}}(Y_i) T_{\sqrt{i}}(Y_{i,i,1}) - \mathbf{E}\{T_{\sqrt{i}}(Y_i) T_{\sqrt{i}}(Y_{i,i,1}) \mid \mathcal{F}_{i-1}\})$$

and

$$J_n = \frac{1}{n} \sum_{i=1}^n \mathbf{E}\{T_{\sqrt{i}}(Y_i) T_{\sqrt{i}}(Y_{i,i,1}) \mid \mathcal{F}_{i-1}\}.$$

I_n is an average of martingale differences such that the a.s. convergence

$$I_n \rightarrow 0 \quad (11)$$

can be derived from the Chow [1] theorem if

$$\sum_{n=1}^{\infty} \frac{\mathbf{Var}\{T_{\sqrt{n}}(Y_n) T_{\sqrt{n}}(Y_{n,n,1})\}}{n^2} < \infty. \quad (12)$$

We have that

$$\begin{aligned} \mathbf{Var}\{T_{\sqrt{n}}(Y_n) T_{\sqrt{n}}(Y_{n,n,1})\} &\leq \mathbf{E}\{(T_{\sqrt{n}}(Y_n))^2 (T_{\sqrt{n}}(Y_{n,n,1}))^2\} \\ &\leq \frac{\mathbf{E}\{(T_{\sqrt{n}}(Y_n))^4\} + \mathbf{E}\{(T_{\sqrt{n}}(Y_{n,n,1}))^4\}}{2}. \end{aligned}$$

Because of $\mathbf{E}\{Y_1^2\} < \infty$,

$$\sum_{n=1}^{\infty} \frac{\mathbf{E}\{(T_{\sqrt{n}}(Y_n))^4\}}{n^2} = \sum_{n=1}^{\infty} \frac{\mathbf{E}\{T_{n^2}(Y_n^4)\}}{n^2} = \sum_{n=1}^{\infty} \frac{\mathbf{E}\{T_{n^2}(Y_1^4)\}}{n^2} < \infty.$$

Recall now the following useful lemma.

Lemma 1. (Györfi et al. [7], Corollary 6.1) *Under the assumption that ties occur with probability zero,*

$$\sum_{i=1}^n \mathbf{I}_{\{\mathbf{X}_i \text{ is the first NN of } \mathbf{X}_i \text{ in } \{\mathbf{X}_1, \dots, \mathbf{X}_{i-1}, \mathbf{X}_i, \mathbf{X}_{i+1}, \dots, \mathbf{X}_n\}\}} \leq \gamma_d$$

a.s., where \mathbf{I} denotes the indicator and $\gamma_d < \infty$ depends only on d .

Lemma 1 implies that

$$\begin{aligned} & \mathbf{E}\{(T_{\sqrt{n}}(Y_{n,n,1}))^4\} \\ &= \mathbf{E}\left\{\sum_{j=1}^{n-1} (T_{\sqrt{n}}(Y_j))^4 \mathbf{I}_{\{\mathbf{X}_j \text{ is the first NN of } \mathbf{X}_n \text{ in } \{\mathbf{X}_1, \dots, \mathbf{X}_{n-1}\}\}}\right\} \\ &= (n-1)\mathbf{E}\left\{(T_{\sqrt{n}}(Y_1))^4 \mathbf{I}_{\{\mathbf{X}_1 \text{ is the first NN of } \mathbf{X}_n \text{ in } \{\mathbf{X}_1, \dots, \mathbf{X}_{n-1}\}\}}\right\} \\ &= (n-1)\mathbf{E}\left\{(T_{\sqrt{n}}(Y_n))^4 \mathbf{I}_{\{\mathbf{X}_n \text{ is the first NN of } \mathbf{X}_1 \text{ in } \{\mathbf{X}_2, \dots, \mathbf{X}_n\}\}}\right\} \\ &= \mathbf{E}\left\{(T_{\sqrt{n}}(Y_n))^4 \sum_{j=1}^{n-1} \mathbf{I}_{\{\mathbf{X}_n \text{ is the first NN of } \mathbf{X}_j \text{ in } \{\mathbf{X}_1, \dots, \mathbf{X}_{j-1}, \mathbf{X}_{j+1}, \dots, \mathbf{X}_n\}\}}\right\} \\ &\leq \mathbf{E}\left\{(T_{\sqrt{n}}(Y_n))^4 \gamma_d\right\}. \end{aligned}$$

Therefore

$$\sum_{n=1}^{\infty} \frac{\mathbf{E}\{(T_{\sqrt{n}}(Y_{n,n,1}))^4\}}{n^2} \leq \sum_{n=1}^{\infty} \frac{\gamma_d \mathbf{E}\{T_{n^2}(Y_n^4)\}}{n^2} = \gamma_d \sum_{n=1}^{\infty} \frac{\mathbf{E}\{T_{n^2}(Y_1^4)\}}{n^2} < \infty,$$

and so (12) is verified, which implies (11). Concerning the term J_n , the derivations below are based on the facts, that the ordinary 1-NN regression estimate is not universally consistent, however, it is strongly Cesàro convergent in the weak topology, and for noiseless observations ($Y_i = m(\mathbf{X}_i)$) it is strongly convergent in L_2 . Introduce the notation

$$m_i(\mathbf{x}) := \mathbf{E}\{T_{\sqrt{i}}(Y) \mid \mathbf{X} = \mathbf{x}\}.$$

