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Abstract

The main objective of this paper is to estimate optimally Sobol' indices at any order when a unique input/output i.i.d. sample is available. Our approach stands on three main ingredients: semi-parametric estimation theory, high-order kernel estimation (inspired by the paper [13]), and mirror-type transformations as introduced in [2, 33]. We propose two different estimators. We prove that these estimators are asymptotically normal and efficient. Furthermore, we illustrate their numerical properties on standard examples.

Keywords: Global sensitivity analysis; Sobol' indices; Given-data estimation; Kernel estimation; One-step estimation; Asymptotic properties.

AMS subject classification: 62G05, 62G08, 62G20.

1 Introduction

The use of complex computer models to simulate and analyse natural systems in physics, engineering and other fields is now commonplace. These models usually depend on many input variables, and it is thus crucial to understand which input parameter or which set of input parameters have an influence on the output. This is the purpose of sensitivity analysis, which has become an essential tool for systems modelling and policy support (see, e.g., [34]). Global sensitivity analysis methods consider the input vector as random and propose a measure of the influence, in terms of output fluctuations, of each subset of its components. We refer to the seminal book [35] for an overview on global sensitivity analysis or to [8] for a synthesis of recent trends in this field. Among the different measures

of global sensitivity analysis, variance-based measures are probably the most commonly used. The so-called Sobol' indices, introduced in [30] and later revisited in the framework of sensitivity analysis in [36, 37], is based on the Hoeffding decomposition of the variance [21]. More precisely, for the output Y of a computer code $Y = G(V_1, \dots, V_p)$ where the inputs V_i are assumed to be mutually independent, the closed Sobol' index of Y with respect to a subset of inputs X of dimension d is defined by

$$S^X = \frac{\mathrm{Var}(\mathbb{E}[Y|X])}{\mathrm{Var}(Y)} = \frac{\mathbb{E}[\mathbb{E}[Y|X]^2] - \mathbb{E}[Y]^2}{\mathrm{Var}(Y)}.$$

Generally, in practice the explicit computation of S^X is out of reach. One of the main tasks in sensitivity analysis is thus to provide statistical estimators of S^X having good asymptotic properties (consistency, asymptotic distribution, asymptotic efficiency...). In recent years a myriad of different estimators have been proposed, we refer to [8, Chapter 4] for a full review. A practical statistical method widely used to construct estimators is based on spectral analysis of the input/output functional relationship and Parseval formulae. We refer to [39] for a basic description of the method and to [8, Chapter 4] for more recent references. It should be noted that the asymptotic properties of these methods have been little studied, as they are based on the theory of non-linear (quadratic) functional estimation. Away from the spectral methods, two families of estimation methods are of particular interest because of the possibility of studying the asymptotic properties of the estimators produced.

The first family of methods is based on the so-called Pick Freeze (PF) design of experiments. The basic idea is to evaluate G repeatedly for input values, fixing those of the vector X, and then to calculate a Monte Carlo estimate of S^X from this particular sampling. The main advantage is that only minimal assumptions are required to derive consistency and central limit theorems. In particular, assumptions of integrability but not regularity on G are necessary (see for example [15, 22]). As an illustration, to estimate at rate $\sqrt{n}$ a single Sobol' index, one needs a design of experiments of size $2n$. This implies that estimating all the p first-order indices corresponding to $d = 1$ involves a sample of size $(p + 1)n$. Notice that recently, this cost has been reduced to $2n$ [40, 17]. The main drawback of this estimation method is that it requires a specific experimental design. In particular, it cannot be used in the case where we only have a classical i.i.d. (vanilla) sample of n input/output observations.

The second class of methods relies on local averaging and tackles this limitation. Among them are kernel estimators, which have been thoroughly studied for the case $d = 1$ [9, 7, 32, 38, 20] with central limit theorems and asymptotic efficiency as soon as G satisfies regularity assumptions. Closely related are nearest neighbor approaches, which have been studied by several authors (see, e.g., [12, 26, 27, 10, 18, 11]). For instance in [11], the authors propose a plug-in estimator with statistical consistency for any d and a central limit theorem with rate $\sqrt{n}$ for $d \leqslant 3$ if, again, regularity assumptions hold. In parallel, [4] consider a variant which is consistent for any d but no rate of convergence is provided. When $d = 1$, a central limit theorem for estimators based on ranks (i.e. nearest neighbors on the right) is also proved in [14].

In a nutshell, on the one hand, the class of PF estimators allows to estimate Sobol' indices at rate $\sqrt{n}$ for any d with minimal assumptions on G but requires a sample with highly

specific structure. On the other hand, local-averaging estimators can handle a vanilla n-sample but need some regularity assumptions on the model and $\sqrt{n}$-parametric rate of convergence is proved only for $d \leqslant 3$ (nearest neighbors method). In this paper, we propose and study a more general local-averaging estimator and show that the rate $\sqrt{n}$ holds for any d.

In our work, we build an optimal estimator. In that view, we correct a plug-in estimator using a high-order kernel and a mirror-type transformation. The correction improves the initial estimator by correcting the bias (see, e.g., [31, 29]), in line with techniques used to improve an estimator in the frame of semi-parametric inference. We refer to [42, Chapter 25] for an exhaustive overview of this theory. As a matter of fact, in our frame, the nonparametric part is the unknown regression function. It is handled by using a very specific kernel estimator. More precisely, on the one hand, we make use of high-order kernels in order to obtain $\sqrt{n}$ rate of convergence, following recent approaches of nonparametric regression (see for example [41]). Note that a high-order kernel has a non-zero negative part thus is not a probability density. Its use allows to kill the bias in the interior of the domain. On the other hand, to remove boundary effects inherent to the kernel estimation procedure, we adapt recent mirror-type transformations [2, 33]. We propose and study two variants for the mirror transformation. In both cases, we show that the proposed estimators satisfy a central limit theorem with the optimal rate and minimal variance. Up to our knowledge, this general optimality result is new in the frame of the estimation of Sobol' indices of any order when using only a vanilla n-sample. Notice that the order one case is tackled in [7] by using another estimator based on classical kernel estimation jointly with a spectral approach. Note finally that our results are closely related to the ones developed in [13] where the boundary issue is tackled using truncation leading to the estimation of a pruned version of S^X.

The paper is organized as follows. The setting and the notation are introduced in Section 2. Then, considering two different mirror-type transformations, we present in Section 3 two kernel-based regression estimators. Section 4 is devoted to the statement of our main results, namely central limit theorems and asymptotic efficiency. A comparison study of asymptotic estimation variance with existing methods is provided in Section 5. Section 6 presents several numerical illustrations of our estimation procedure. The proofs are postponed to Appendix A. Moreover, extended numerical studies discussing numerical stability of high-order kernels can be found on the following link `https://hal.science/hal-04052837`.