Let $\mathbf{X}_{i-1,1}(\mathbf{x})$ denote the 1-NN (first nearest neighbor) of \mathbf{x} among $\{\mathbf{X}_1, \dots, \mathbf{X}_{i-1}\}$ and $Y_{i-1,1}(\mathbf{x})$ denote the corresponding label ($x \in \mathbf{R}^d$, $i \geq 2$), then

$$Y_{i-1,1}(\mathbf{X}_i) = Y_{i,i,1} \quad \text{and} \quad \mathbf{X}_{i-1,1}(\mathbf{X}_i) = \mathbf{X}_{i,i,1}.$$

The representation

$$J_n = \frac{1}{n} \sum_{i=1}^n \int_{\mathbf{R}^d} m_i(\mathbf{x}) T_{\sqrt{i}}(Y_{i-1,1}(\mathbf{x})) \mu(d\mathbf{x})$$

holds, where $Y_{0,1}(\mathbf{x}) := 0$. It remains to show that

$$J_n \rightarrow \mathbf{E}\{m(\mathbf{X})^2\} \quad \text{a.s.} \tag{13}$$

Before proving (13) we use two lemmas. Let μ denote the distribution of \mathbf{X} .

Lemma 2. *If $\mathbf{E}\{Y^2\} < \infty$ then*

$$\int |m(\mathbf{X}_{n-1,1}(\mathbf{x})) - m(\mathbf{x})|^2 \mu(d\mathbf{x}) \rightarrow 0 \quad \text{a.s.}$$

Proof. The proof is in the spirit of the proof of Theorem 4.1 and Problems 4.5 and 6.3 in Györfi et al. [7]. \square

The following lemma is a reformulation of a classic deterministic Tauberian theorem of Landau [8] in summability theory. For a proof and further references, see Lemma 1 in Walk [16].

Lemma 3. *If the sequence a_n , $n = 1, 2, \dots$ of real numbers is bounded from below and satisfies*

$$\sum_{n=1}^{\infty} \frac{(\sum_{i=1}^n a_i)^2}{n^3} < \infty,$$

then

$$\frac{1}{n} \sum_{i=1}^n a_i \rightarrow 0.$$

Proof of (13). It suffices to show

$$J_n^* := \frac{1}{n} \sum_{i=1}^n \int_{R^d} m(\mathbf{x}) T_{\sqrt{i}}(Y_{i-1,1}(\mathbf{x})) \mu(d\mathbf{x}) \rightarrow \mathbf{E}\{m(\mathbf{X})^2\} \quad a.s. \quad (14)$$

In fact, we notice that for each $\alpha > 0$

$$\begin{aligned} & \int_{R^d} |m_i(\mathbf{x}) - m(\mathbf{x})| |T_{\sqrt{i}}(Y_{i-1,1}(\mathbf{x}))| \mu(d\mathbf{x}) \\ & \leq \frac{1}{2} \frac{1}{\alpha} \int_{R^d} |m_i(\mathbf{x}) - m(\mathbf{x})|^2 \mu(d\mathbf{x}) + \frac{1}{2} \alpha \int_{R^d} T_i(Y_{i-1,1}(\mathbf{x})^2) \mu(d\mathbf{x}). \end{aligned}$$

If we can show

$$\limsup \frac{1}{n} \sum_{i=1}^n \int T_i(Y_{i-1,1}(\mathbf{x})^2) \mu(d\mathbf{x}) \leq c \mathbf{E}\{Y^2\} \quad a.s., \quad (15)$$

for some constant c , then this together with $\int_{R^d} |m_i(\mathbf{x}) - m(\mathbf{x})|^2 \mu(d\mathbf{x}) \rightarrow 0$ implies

$$\limsup \frac{1}{n} \sum_{i=1}^n \int_{R^d} |m_i(\mathbf{x}) - m(\mathbf{x})| |T_{\sqrt{i}}(Y_{i-1,1}(\mathbf{x}))| \mu(d\mathbf{x}) \leq \frac{1}{2} \alpha c \mathbf{E}\{Y^2\} \quad a.s.$$

But $\alpha \rightarrow 0$ yields that left-hand side equals 0 a.s. This, together with (14), implies (13). Therefore, to complete the proof it remains to show (15) and (14). In the first part we show (15). Set $r(\mathbf{x}) := \mathbf{E}\{Y^2 | \mathbf{X} = \mathbf{x}\}$, $r_i(\mathbf{x}) := \mathbf{E}\{T_i(Y^2) | \mathbf{X} = \mathbf{x}\}$. In order to get (15) it is enough to show

$$\frac{1}{n} \sum_{i=1}^n \int (T_i(Y_{i-1,1}(\mathbf{x})^2) - r_i(\mathbf{X}_{i-1,1}(\mathbf{x}))) \mu(d\mathbf{x}) \rightarrow 0 \quad a.s., \quad (16)$$

where $r_1(\mathbf{X}_{0,1}(\mathbf{x})) := 0$, and

$$\limsup \frac{1}{n} \sum_{i=1}^n \int r_i(\mathbf{X}_{i-1,1}(\mathbf{x})) \mu(d\mathbf{x}) \leq c \mathbf{E}\{Y^2\} \quad a.s.$$