2 Setting

2.1 Model and purpose

The output Y is obtained from a regression model (generally computed by a numerical code or a machine learning estimated model), and is regarded as a function G of the vector of random inputs $(V_i)_{i=1,\dots,p}$:

$$Y = G(V_1, \dots, V_p),$$

where the function G is defined on a compact subset of $\mathbb{R}^p$, $p \geqslant 2$ and is real-valued. Classically we assume that the V_i's are independent random variables and that $Y \in \mathbb{L}^2(\mathbb{R})$:

global sensitivity analysis is then performed using Hoeffding decomposition [1, 42] which leads to standard Sobol' indices introduced below [36].

For any $u \subsetneq \{1, \dots, p\}$, $u \neq \emptyset$ we denote $X = (V_i)_{i \in u}$ a group of inputs with cardinality $|u| = d < p$. The *first-order Sobol' index* of output Y associated to the d-dimensional vector X is defined as

$$S^X = \frac{\mathrm{Var}(\mathbb{E}[Y|X])}{\mathrm{Var}(Y)} = \frac{\mathbb{E}[\mathbb{E}[Y|X]^2] - \mathbb{E}[Y]^2}{\mathrm{Var}(Y)}. \tag{1}$$

For the specific case $u = \{i_0\}$ with $i_0 \in \{1, \dots, p\}$, that is for $X = V_{i_0}$, $S^{i_0} = S^X$ is the first-order Sobol' index associated to the input V_{i_0}. In addition, the *total Sobol' index* associated to V_{i_0} writes

$$S^{\mathrm{tot},i_0} = 1 - S^{V_{\sim i_0}} \tag{2}$$

where $V_{\sim i_0} = (V_1, \cdots, V_{i_0-1}, V_{i_0+1}, \cdots, V_p)$.

Our goal is to estimate S^X from a n-sample $(X_j, Y_j)_{j=1,\dots,n}$ of the pair (X, Y) with joint distribution $\mathcal{P}$. Since $\mathbb{E}[Y]$ and $\mathrm{Var}(Y)$ can naturally be estimated with classical empirical moments, we focus here on the estimation in (1) of

$$T = \mathbb{E}[\mathbb{E}[Y|X]^2]. \tag{3}$$

2.2 Notation and assumptions

In this section, we give the general assumptions made in the paper.

($\mathcal{A}$1) The support of $(V_1, \dots, V_p)$ is $[0,1]^p$. We assume that X is absolutely continuous with respect to the Lebesgue measure on $[0,1]^d$ with density function f_X.

One actually only needs to assume that the support of $(V_1, \dots, V_p)$ is of the form $[B_1, C_1] \times \cdots \times [B_p, C_p]$ where $B_i < C_i$ for all $i \in \{1, \dots, p\}$, but for simpler notation here we only consider $[0,1]^p$.

($\mathcal{A}$2) $\exists\, \delta > 0$ such that $\inf_{x \in [0,1]^d} f_X(x) \geqslant \delta$ for some $\delta > 0$.

($\mathcal{A}$3) $\mathbb{E}[Y^4] < \infty$ and $\sigma^2(x) = \mathrm{Var}(Y|X = x)$ is bounded on $[0,1]^d$.

Note that under Assumption **($\mathcal{A}$3)** the regression function $m(\cdot) = \mathbb{E}[Y|X = \cdot]$ exists and is bounded on the support of X by Cauchy-Schwartz inequality. Furthermore, we define the function $g := f_X m$.

For any integer d, we introduce the following multi-index notation. For any $\beta = (\beta_1, \dots, \beta_d) \in (\mathbb{R}_{>0})^d$, let $\lfloor \beta \rfloor$ be the largest integer stricly lower than β: $\lfloor \beta \rfloor = (\lfloor \beta_1 \rfloor, \dots, \lfloor \beta_d \rfloor) =: \gamma \in \mathbb{N}^d$. In addition, we introduce

$$|\gamma| = \gamma_1 + \cdots + \gamma_d\,,\ \gamma! = \gamma_1! \dots \gamma_d!,\ \text{and } v^\beta = v_1^{\beta_1} \dots v_d^{\beta_d} \text{ for any } v \in \mathbb{R}^d\,.$$

For $\alpha > 0$ let $\mathcal{C}^\alpha([0,1]^d)$ be the set of functions $\phi\colon [0,1]^d \to \mathbb{R}$ that have derivatives up to order $\lfloor \alpha \rfloor$ and for which partial derivative of order $\lfloor \alpha \rfloor$ is $\alpha - \lfloor \alpha \rfloor$-Hölder. Namely, there exists $C_\phi > 0$ such that, for any x and $x' \in [0,1]^d$, one has

$$\left| \frac{\partial^\beta \phi}{\partial x^\beta}(x) - \frac{\partial^\beta \phi}{\partial x^\beta}(x') \right| \leqslant C_\phi \left\| x - x' \right\|_\infty^{\alpha - \lfloor \alpha \rfloor} \tag{4}$$

for any $\beta \in \mathbb{N}^d$ such that $\beta = \lfloor \alpha \rfloor$ where $(\partial^\beta \cdot / \partial x^\beta)$ stands for the partial derivative of order β and $\|\cdot\|_\infty$ for the supremum norm on $[0,1]^d$.

($\mathcal{A}4$) The density f_X of X belongs to $\mathcal{C}^\alpha([0,1]^d)$ for some $\alpha > 0$.

($\mathcal{A}5$) The regression function m belongs to $\mathcal{C}^\alpha([0,1]^d)$.

Notice that, if the model G belongs to $\mathcal{C}^\alpha$, then Assumption **($\mathcal{A}5$)** is satisfied.

($\mathcal{A}6$) Let $k\colon [0,1] \to \mathbb{R}$ be a univariate kernel such that $\|k\|_\infty < \infty$ and $\int_0^1 k(u)du = 1$. We assume that k is of order $(\lfloor \alpha \rfloor + 1)$ which means that $\int_0^1 u^\ell k(u)du = 0$ for any $\ell \in \mathbb{N}$ such that $0 < \ell \leqslant \lfloor \alpha \rfloor$ and $\int_0^1 u^{\lfloor \alpha \rfloor + 1} k(u)du \neq 0$. Furthermore, we define the multivariate kernel $K\colon [0,1]^d \to \mathbb{R}$ as: $K(u) = \prod_{k=1}^d k(u_k)$ for any $u = (u_1, \ldots, u_d) \in [0,1]^d$. Finally, we define $K_h(u) = K(u/h)/h^d = \prod_{k=1}^d k(u_k/h)/h^d$ for any $u = (u_1, \ldots, u_d) \in [0,1]^d$.

Observe that $\int_{[0,1]^d} u^\beta K(u)du = 0$ for any $\beta \in \mathbb{N}^d$ such that $0 < |\beta| \leqslant \lfloor \alpha \rfloor$ and $\int_{[0,1]^d} u^\beta K(u)du \neq 0$ for some β such that $|\beta| = \lfloor \alpha \rfloor + 1$.