The latter follows from

$$\limsup \int r_n(\mathbf{X}_{n-1,1}(\mathbf{x})) \mu(d\mathbf{x}) \leq \lim \int r(\mathbf{X}_{n-1,1}(\mathbf{x})) \mu(d\mathbf{x}) = \mathbf{E}\{r(\mathbf{X})\} = \mathbf{E}\{Y^2\}$$

a.s. (where the first equality holds by Lemma 2), which further yields that the sequence

$$\int (T_n(Y_{n-1,1}(\mathbf{x})^2) - r_n(\mathbf{X}_{n-1,1}(\mathbf{x}))) \mu(d\mathbf{x})$$

$n = 1, 2, \dots$, is a.s. bounded from below. In order to get (16) and therefore (15), by Lemma 3, it suffices to show

$$\sum_{n=1}^{\infty} \frac{\mathbf{E} \left\{ \left[\sum_{i=1}^n \int_{R^d} (T_i(Y_{i-1,1}(\mathbf{x})^2) - r_i(\mathbf{X}_{i-1,1}(\mathbf{x}))) \mu(d\mathbf{x}) \right]^2 \right\}}{n^3} < \infty. \quad (17)$$

We now show (17). Set for it $A_{i,j} := \{\mathbf{x}; \mathbf{X}_{i-1,1}(\mathbf{x}) = \mathbf{X}_j\}$. We note

$$\begin{aligned} & \sum_{i=1}^n \int_{R^d} (T_i(Y_{i-1,1}(\mathbf{x})^2) - r_i(\mathbf{X}_{i-1,1}(\mathbf{x}))) \mu(d\mathbf{x}) \\ &= \sum_{i=1}^n \int_{R^d} \sum_{j=1}^{i-1} \mathbf{1}_{\{\mathbf{X}_{i-1,1}(\mathbf{x}) = \mathbf{X}_j\}} \mu(d\mathbf{x}) (T_i(Y_j^2) - r_i(\mathbf{X}_j)) \\ &= \sum_{i=1}^n \sum_{j=1}^{i-1} \mu(A_{i,j}) (T_i(Y_j^2) - r_i(\mathbf{X}_j)) \\ &= \sum_{j=1}^{n-1} \left(\sum_{i=j+1}^n \mu(A_{i,j}) (T_i(Y_j^2) - r_i(\mathbf{X}_j)) \right), \end{aligned}$$

where the $(n-1)$ summands in brackets are orthogonal, because $\mathbf{E}\{T_i(Y_j^2) - r_i(\mathbf{X}_j) \mid \mathbf{X}_1, \dots, \mathbf{X}_{n-1}, Y'_j\} = 0$ for all i and all $j' \neq j$ ($j, j' \in \{1, \dots, n-1\}$). Thus (17) is equivalent to

$$\sum_{n=1}^{\infty} \frac{1}{n^3} \sum_{j=1}^{n-1} \mathbf{E} \left\{ \left(\sum_{i=j+1}^n \mu(A_{i,j}) (T_i(Y_j^2) - r_i(\mathbf{X}_j)) \right)^2 \right\} < \infty. \quad (18)$$

Let the cones C_1, \dots, C_{γ_d} have top $\mathbf{0}$ and angle $\frac{\pi}{3}$, which cover \mathbf{R}^d , and let $B_{i,j,l}$ be the subset of $C_{j,l} := \mathbf{X}_j + C_l$ ($j = 1, \dots, i-1$; $l = 1, \dots, \gamma_d$) consisting of all \mathbf{x} that are closer to \mathbf{X}_j than the 1-NN of \mathbf{X}_j in $\{\mathbf{X}_1, \dots, \mathbf{X}_{j-1}, \mathbf{X}_{j+1}, \dots, \mathbf{X}_{i-1}\} \cap C_{j,l}$. For $j \leq i-1$ a covering result of Devroye et al. [2], and also pp. 489, 490 in Györfi et al. [7], holds:

$$\mu(A_{i,j}) \leq \sum_{l=1}^{\gamma_d} \mu(B_{i,j,l}).$$

It suffices to show, for each $l \in \{1, \dots, \gamma_d\}$

$$\sum_{n=1}^{\infty} \frac{1}{n^3} \sum_{j=1}^{n-1} \mathbf{E} \left\{ \left(\sum_{i=j+1}^n \mu(B_{i,j,l}) (T_i(Y_j^2) - r_i(\mathbf{X}_j)) \right)^2 \right\} < \infty. \quad (19)$$