($\mathcal{A}7$) The sequence $(h_n)_{n\in\mathbb{N}}$ of bandwidths is positive and such that $h_n \to 0$ as $n \to \infty$.

In the rest of the paper, C denotes a generic constant (deterministic and finite) which may vary from line to line.

3 Estimation procedure and preliminary results

In this section, we propose an estimator of T based on two main ingredients: (a) estimation based on the efficient influence function of T (see, e.g., [3, 13, 42]) and (b) mirror-type kernel estimators (see, e.g., [2, 33]).
Let us first exhibit the general form of the estimator of T considered in this paper:

$$T_n = \frac{1}{n}\sum_{i=1}^n (2Y_i - m_n(X_i))\, m_n(X_i). \tag{5}$$

Here, m_n is an estimator of the regression function m of Y on X (with properties to be discussed later), and $(X_i, Y_i)_{1\leqslant i\leqslant n}$ are independent copies of (X, Y).
Such a form can actually be justified and inferred from a heuristic based on efficient influence functions. Indeed, let $\mathcal{P}$ be the set of probability distributions on $[0,1]^d \times \mathbb{R}$ satisfying Assumptions **($\mathcal{A}2$)**, **($\mathcal{A}3$)**, **($\mathcal{A}4$)** and **($\mathcal{A}5$)**. Then we know from [13] that

$$(x, y) \mapsto (2y - m(x))m(x) - \mathbb{E}[\mathbb{E}[Y|X]]$$

is the efficient influence function of T under the nonparametric model $\mathcal{P}$ (see [24] for detailed computations). Thus, if the probability distribution of (X, Y) is in $\mathcal{P}$ and if m is known, we can state, from [42, Equation (25.22)], that the estimator

$$T_n = \frac{1}{n}\sum_{i=1}^n (2Y_i - m(X_i))\, m(X_i) \tag{6}$$

is asymptotically efficient with optimal variance equal to $\mathrm{Var}\left((2Y - m(X))\, m(X)\right)$. Unfortunately, the estimator in (6) is only an oracle, as m is unknown in our case and needs then to be estimated, but this explains the intuition behind our focus on (5). As for the

choice of the estimator of m, since we assume that the domain of the inputs is compact, the crucial point is to handle possible boundary effects. To do so, in [13] the authors estimate a truncated version of T defined as $T^{\text{trunc},\varepsilon} = \mathbb{E}[\mathbb{E}[Y|X]^2 \mathbb{1}_{X\in(\varepsilon,1-\varepsilon)^d}]$. Even if $T^{\text{trunc},\varepsilon} \to T$ as $\varepsilon \to 0$ under mild assumptions, the practical tuning of the parameter ε depends on the unknown function G and its choice has a large impact, see Figure 7 in the numerical experiment section. Here, we therefore prefer the use of plugging mirror-type kernel estimators for $m(\cdot)$ in (6). Mirror-type transformations have been used, e.g., in [2, 33] in the framework of density estimation. In the following, we adapt these works to propose two nonparametric estimators of m, denoted as $\widehat{m}$ and $\widetilde{m}$. We then prove that both estimators $\widehat{T}_n$ and $\tilde{T}_n$ satisfy a central limit theorem with optimal asymptotic variance $\text{Var}\left((2Y - m(X))\, m(X)\right)$.

3.1 A mirror-type kernel estimator for the regression function

To estimate the regression function m, we consider a leave-one-out kernel estimator together with a mirror-type transformation introduced in [2] to bypass boundary issues. More precisely, the regression function estimator is defined as follows:

$$\widehat{m}_{n,h_n,i}(X_i) = \frac{\sum_{j\neq i} Y_j K_{h_n} \circ A_{X_i}(X_j - X_i)}{\sum_{j\neq i} K_{h_n} \circ A_{X_i}(X_j - X_i)} \mathbb{1}_{\sum_{j\neq i} K_{h_n}\circ A_{X_i}(X_j - X_i)\neq 0} \tag{7}$$

for a bandwidth $h_n > 0$, a mirror-type transformation A, and a kernel K_{h_n} satisfying Assumption **($\mathcal{A}$6)** presented in Section 2.2. Then, (6) is adapted as

$$\widehat{T}_{n,h_n} = \frac{1}{n}\sum_{i=1}^{n} (2Y_i - \widehat{m}_{n,h_n,i}(X_i))\widehat{m}_{n,h_n,i}(X_i)\,. \tag{8}$$

As for the mirror-transformation, for $x \in [0,1]^d$, one may consider for instance

$$A_x \colon \left\{ \begin{array}{ccc} \mathbb{R}^d & \to & \mathbb{R}^d \\ u = (u_1, \ldots, u_d) & \mapsto & (a_1(x_1)u_1, \ldots, a_d(x_d)u_d) \end{array} \right. \tag{9}$$

with $a_i(s) := 1 - 2\mathbb{1}_{(\frac{1}{2},1]}(s) \in \{-1, 1\}$, see Figure 1 for an illustration. Observe that $\mathcal{A} = \{A_x, x \in [0,1]^d\}$ is a finite subset of $GL_d(\mathbb{R})$ (where $GL_d(\mathbb{R})$ is the general linear group on $\mathbb{R}$), $\mathcal{A} = \{A_1, \ldots, A_\kappa\}$, with cardinality $\kappa = 2^d$. Moreover, it satisfies

(i) for any $\ell = 1, \ldots, \kappa$, $|\det(A_\ell)| = 1$;

(ii) **Mirror property**:

$$\forall x \in [0,1]^d,\ x + A_x^{-1}([0,1/2]^d) \subset [0,1]^d. \tag{10}$$

The $\mathcal{C}^\alpha([0,1]^d)$ regularity assumption can be relaxed to piecewise regularity as soon as the number k of pieces is finite. The cardinality of $\mathcal{A}$ is then increased to $\kappa = (2k)^d$.
Let $\widehat{f}_{n,h_n,i}$ be the leave-one-out estimator of the density function f_X based on the $(n-1)$-sample $(X_1, \cdots, X_{i-1}, \cdots, X_{i+1}, \cdots, X_n)$:

$$\widehat{f}_{n,h_n,i}(x) = \frac{1}{n-1}\sum_{j\neq i} K_{h_n} \circ A_x(X_j - x). \tag{11}$$

The following lemmas establish classical controls on the bias and on the variance of $\widehat{f}_{n,h_n,i}$ for all $i \in \{1, \cdots, d\}$. The proofs are postponed to Appendix A.1.