We have that

$$\begin{aligned} & \mathbf{E} \left\{ \left(\sum_{i=j+1}^n \mu(B_{i,j,l}) (T_i(Y_j^2) - r_i(\mathbf{X}_j)) \right)^2 \right\} \\ &= \mathbf{E} \left\{ \sum_{i,i'=j+1}^n \mathbf{E} \{ \mu(B_{i,j,l}) \mu(B_{i',j,l}) (T_i(Y_j^2) - r_i(\mathbf{X}_j)) (T_{i'}(Y_j^2) - r_{i'}(\mathbf{X}_j)) \mid \mathbf{X}_j \} \right\} \\ &= \mathbf{E} \left\{ \sum_{i,i'=j+1}^n \mathbf{E} \{ \mu(B_{i,j,l}) \mu(B_{i',j,l}) \mid \mathbf{X}_j \} \mathbf{E} \{ (T_i(Y_j^2) - r_i(\mathbf{X}_j)) (T_{i'}(Y_j^2) - r_{i'}(\mathbf{X}_j)) \mid \mathbf{X}_j \} \right\} \\ &\leq \int_{i,i'=j+1}^n \sqrt{\mathbf{E}\{\mu(B_{i,j,l})^2 \mid \mathbf{X}_j = \mathbf{x}\}} \sqrt{\mathbf{E}\{\mu(B_{i',j,l})^2 \mid \mathbf{X}_j = \mathbf{x}\}} \\ &\quad \cdot \sqrt{\mathbf{E}\{(T_i(Y^2))^2 \mid \mathbf{X} = \mathbf{x}\}} \sqrt{\mathbf{E}\{(T_{i'}(Y^2))^2 \mid \mathbf{X} = \mathbf{x}\}} \mu(d\mathbf{x}) \end{aligned}$$

$$= \int \left(\sum_{i=j+1}^n \sqrt{\mathbf{E}\{\mu(B_{i,j,l})^2 | \mathbf{X}_j = \mathbf{x}\}} \sqrt{\mathbf{E}\{(T_i(Y^2))^2 | \mathbf{X} = \mathbf{x}\}} \right)^2 \mu(d\mathbf{x})$$

According to [2] and pp. 489, 490 in [7], one has that $\mathbf{P}\{\mu(B_{i,j,l}) > \sqrt{p}\}$ equals the probability that a $\text{Binom}(i-2, \sqrt{p})$ -distributed random variable takes the value 0, i.e., $(1 - \sqrt{p})^{i-2}$ ($0 < p < 1$). Thus,

$$\begin{aligned} & \mathbf{E} \left\{ \left(\sum_{i=j+1}^n \mu(B_{i,j,l}) (T_i(Y_j^2) - r_i(\mathbf{X}_j)) \right)^2 \right\} \\ & \leq \int \left(\sum_{i=j+1}^n \sqrt{\int_0^1 \mathbf{P}\{\mu(B_{i,j,l}) > \sqrt{p} | \mathbf{X}_j = \mathbf{x}\} dp} \sqrt{\mathbf{E}\{(T_i(Y^2))^2 | \mathbf{X} = \mathbf{x}\}} \right)^2 \mu(d\mathbf{x}) \\ & = \int \left(\sum_{i=j+1}^n \sqrt{\int_0^1 (1 - \sqrt{p})^{i-2} dp} \sqrt{\mathbf{E}\{(T_i(Y^2))^2 | \mathbf{X} = \mathbf{x}\}} \right)^2 \mu(d\mathbf{x}) \\ & = \int \left(\sum_{i=j+1}^n \sqrt{\frac{2}{(i-1)i}} \sqrt{\mathbf{E}\{(T_i(Y^2))^2 | \mathbf{X} = \mathbf{x}\}} \right)^2 \mu(d\mathbf{x}) \\ & \leq 8 \int \left(\sum_{i=j+1}^n \frac{1}{i} \sqrt{\mathbf{E}\{(T_n(Y^2))^2 | \mathbf{X} = \mathbf{x}\}} \right)^2 \mu(d\mathbf{x}) \\ & \leq 8 \left(\ln \frac{n}{j} \right)^2 \int \mathbf{E}\{(T_n(Y^2))^2 | \mathbf{X} = \mathbf{x}\} \mu(d\mathbf{x}) \\ & = 8 \left(\ln \frac{n}{j} \right)^2 \mathbf{E}\{(T_n(Y^2))^2\}. \end{aligned}$$

Thus the left-hand side of (19) is bounded by

$$8 \sum_{n=1}^{\infty} \frac{1}{n^3} \sum_{j=1}^{n-1} \left(\ln \frac{n}{j} \right)^2 \mathbf{E}\{(T_n(Y^2))^2\} \leq 8 \text{const} \sum_{n=1}^{\infty} \frac{\mathbf{E}\{(T_n(Y^2))^2\}}{n^2} < \infty,$$

(because of $\mathbf{E}\{Y^2\} < \infty$), having used the fact that $\frac{1}{n} \sum_{j=1}^{n-1} \left(\ln \frac{n}{j} \right)^2 \rightarrow \int_0^1 (\ln \frac{1}{t})^2 dt = \int_0^1 (\ln t)^2 dt < \infty$. Thus (19), and therefore (15), is proved. In the second part, it remains to show (14). In order to get it, according to the proof of Lemma 23.3 in Györfi et al. [7], it suffices to show

$$\limsup_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n \int |m(\mathbf{x}) T_{\sqrt{i}}(Y_{i-1,1}(\mathbf{x}))| \mu(d\mathbf{x}) \leq c^* \mathbf{E}\{Y^2\} \quad \text{a.s.} \quad (20)$$

for some constant c^* and to show (14) for bounded Y . We prove first (20). Notice that

$$\int |m(\mathbf{x}) T_{\sqrt{i}}(Y_{i-1,1}(\mathbf{x}))| \mu(d\mathbf{x}) \leq \frac{1}{2} \int m(\mathbf{x})^2 \mu(d\mathbf{x}) + \frac{1}{2} \int T_i(Y_{i-1,1}(\mathbf{x}))^2 \mu(d\mathbf{x}).$$

From $\int m(\mathbf{x})^2 \mu(d\mathbf{x}) \leq \mathbf{E}\{Y^2\}$ and from (15) we obtain (20), with $c^* = \frac{1}{2} + \frac{1}{2}c$. By boundedness of Y , from some index on we have that $T_{\sqrt{i}}(Y) = Y$. Therefore and because of Lemma 2 it suffices to show

$$\frac{1}{n} \sum_{i=1}^n \int_{\mathbb{R}^d} m(\mathbf{x}) (Y_{i-1,1}(\mathbf{x}) - m(\mathbf{X}_{i-1,1}(\mathbf{x}))) \mu(d\mathbf{x}) \rightarrow 0 \quad \text{a.s.},$$

where $m(\mathbf{X}_{0,1}(\mathbf{x})) := 0$. By boundedness, because of Lemma 3 it is enough to show

$$\sum_{n=1}^{\infty} \frac{\mathbf{E}\{[\sum_{i=1}^n \int_{R^d} m(\mathbf{x}) (Y_{i-1,1}(\mathbf{x}) - m(\mathbf{X}_{i-1,1}(\mathbf{x}))) \mu(d\mathbf{x})]^2\}}{n^3} < \infty. \quad (21)$$

Noticing

$$\begin{aligned} & \int_{R^d} m(\mathbf{x}) (Y_{i-1,1}(\mathbf{x}) - m(\mathbf{X}_{i-1,1}(\mathbf{x}))) \mu(d\mathbf{x}) \\ &= \int_{R^d} m(\mathbf{x}) \sum_{j=1}^{i-1} \mathbf{I}_{\{\mathbf{X}_{i-1,1}(\mathbf{x}) = \mathbf{x}_j\}} \mu(d\mathbf{x}) (Y_j - m(\mathbf{X}_j)) \\ &= \sum_{j=1}^{i-1} \int_{A_{i,j}} m(\mathbf{x}) \mu(d\mathbf{x}) (Y_j - m(\mathbf{X}_j)), \end{aligned}$$

we obtain, with suitable constants c' and c'' , that the left-hand side of (21) equals

$$\begin{aligned} & \sum_{n=1}^{\infty} \frac{1}{n^3} \mathbf{E} \left\{ \left[\sum_{i=1}^n \sum_{j=1}^{i-1} \int_{A_{i,j}} m(\mathbf{x}) \mu(d\mathbf{x}) (Y_j - m(\mathbf{X}_j)) \right]^2 \right\} \\ &= \sum_{n=1}^{\infty} \frac{1}{n^3} \mathbf{E} \left\{ \left[\sum_{j=1}^{n-1} \left(\sum_{i=j+1}^n \int_{A_{i,j}} m(\mathbf{x}) \mu(d\mathbf{x}) \right) (Y_j - m(\mathbf{X}_j)) \right]^2 \right\} \\ &= \sum_{n=1}^{\infty} \frac{1}{n^3} \sum_{j=1}^{n-1} \mathbf{E} \left\{ \left(\sum_{i=j+1}^n \int_{A_{i,j}} m(\mathbf{x}) \mu(d\mathbf{x}) (Y_j - m(\mathbf{X}_j)) \right)^2 \right\} \\ &\quad (\text{by orthogonality of the } (n-1) \text{ summands in the brackets}) \\ &\leq c' \sum_{n=1}^{\infty} \frac{1}{n^3} \sum_{j=1}^{n-1} \mathbf{E} \left\{ \left(\sum_{i=j+1}^n \mu(A_{i,j}) \right)^2 \right\} \\ &\leq c'' \sum_{n=1}^{\infty} \frac{1}{n^3} \sum_{j=1}^{n-1} \left(\ln \frac{n}{j} \right)^2 < \infty, \end{aligned}$$

the latter is as in the proof of (15). Thus (14) is proved for bounded Y . Therefore altogether (13) and thus the assertion have been verified. \square

3 Rate of convergence

Next we bound the rate of convergence:

Theorem 3. Assume that Y and \mathbf{X} are bounded ($|Y| < L$, $\|\mathbf{X}\| < K$) and m is Lipschitz continuous and ties occur with probability zero. In addition, suppose that

- (i) μ has a Lipschitz continuous density f ,
- (ii) For any \mathbf{x} from the support of μ and $0 < r < 2K$,

$$\mu(S_{\mathbf{x},r}) \geq \gamma r^d,$$

with $\gamma > 0$.