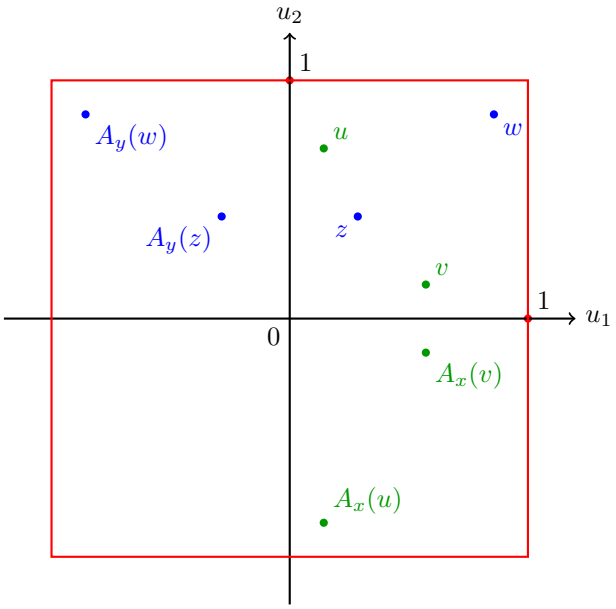


Figure 1: Mirror-type transformation with $d = 2$, for $x = (1/3, 3/4)$, and for $y = (2/3, 1/5)$.

Lemma 3.1. *Under Assumptions* **(A1)**, **(A4)**, *and* **(A6)**, *for all* $i \in \{1, \cdots, d\}$,

$$\left\|\mathbb{E}\left[\widehat{f}_{n,h_n,i}\right] - f_X\right\|_\infty = \left\|\mathbb{E}\left[\widehat{f}_{n,h_n,1}\right] - f_X\right\|_\infty = O\Big(h_n^\alpha\Big). \tag{12}$$

To control the variance, one needs to define a supplementary assumption.

(A8) Assume that the family of functions

$$\mathcal{F} = \{K_{h,x} \colon y \in [0,1]^d \mapsto K_h(y - x) \in \mathbb{R},\ h > 0, x \in [0,1]^d\} \tag{13}$$

is a uniformly bounded Vapnik-Chervonenkis (VC)-class of functions, i.e. there exists positive numbers A, B, and v such that, for all $K \in \mathcal{F}$, $\|K\|_\infty < \infty$ and the ε-covering number $\mathcal{N}(\mathcal{F}, L^2(Q), \varepsilon)$ of $\mathcal{F}$ for the $L^2(Q)$-distance satisfies

$$\mathcal{N}(\mathcal{F}, L^2(Q), \varepsilon) \leqslant \left(\frac{AB}{\varepsilon}\right)^v$$

for every probability measure Q on $[0,1]^d$ and for every $\varepsilon \in (0, B)$.

Lemma 3.2. *Let* $\delta_n \in (0,1)$. *Under Assumptions* **(A1)**, **(A6)**, *and* **(A8)**, *there exists a constant* $C > 0$ *such that we have, with probability* $1 - \delta_n$,

$$\left\|\widehat{f}_{n,h_n,i} - \mathbb{E}\left[\widehat{f}_{n,h_n,i}\right]\right\|_\infty^2 \leqslant C\ \frac{\log(\frac{1}{h_n}) + \log(\frac{2}{\delta_n})}{nh_n^d} \tag{14}$$

for all $i \in \{1, \cdots, d\}$.

Remark 3.3. Choosing $h_n = n^{-1/(2\alpha+d)}$ and $\delta_n = 1/n$ in Lemmas 3.1 and 3.2, we get the following bound with probability $1 - 1/n$:

$$\left\| \widehat{f}_{n,h_n,i} - f_X \right\|_\infty \leqslant C \sqrt{\log(n)} n^{-\alpha/(2\alpha+d)}$$

which corresponds to the optimal nonparametric rate up to the log factor.

Now, we can control the mean integrated squared error of $\widehat{f}_{n,h_n,i}$ together with its infimum.

Corollary 3.4. *Under Assumptions* **(A1)**, **(A2)**, **(A4)**, **(A6)**, *and* **(A8)**, *one has, for all* $i \in \{1, \cdots, d\}$,

$$\mathbb{E}\Big[\int_{[0,1]^d} (\widehat{f}_{n,h_n,i}(x) - f_X(x))^2 dx\Big] = o(n^{-1/2}) \tag{15}$$

and

$$\frac{1}{\inf_{x\in[0,1]^d} \left|\widehat{f}_{n,h_n,i}(x)\right|} = O_{\mathbb{P}}(1) \tag{16}$$

as soon as $nh_n^{2d} \to \infty$ *and* $nh_n^{4\alpha} \to 0$ *as* $n \to \infty$.

Assuming $h_n = n^{-\gamma}$ with $\gamma > 0$, the conditions $nh_n^{2d} \to \infty$ and $nh_n^{4\alpha} \to 0$ lead to $1/(4\alpha) < \gamma < 1/(2d)$ and $\alpha > d/2$. The proof of Corollary 3.4 is postponed to Appendix A.1.

3.2 An alternative regression estimator

This alternative estimator is based on the mirror-image kernel density estimator in [33], introduced as a generalization to dimension $d \geqslant 2$ of the estimator in [28]. More precisely, we consider the following transformations: for any $z \in [0,1]$,

$$m^{-1}(z) = -z, \quad m^0(z) = z, \quad \text{and} \quad m^1(z) = 2 - z,$$

and, for any $a \in \{-1,0,1\}^d$ and $x \in [0,1]^d$, the d-dimensional vector

$$M^a(x) = (m^{a_1}(x_1), \cdots, m^{a_d}(x_d)).$$

Then, let

$$\widetilde{f}_{n,h_n,i}(x) = \mathbb{1}_{[0,1]^d}(x) \frac{1}{(n-1)} \sum_{j\neq i} \sum_{a\in\{-1,0,1\}^d} \widetilde{K}_{h_n}\Big(M^a(X_j) - x\Big), \tag{17}$$

and

$$\widetilde{g}_{n,h_n,i}(x) = \mathbb{1}_{[0,1]^d}(x) \frac{1}{(n-1)} \sum_{j\neq i} Y_j \sum_{a\in\{-1,0,1\}^d} \widetilde{K}_{h_n}\Big(M^a(X_j) - x\Big). \tag{18}$$

Here, the bandwidth $h_n > 0$ and the multivariate kernel $\widetilde{K}$ satisfy Assumption **(A′5)** stated below. Now we propose the following regression function estimator:

$$\widetilde{m}_{n,h_n,i}(X_i) = \frac{\widetilde{g}_{n,h_n,i}(X_i)}{\widetilde{f}_{n,h_n,i}(X_i)} \tag{19}$$

if $\widetilde{f}_{n,h_n,i}(X_i) \neq 0$ and 0 otherwise. The associated plug-in estimator then becomes:

$$\widetilde{T}_{n,h_n} = \frac{1}{n} \sum_{i=1}^n (2Y_i - \widetilde{m}_{n,h_n,i}(X_i)) \widetilde{m}_{n,h_n,i}(X_i). \tag{20}$$

The assumptions on f_X and g are strengthened as follows.