Then for $d \geq 2$, we have that

$$\mathbf{E}\{|\tilde{L}_n - L^*|\} \leq c_1 n^{-1/2} + c_2 n^{-2/d}. \quad (22)$$

Proof. Apply the decomposition

$$\mathbf{E}\{|\tilde{L}_n - L^*|\} \leq \mathbf{E}\{|\tilde{L}_n - \mathbf{E}\{\tilde{L}_n\}|\} + |\mathbf{E}\{\tilde{L}_n\} - L^*| \leq \sqrt{\mathbf{Var}(\tilde{L}_n)} + |\mathbf{E}\{\tilde{L}_n\} - L^*|.$$

For the variance term $\mathbf{Var}(\tilde{L}_n)$, introduce the notation

$$R_n := -\frac{1}{n} \sum_{i=1}^n Y_i Y_{n,i,1}.$$

For bounded Y ($|Y| \leq L$), we show that

$$\mathbf{Var}(R_n) \leq \frac{2(1+2\gamma_d)^2 L^4}{n}, \quad (23)$$

from which we get that

$$\begin{aligned} \mathbf{Var}(\tilde{L}_n) &= \mathbf{Var}\left(\frac{1}{n} \sum_{i=1}^n Y_i^2 + R_n\right) \\ &\leq 2\mathbf{Var}\left(\frac{1}{n} \sum_{i=1}^n Y_i^2\right) + 2\mathbf{Var}(R_n) \leq \frac{2L^4}{n} + \frac{4(1+2\gamma_d)^2 L^4}{n}, \end{aligned}$$

and thus,

$$\sqrt{\mathbf{Var}(\tilde{L}_n)} \leq \frac{c_1}{\sqrt{n}}.$$

In the same way as in Liitiäinen et al. [9], we show (23) using the Efron-Stein inequality [5]. Replacement of (\mathbf{X}_j, Y_j) by (\mathbf{X}'_j, Y'_j) for fixed $j \in \{1, \dots, n\}$ (where $(\mathbf{X}_1, Y_1), \dots, (\mathbf{X}_n, Y_n), (\mathbf{X}'_1, Y'_1), \dots, (\mathbf{X}'_n, Y'_n)$ are independent and identically distributed) leads to the estimator

$$R_{n,j} = \frac{1}{n} \left(Y'_j Y'_{n,j,1} + \sum_{i \neq j} Y_i Y'_{n,i,1} \right).$$

According to the Efron-Stein inequality we have that

$$\mathbf{Var}(R_n) \leq \frac{1}{2} \sum_{i=1}^n \mathbf{E}\{(R_n - R_{n,i})^2\} = \frac{n}{2} \mathbf{E}\{(R_n - R_{n,1})^2\}.$$

Evaluate the difference $R_n - R_{n,1}$:

$$\begin{aligned} R_n - R_{n,1} &= \frac{1}{n} \left(Y_1 Y_{n,1,1} + \sum_{i \neq 1} Y_i Y_{n,i,1} \right) - \frac{1}{n} \left(Y'_1 Y'_{n,1,1} + \sum_{i \neq 1} Y_i Y'_{n,i,1} \right) \\ &= \frac{1}{n} (Y_1 Y_{n,1,1} - Y'_1 Y'_{n,1,1}) + \frac{1}{n} \sum_{i \neq 1} Y_i (Y_{n,i,1} - Y'_{n,i,1}). \end{aligned}$$

One can check that $|Y_1 Y_{n,1,1} - Y'_1 Y'_{n,1,1}| \leq 2L^2$. Introduce the following notations. Let $n[i]$ be the index of the first nearest neighbor of \mathbf{X}_i from the set $\{\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_n\} \setminus \{\mathbf{X}_i\}$. Similarly, let $n'[i]$ be the index of the first nearest neighbor of \mathbf{X}_i from the set $\{\mathbf{X}'_1, \mathbf{X}'_2, \dots, \mathbf{X}'_n\} \setminus \{\mathbf{X}'_i\}$. For fixed $i \neq 1$, notice

$$\{Y_{n,i,1} - Y'_{n,i,1} \neq 0\} \subset \{n[i] = 1\} \cup \{n'[i] = 1\}.$$

Thus

$$\left| \sum_{i \neq 1} Y_i (Y_{n,i,1} - Y'_{n,i,1}) \right| \leq L \sum_{i \neq 1} |Y_{n,i,1} - Y'_{n,i,1}|$$

$$\leq 2L^2 \left(\sum_{i \neq 1} \mathbf{1}_{n[i]=1} + \sum_{i \neq 1} \mathbf{1}_{n'[i]=1} \right) \leq 2L^2 (\gamma_d + \gamma_d) = 4L^2 \gamma_d$$

a.s., where in the last step we applied Lemma 1. Summarizing these bounds we get that

$$\text{Var}(R_n) \leq \frac{n}{2} \left(\frac{1}{n} 2L^2 + \frac{1}{n} 4L^2 \gamma_d \right)^2 = \frac{2(1+2\gamma_d)^2 L^4}{n}$$

a.s., and the proof of (23) is complete. For the bias term $\mathbf{E}\{\tilde{L}_n\} - L^*$, notice that

$$\mathbf{E}\{\tilde{L}_n\} - L^* = \mathbf{E}\{m(\mathbf{X}_1)m(\mathbf{X}_{n,1,1})\} - \mathbf{E}\{m(\mathbf{X}_1)^2\}. \quad (24)$$

Because of

$$m(\mathbf{X}_1)m(\mathbf{X}_{n,1,1}) - m(\mathbf{X}_1)^2 = \frac{1}{2}(m(\mathbf{X}_{n,1,1})^2 - m(\mathbf{X}_1)^2) - \frac{1}{2}(m(\mathbf{X}_{n,1,1}) - m(\mathbf{X}_1))^2,$$

the Lipschitz condition (1) implies that

$$\begin{aligned} & |\mathbf{E}\{m(\mathbf{X}_1)m(\mathbf{X}_{n,1,1})\} - \mathbf{E}\{m(\mathbf{X}_1)^2\}| \\ & \leq \frac{1}{2}|\mathbf{E}\{m(\mathbf{X}_{n,1,1})^2\} - \mathbf{E}\{m(\mathbf{X}_1)^2\}| + \frac{1}{2}\mathbf{E}\{(m(\mathbf{X}_{n,1,1}) - m(\mathbf{X}_1))^2\} \\ & \leq \frac{1}{2}|\mathbf{E}\{m(\mathbf{X}_{n,1,1})^2\} - \mathbf{E}\{m(\mathbf{X}_1)^2\}| + \frac{C}{2}\mathbf{E}\{\|\mathbf{X}_{n,1,1} - \mathbf{X}_1\|^2\}, \end{aligned}$$

where C is the Lipschitz constant in (1). For $d \geq 3$, Lemma 6.4 in Györfi et al. [7] and for $d \geq 2$, Theorem 3.2 in Liitiäinen et al. [10] say that

$$\mathbf{E}\{\|\mathbf{X}_{n,1,1} - \mathbf{X}_1\|^2\} \leq c_3 n^{-2/d}. \quad (25)$$

Therefore

$$|\mathbf{E}\{m(\mathbf{X}_1)m(\mathbf{X}_{n,1,1})\} - \mathbf{E}\{m(\mathbf{X}_1)^2\}| \leq \frac{1}{2}|\mathbf{E}\{m(\mathbf{X}_{n,1,1})^2\} - \mathbf{E}\{m(\mathbf{X}_1)^2\}| + c_4 n^{-2/d},$$

and so we have to prove that

$$|\mathbf{E}\{m(\mathbf{X}_{n,1,1})^2\} - \mathbf{E}\{m(\mathbf{X}_1)^2\}| \leq c_4 n^{-1/2} + c_5 n^{-2/d}. \quad (26)$$

In order to show (26), let's calculate the density f_n of $(\mathbf{X}_1, \mathbf{X}_{n,1,1})$ with respect to $\mu \times \mu$. We have that

$$\begin{aligned} & \mathbf{P}\{\mathbf{X}_1 \in A, \mathbf{X}_{n,1,1} \in B\} \\ & = \sum_{i=2}^n \mathbf{P}\{\mathbf{X}_1 \in A, \mathbf{X}_i \in B, \mathbf{X}_{n,1,1} = \mathbf{X}_i\} \\ & = (n-1)\mathbf{P}\{\mathbf{X}_1 \in A, \mathbf{X}_2 \in B, \mathbf{X}_{n,1,1} = \mathbf{X}_2\} \\ & = (n-1)\mathbf{E}\{\mathbf{P}\{\mathbf{X}_1 \in A, \mathbf{X}_2 \in B, \mathbf{X}_{n,1,1} = \mathbf{X}_2 | \mathbf{X}_1, \mathbf{X}_2\}\} \\ & = (n-1)\mathbf{E}\{\mathbf{P}\{\cap_{i=3}^n \{\|\mathbf{X}_1 - \mathbf{X}_i\| \geq \|\mathbf{X}_1 - \mathbf{X}_2\|\} | \mathbf{X}_1, \mathbf{X}_2\} \mathbf{I}_{\{\mathbf{X}_1 \in A, \mathbf{X}_2 \in B\}}\}\} \\ & = (n-1)\mathbf{E}\left\{(1 - \mu(S_{\mathbf{X}_1, \|\mathbf{X}_1 - \mathbf{X}_2\|}))^{n-2} \mathbf{I}_{\{\mathbf{X}_1 \in A, \mathbf{X}_2 \in B\}}\right\}. \end{aligned}$$

Therefore

$$f_n(\mathbf{x}_1, \mathbf{x}_2) = (n-1) (1 - \mu(S_{\mathbf{x}_1, \|\mathbf{x}_1 - \mathbf{x}_2\|}))^{n-2}.$$

It implies that

$$\mathbf{E}\{m(\mathbf{X}_1)^2\} = \mathbf{E}\{m(\mathbf{X}_1)^2 f_n(\mathbf{X}_1, \mathbf{X}_2)\}$$

and

$$\mathbf{E}\{m(\mathbf{X}_{n,1,1})^2\} = \mathbf{E}\{m(\mathbf{X}_2)^2 f_n(\mathbf{X}_1, \mathbf{X}_2)\} = \mathbf{E}\{m(\mathbf{X}_1)^2 f_n(\mathbf{X}_2, \mathbf{X}_1)\}.$$