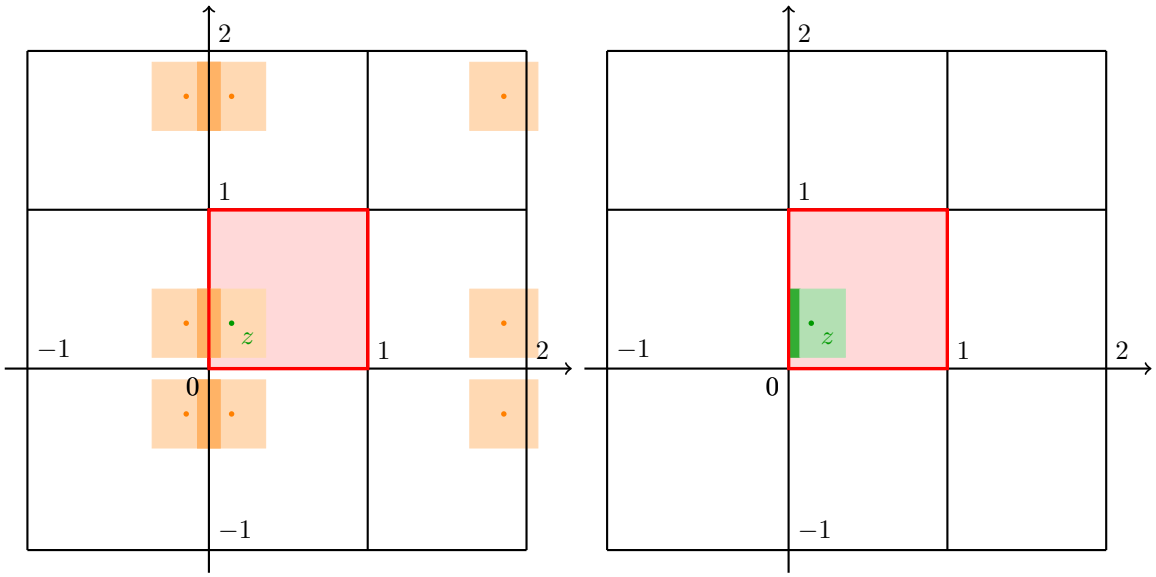


Figure 2: Mirror-image transformation with $d = 2$ in red. In the left-hand side of the figure, a data-point in $[0,1]^d$ (in green) and its 8 mirror-images (in orange). A kernel is fitted over all points of the augmented dataset (orange areas). The darker orange regions correspond to the regions where several kernels overlap. In the right-hand side of the figure, the data-point (in green) and the restriction to $[0,1]^d$ of the augmented dataset (in green).

($\mathcal{A}'$4) The density function $f_X \in \mathcal{C}^\alpha([0,1]^d)$ for some $\alpha > 0$. Its derivatives of order β, with $0 < \beta \leqslant \lfloor \alpha \rfloor$, vanish near the boundary.

The assumptions on K are listed below.

($\mathcal{A}'$5) Let $\widetilde{k}\colon [-1,1] \to \mathbb{R}$ be a univariate kernel such that $\left\|\widetilde{k}\right\|_\infty < \infty$ and $\int_{-1}^1 \widetilde{k}(u)du = 1$. We assume that k is of order $(\lfloor \alpha \rfloor + 1)$ which means that $\int_{-1}^1 u^\ell \widetilde{k}(u)du = 0$ for any $\ell \in \mathbb{N}$ such that $0 < \ell \leqslant \lfloor \alpha \rfloor$ and $\int_{-1}^1 u^{\lfloor \alpha \rfloor + 1} \widetilde{k}(u)du \neq 0$. Furthermore, we define the multivariate kernel $\widetilde{K}\colon [-1,1]^d \to \mathbb{R}$ as: $\widetilde{K}(z) = \prod_{k=1}^d \widetilde{k}(u_k)$. Finally, we define $\widetilde{K}_h(u) = \widetilde{K}(u/h)/h^d = \prod_{k=1}^d \widetilde{k}(u_k/h)/h^d$ for any $u \in [-1,1]^d$.

Both numerator and denominator of the estimator defined in (19) are the sum of 3^d terms; one corresponds to the original data in the unit hypercube $[0,1]^d$, and each of the remaining terms corresponds to reflected data across one of the 0-faces, 1-faces, ..., $d-1$-faces of the unit hypercube as illustrated in Figure 2 for $d = 2$.

Note that the function $\widetilde{f}_{n,h_n,i}$ is supported on $[0,1]^d$ and $\int_{[0,1]^d} \widetilde{f}_{n,h_n,i}(x)dx = 1$. Moreover, it satisfies the two following lemmas.

Lemma 3.5. *Let $h_n \in (0, 1/2)$. Under Assumptions the* **($\mathcal{A}$1)**, **($\mathcal{A}'$4)**, *and* **($\mathcal{A}'$5)**, *for all $i \in \{1, \cdots, d\}$, we have*

$$\left\|\mathbb{E}\left[\widetilde{f}_{n,h_n,i}\right] - f_X\right\|_\infty = \left\|\mathbb{E}\left[\widetilde{f}_{n,h_n,1}\right] - f_X\right\|_\infty = O(h_n^\alpha). \tag{21}$$

Lemma 3.5 is an extension of [33, Proposition 5.2] to every $\alpha > 0$ in Assumption **($\mathcal{A}'$4)** (itself an extension to every dimension and every $\alpha \in (0,2]$ of [28, Lemma 3.1]). Its proof is postponed to Appendix A.2.

Lemma 3.6. *[33, Proposition 5.3] Let $h_n \in (0, 1/2)$ and $\delta_n \in (0, 1)$. Under the Assumptions* $(\mathcal{A}\mathbf{1})$, $(\mathcal{A}'\mathbf{5})$, *and* $(\mathcal{A}\mathbf{8})$ *and with the kernel $\widetilde{K}$, there exists a constant $C > 0$ such that we have, with probability $1 - \delta_n$,*

$$\left\| \widetilde{f}_{n,h_n,i} - \mathbb{E}\left[\widetilde{f}_{n,h_n,i}\right] \right\|_\infty^2 \leqslant C \, \frac{\left(\log(\frac{1}{h_n})\right)_+ + \log(\frac{2}{\delta_n})}{nh_n^d} \tag{22}$$

for all $i \in \{1, \cdots, d\}$.

Once more, choosing $h_n = n^{-1/(2\alpha+d)}$ and $\delta_n = 1/n$ in Lemmas 3.5 and 3.6, we recover the optimal nonparametric rate up to the log factor. As before, we can deduce from Lemmas 3.5 and 3.6 the control of the mean integrated squared error of $\widetilde{f}_{n,h_n,i}$ together with its infimum.