Thus,

$$\mathbf{E}\{m(\mathbf{X}_{n,1,1})^2\} - \mathbf{E}\{m(\mathbf{X}_1)^2\} = \mathbf{E}\{m(\mathbf{X}_1)^2(f_n(\mathbf{X}_2, \mathbf{X}_1) - f_n(\mathbf{X}_1, \mathbf{X}_2))\},$$

and interchanging \mathbf{X}_1 and \mathbf{X}_2 we get that

$$\mathbf{E}\{m(\mathbf{X}_{n,1,1})^2\} - \mathbf{E}\{m(\mathbf{X}_1)^2\} = -\mathbf{E}\{m(\mathbf{X}_2)^2(f_n(\mathbf{X}_2, \mathbf{X}_1) - f_n(\mathbf{X}_1, \mathbf{X}_2))\},$$

and so

$$\mathbf{E}\{m(\mathbf{X}_{n,1,1})^2\} - \mathbf{E}\{m(\mathbf{X}_1)^2\} = \frac{1}{2}\mathbf{E}\{(m(\mathbf{X}_1)^2 - m(\mathbf{X}_2)^2)(f_n(\mathbf{X}_2, \mathbf{X}_1) - f_n(\mathbf{X}_1, \mathbf{X}_2))\}. \quad (27)$$

m satisfies the Lipschitz condition (1). Therefore

$$|m(\mathbf{x})^2 - m(\mathbf{z})^2| \leq |m(\mathbf{x}) - m(\mathbf{z})|(|m(\mathbf{x})| + |m(\mathbf{z})|) \leq 2LC\|\mathbf{x} - \mathbf{z}\|,$$

and so (27) implies that

$$|\mathbf{E}\{m(\mathbf{X}_{n,1,1})^2\} - \mathbf{E}\{m(\mathbf{X}_1)^2\}| \leq LC\mathbf{E}\{\|\mathbf{X}_1 - \mathbf{X}_2\| \cdot |f_n(\mathbf{X}_2, \mathbf{X}_1) - f_n(\mathbf{X}_1, \mathbf{X}_2)|\}.$$

For any $0 < a < b < 1$, we have the inequality

$$0 < (1-a)^n - (1-b)^n < n(b-a)(1-a)^{n-1}.$$

Therefore

$$\begin{aligned} & |\mathbf{E}\{m(\mathbf{X}_{n,1,1})^2\} - \mathbf{E}\{m(\mathbf{X}_1)^2\}| \\ & \leq LCn^2\mathbf{E}\left\{\|\mathbf{X}_1 - \mathbf{X}_2\| \cdot |\mu(S_{\mathbf{X}_1, \|\mathbf{X}_1 - \mathbf{X}_2\|}) - \mu(S_{\mathbf{X}_2, \|\mathbf{X}_1 - \mathbf{X}_2\|})| \right. \\ & \quad \cdot \left. \left(e^{-(n-2)\mu(S_{\mathbf{X}_1, \|\mathbf{X}_1 - \mathbf{X}_2\|})} + e^{-(n-2)\mu(S_{\mathbf{X}_2, \|\mathbf{X}_1 - \mathbf{X}_2\|})}\right)\right\}. \end{aligned}$$

If $c_d := Vol(S_{\mathbf{0},1})$ then the Condition (i) implies that

$$\begin{aligned} |\mu(S_{\mathbf{X}_1, \|\mathbf{X}_1 - \mathbf{X}_2\|}) - \mu(S_{\mathbf{X}_2, \|\mathbf{X}_1 - \mathbf{X}_2\|})| & \leq c_d \|\mathbf{X}_1 - \mathbf{X}_2\|^d \max_{\|\mathbf{x} - \mathbf{z}\| \leq 2\|\mathbf{X}_1 - \mathbf{X}_2\|} |f(\mathbf{x}) - f(\mathbf{z})| \\ & \leq c_9 \|\mathbf{X}_1 - \mathbf{X}_2\|^{d+1}. \end{aligned}$$

Because of Condition (ii), both $e^{-(n-2)\mu(S_{\mathbf{X}_1, \|\mathbf{X}_1 - \mathbf{X}_2\|})}$ and $e^{-(n-2)\mu(S_{\mathbf{X}_2, \|\mathbf{X}_1 - \mathbf{X}_2\|})}$ are upper bounded by $e^{-(n-1)\gamma\|\mathbf{X}_1 - \mathbf{X}_2\|^d}$. Therefore

$$|\mathbf{E}\{m(\mathbf{X}_{n,1,1})^2\} - \mathbf{E}\{m(\mathbf{X}_1)^2\}| \leq c_{10}n^2\mathbf{E}\left\{\|\mathbf{X}_1 - \mathbf{X}_2\|^{d+2}e^{-(n-1)\gamma\|\mathbf{X}_1 - \mathbf{X}_2\|^d}\right\}.$$

Note that the random variable $R := \|\mathbf{X}_1 - \mathbf{X}_2\|$ has a density on $[0, 2K]$ bounded above by $c_{11}r^{d-1}$. Therefore

$$\begin{aligned} |\mathbf{E}\{m(\mathbf{X}_{n,1,1})^2\} - \mathbf{E}\{m(\mathbf{X}_1)^2\}| & \leq c_{12}n^2 \int_0^{2K} r^{d+2}e^{-n\gamma r^d}r^{d-1}dr \\ & \leq c_{12}n^{-2/d} \int_0^\infty r^{1+2/d}e^{-\gamma r}dr. \end{aligned}$$

□

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