Corollary 3.7. *Assume that Assumptions* $(\mathcal{A}\mathbf{1})$, $(\mathcal{A}\mathbf{2})$, $(\mathcal{A}'\mathbf{4})$, *and* $(\mathcal{A}'\mathbf{5})$ *are satisfied, as well as Assumption* $(\mathcal{A}\mathbf{8})$ *with kernel $\widetilde{K}$. Then one has, for all $i \in \{1, \cdots, d\}$,*

$$\mathbb{E}\Big[\int_{[0,1]^d} (\widetilde{f}_{n,h_n,i}(x) - f_X(x))^2 dx\Big] = o(n^{-1/2}) \tag{23}$$

and

$$\frac{1}{\inf_{x\in[0,1]^d} \left|\widetilde{f}_{n,h_n,i}(x)\right|} = O_{\mathbb{P}}(1) \tag{24}$$

as soon as $nh_n^{2d} \to \infty$ and $nh_n^{4\alpha} \to 0$ as $n \to \infty$.

Assuming $h_n = n^{-\gamma}$ with $\gamma > 0$, the conditions $nh_n^{2d} \to \infty$ and $nh_n^{4\alpha} \to 0$ lead once more to $1/(4\alpha) < \gamma < 1/(2d)$ and $\alpha > d/2$.

The proof of Corollary 3.7 comes from Lemmas 3.5 and 3.6 and is similar to the proof of Corollary 3.4 from Lemmas 3.1 and 3.2. It is thus skipped.

4 Central limit theorems

In this section, we prove a central limit theorem for both estimators defined in (8) and (20).

Theorem 4.1 (Central limit theorem for $\widehat{T}_{n,h_n}$)**.** *Under Assumptions* $(\mathcal{A}\mathbf{1})$ *to* $(\mathcal{A}\mathbf{8})$, *one has*

$$\sqrt{n}\Big(\widehat{T}_{n,h_n} - \mathbb{E}[\mathbb{E}[Y|X]^2]\Big) \xrightarrow[n\to\infty]{\mathcal{L}} \mathcal{N}\Big(0, \, Var((2Y - m(X))m(X))\Big) \tag{25}$$

as soon as $\alpha > d/2$ and $h_n = n^{-\gamma}$ with $1/(4\alpha) < \gamma < 1/(2d)$.

Theorem 4.2 (Central limit theorem for $\widetilde{T}_{n,h_n}$)**.** *Replacing Assumptions* $(\mathcal{A}\mathbf{4})$ *and* $(\mathcal{A}\mathbf{6})$ *respectively by Assumptions* $(\mathcal{A}'\mathbf{4})$ *and* $(\mathcal{A}'\mathbf{5})$ *in the statement of Theorem 4.1, one has*

$$\sqrt{n}\Big(\widetilde{T}_{n,h_n} - \mathbb{E}[\mathbb{E}[Y|X]^2]\Big) \xrightarrow[n\to\infty]{\mathcal{L}} \mathcal{N}\Big(0, \, Var((2Y - m(X))m(X))\Big) \tag{26}$$

as soon as $\alpha > d/2$ and $h_n = n^{-\gamma}$ with $1/(4\alpha) < \gamma < 1/(2d)$.

The proofs of Theorems 4.1 and 4.2 are postponed to Appendix A.3 while the proofs of the following results are postponed to Appendix A.4.

Proposition 4.3 (Asymptotic efficiency for $\widehat{T}_{n,h_n}$ and $\widetilde{T}_{n,h_n}$)**.** *Under the assumptions of Theorems 4.1 and 4.2 respectively, $\widetilde{T}_{n,h_n}$ and $\widetilde{T}_{n,h_n}$ are asymptotically efficient to estimate $\mathbb{E}[\mathbb{E}[Y|X]^2]$ from an i.i.d. sample $(X_i, Y_i)_{i=1,\cdots,n}$ of the pair (X, Y).*

Using the delta method [42, Theorem 3.1], we are now able to get the asymptotic behavior of the estimators of S^X derived respectively from (8) and (20). Let

$$\widehat{S}_{n,h_n} := \frac{\widehat{T}_{n,h_n} - \left(\frac{1}{n}\sum_{j=1}^n Y_j\right)^2}{\frac{1}{n}\sum_{j=1}^n Y_j^2 - \left(\frac{1}{n}\sum_{j=1}^n Y_j\right)^2} \quad \text{and} \quad \widetilde{S}_{n,h_n} := \frac{\widetilde{T}_{n,h_n} - \left(\frac{1}{n}\sum_{j=1}^n Y_j\right)^2}{\frac{1}{n}\sum_{j=1}^n Y_j^2 - \left(\frac{1}{n}\sum_{j=1}^n Y_j\right)^2}.$$

Corollary 4.4 (Central limit theorem and asymptotic efficiency for $\widehat{S}_{n,h_n}$ and $\widetilde{S}_{n,h_n}$)**.**
(i) Under the assumptions of Theorem 4.1, one has

$$\sqrt{n}\left(\widehat{S}_{n,h_n} - S^X\right) \xrightarrow[n\to\infty]{\mathcal{L}} \mathcal{N}(0, \sigma^2), \tag{27}$$

where the limiting variance σ^2 has an explicit expression given in the proof.
(ii) Under the assumptions of Theorem 4.2, the same result holds for $\widetilde{S}_{n,h_n}$.
(iii) Moreover, $\widehat{S}_{n,h_n}$ and $\widetilde{S}_{n,h_n}$ are asymptotically efficient to estimate S^X from an i.i.d. sample $(X_i, Y_i)_{i=1,\cdots,n}$ of the pair (X, Y).

Using once more the delta method, we deduce the asymptotic behavior of the vector of the p first-order Sobol' indices. Let us denote by S^i the first-order Sobol' index associated to $X = V_i$ and its estimators $\widehat{S}^i$ and $\widetilde{S}^i$ given by:

$$\widehat{S}^i_{n,h_n} := \frac{\widehat{T}_{n,h_n} - \left(\frac{1}{n}\sum_{j=1}^n Y_j\right)^2}{\frac{1}{n}\sum_{j=1}^n Y_j^2 - \left(\frac{1}{n}\sum_{j=1}^n Y_j\right)^2}, \; \widetilde{S}^i_{n,h_n} := \frac{\widetilde{T}_{n,h_n} - \left(\frac{1}{n}\sum_{j=1}^n Y_j\right)^2}{\frac{1}{n}\sum_{j=1}^n Y_j^2 - \left(\frac{1}{n}\sum_{j=1}^n Y_j\right)^2}.$$

Corollary 4.5. *(i) Under the assumptions of Theorem 4.1, one has*

$$\sqrt{n}\Big((\widehat{S}^1_{n,h_n}, \ldots, \widehat{S}^p_{n,h_n})^T - (S^1, \ldots, S^p)^T\Big) \xrightarrow[n\to\infty]{\mathcal{L}} \mathcal{N}_p(0, \Sigma), \tag{28}$$

where the limiting covariance matrix Σ has an explicit expression.
(ii) Under the assumptions of Theorem 4.2, the same result holds for $(\widetilde{S}^1_{n,h_n}, \ldots, \widetilde{S}^p_{n,h_n})$.
(iii) Moreover, $(\widehat{S}^1_{n,h_n}, \ldots, \widehat{S}^p_{n,h_n})$ and $(\widetilde{S}^1_{n,h_n}, \ldots, \widetilde{S}^p_{n,h_n})$ are asymptotically efficient to estimate $(S^1, \ldots, S^p)$ from an i.i.d. sample $(X_i, Y_i)_{i=1,\cdots,n}$ of the pair (X, Y).

The proof of Corollary 4.5 does not rely on the fact that we are dealing with first-order Sobol' indices. Hence if $u_1, \ldots, u_r$ are distinct subsets of $\{1, \ldots, p\}$, we also have under the same assumptions that

$$\sqrt{n}\Big((\widehat{S}^{u_1}_{n,h_n}, \ldots, \widehat{S}^{u_r}_{n,h_n})^T - (S^{u_1}, \ldots, S^{u_r})^T\Big) \xrightarrow[n\to\infty]{\mathcal{L}} \mathcal{N}_r(0, \Sigma_r), \tag{29}$$

where the limiting covariance matrix Σ_r has an explicit expression. The same result naturally holds for $(\widetilde{S}^{u_1}_{n,h_n}, \ldots, \widetilde{S}^{u_r}_{n,h_n})$.

5 Comparison with existing methods

In this section, we compare several estimators of $\mathbb{E}[\mathbb{E}[Y|X]^2]$ proposed in the literature in terms of asymptotic variance in the central limit theorem.

A seminal kernel-based method As mentioned in Section 3, the authors of [13] consider a truncated version of T defined as $T^{\mathrm{trunc},\varepsilon} = \mathbb{E}[\mathbb{E}[Y|X]^2 \mathbb{1}_{X\in(\varepsilon,1-\varepsilon)^d}]$ to bypass boundary issues.

Proposition 5.1 (Remark 2.2 in [13]). *Under the assumptions of [13, Corollary 2.1] and, for $d \geqslant \alpha$, the limiting variance is given by*

$$Var\left(\mathbb{1}_{X\in(\varepsilon,1-\varepsilon)^d} m^2(X)\right) + 4\mathbb{E}[\mathbb{1}_{X\in(\varepsilon,1-\varepsilon)^d} m^2(X)\sigma^2(X)]$$

recalling that m is the regression function.

As mentioned before, notice that the fine tuning of ε is cumbersome. Moreover, the estimated quantity is not exactly T but only its pruned version.

An alternative kernel-based method in dimension one An alternative procedure has been introduced in [7, page 11]. Anyway, note that the estimator $\widehat{T}_n$ defined in [7, page 11] is not easily tractable in practice. More precisely, the initial n-sample is split into two samples of sizes $n_1 = \lfloor n/\log n \rfloor$ and $n_2 = n - n_1 \approx n$. The first sample is used to estimate the joint density of (X, Y) while the second one is used in an outer loop to estimate the integral term by Monte-Carlo. Asymptotic guarantees are provided in [7] and we recall the form of the asymptotic variance in Proposition 5.2 below.

Proposition 5.2 (Theorems 3.4 and 3.5 in [7]). *The limiting variance is given by*

$$Var((2Y - m(X))m(X)) = Var(m^2(X)) + 4\mathbb{E}[m^2(X)\sigma^2(X)].$$

In addition, the sequence of estimators $(\widehat{T}_n)_{n\geqslant 1}$ is proved to be asymptotically efficient to estimate $\mathbb{E}[\mathbb{E}[Y|X]^2]$. We refer the reader to [7, Theorems 3.4 and 3.5] and [14].

Nearest neighbor-based method One may also compare our results to the estimation procedure proposed in [11], based on nearest neighbors. Here again, the initial $2n$-sample is split into two samples of equal size n. The first sample allows to estimate the regression function $m(\cdot) = \mathbb{E}[Y|X = \cdot]$ using the first nearest neighbor of x among the points of the first sample while the second sample is used as a plug-in estimator. They proved that their estimator S_n is consistent for any dimension d of X and that $\sqrt{n}(S_n - \mathbb{E}[S_n])$ is asymptotically Gaussian. Nevertheless, the bias term is negligible only if $d \leqslant 3$ and in the setting where f_X is Lipschitz continuous and bounded away from zero. Thus it may happen that the central limit theorem does not hold true for $\sqrt{n}(S_n - \mathbb{E}[\mathbb{E}[Y|X]^2])$ if $d \geqslant 4$. In the following proposition, we give the limiting variance obtained with this estimation procedure. The multiplicative factor 2 in front of $\mathrm{Var}(m^2(X))$ takes into account that we have considered two samples of size n.

Proposition 5.3 (Theorem 2.1 in [11]). *Under the assumptions of [11, Theorem 2.1] and for $d \leqslant 3$, the limiting variance is given by*

$$2\,Var(m^2(X)) + 5\mathbb{E}[m^2(X)\sigma^2(X)] + 2\mathbb{E}[\sigma^2(X)].$$

When $d = 1$, one may also use the estimation procedure based on ranks introduced in [5] and studied in [14].

Proposition 5.4 (Proof of Theorem 4.1 in [14, 16])**.** *Under the assumptions of [14, Theorem 4.1], the limiting variance is given by*

$$Var(m^2(X)) + 4\mathbb{E}[m^2(X)\sigma^2(X)] + \mathbb{E}[\sigma^2(X)].$$

This asymptotic variance is not the efficient one. Anyway, this methodology has been proven to perform numerically particularly well.

Pick-Freeze method The limiting variance involved in the central limit theorem of the Pick-Freeze estimation, based on the particular Pick-Freeze design, is given by

$$\mathrm{Var}(m^2(X)) + 2\mathbb{E}[m^2(X)\sigma^2(X)] + \mathbb{E}[\sigma^2(X)].$$

6 Numerical applications

In this section, we illustrate the practical performances of one of our estimators on several analytical test cases coming from the sensitivity analysis literature. Recall that both estimators are based on a high-order kernel supported on $[0, 1]^d$ for the first estimator and on $[-1, 1]^d$ for the second one. From a theoretical perspective both of them lead to equivalent convergence results, but the first one actually suffers from strong numerical instabilities as discussed in `https://hal.science/hal-04052837`. This explains why we focus on the second one in what follows.

For all test cases:

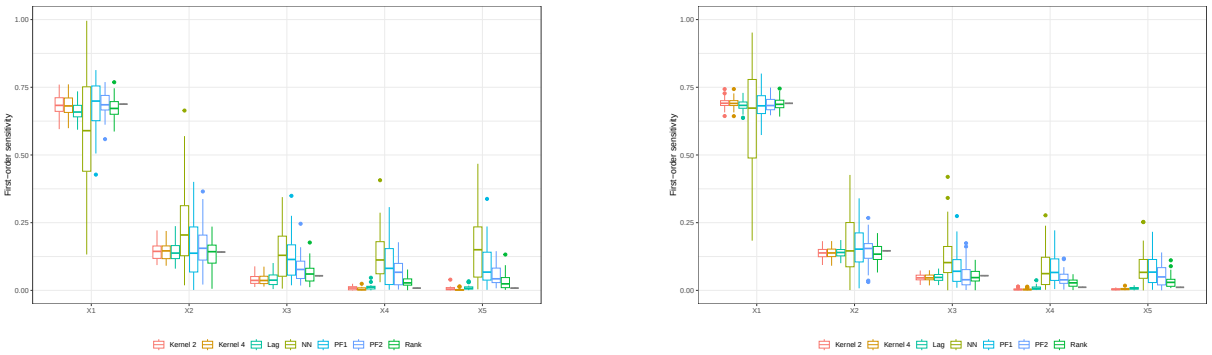
- We will focus on estimators for first-order and total-order Sobol' indices for each input variable V_i, corresponding to (1) with $X = V_i$ and $X = V_{-i}$ respectively.
- We compute our second mirror-type estimator (20) with an Epanechnikov kernel of order 2 and 4 (see [19] for a definition), with the kernel bandwidth being optimized via leave-one-out on the regression function ("Kernel 2" and "Kernel 4").
- We also consider concurrent estimators, namely the nearest-neighbor estimator of [11] ("NN") and the asymptotically efficient version of Pick-Freeze estimator studied in [22] ("PF1") for first-order indices and for total-order indices, and also the replicated version of Pick-Freeze estimator proposed in [40] ("PF2"), the rank estimator of [14] ("Rank"), and the lag estimator of [25] ("Lag") for first-order indices.
- For all estimators, we generate a standard n-sample $(X_1, Y_1), \cdots, (X_n, Y_n)$ except for the Pick-Freeze method since it relies on a structured design of experiments.
- Each experiment is repeated 50 times with a number of model evaluations fixed to $n = 500$ (then to $n = 1000$). The reference value is obtained from a Pick-Freeze estimation with very large sample size.

The Bratley function First, we consider the Bratley function defined by:

$$g_{\text{Bratley}}(V_1, \dots, V_p) = \sum_{i=1}^{p} (-1)^i \prod_{j=1}^{i} V_j, \tag{30}$$

with $V_i \sim \mathcal{U}([0,1])$ i.i.d. and $p = 5$. The results of the 50 experiments for all estimators of first-order indices are given as boxplots in Figure 3. We observe several trends.

- The nearest-neighbor estimator exhibits both large bias and large variance.
- The Pick-Freeze estimators and the rank one perform well except when the sensitivity index is small.
- Both the lag estimator and our mirror-type one have very small bias and variance.



(a) $n = 500$ (b) $n = 1000$

Figure 3: Estimators for first-order indices of the Bratley function with $n = 500$ (left) and $n = 1000$ (right). The reference value is represented with a gray line.

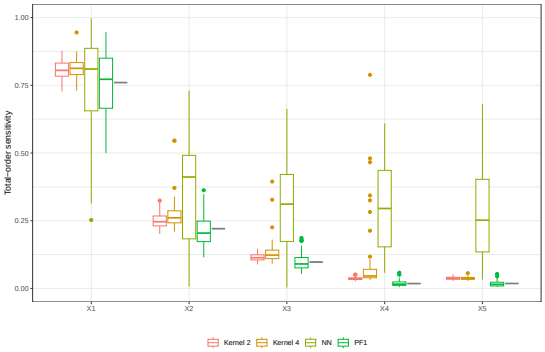
For total-order indices in Figure 4, recall that the only concurrent estimators are nearest-neighbor and Pick-Freeze estimators. Once again Pick-freeze estimators perform well, but the bias of the nearest-neighbor one is very large (here $d = p - 1 = 4$), this bias increasing dramatically when the sensitivity index is small. Our mirror-type estimator still has small bias and very small variance for all input variables.

The g-Sobol function Then, we investigate the g-Sobol function defined by

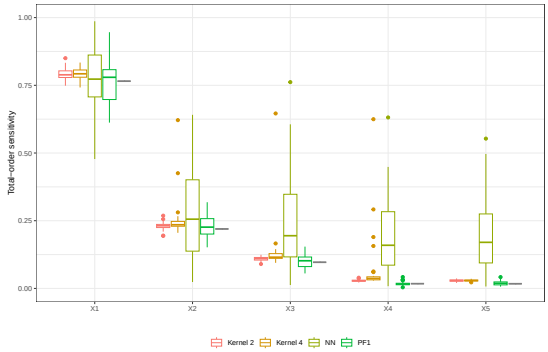
$$g_{\text{g-Sobol}}(V_1, \dots, V_p) = \prod_{i=1}^{p} \frac{|4V_i - 2| + a_i}{1 + a_i}, \tag{31}$$

with $V_i \sim \mathcal{U}([0,1])$ i.i.d., $p = 5$ and $a = (0, 1, 4.5, 9, 99)$. Notice that it is non-differentiable at any input value with a component equal to 0.5, but the impact on our estimator performance is negligible, as can be seen in Figure 5 for first-order indices. Except for the degraded performance of the lag estimator, the conclusions are the same as for the Bratley function, even for total indices displayed in Figure 6.

Finally, we illustrate numerically that the choice of the ϵ tuning parameter of the estimator proposed in [13] is very sensitive, thus limiting its practical use as opposed to our mirror-type estimator. We consider Example 3.2 from [13] and test $\epsilon = 10^{-1}, 10^{-2}, 10^{-3}$. The

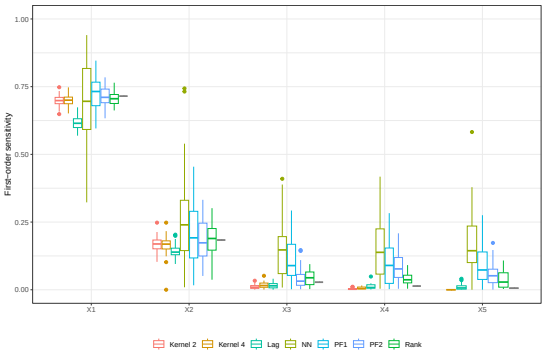


(a) $n = 500$

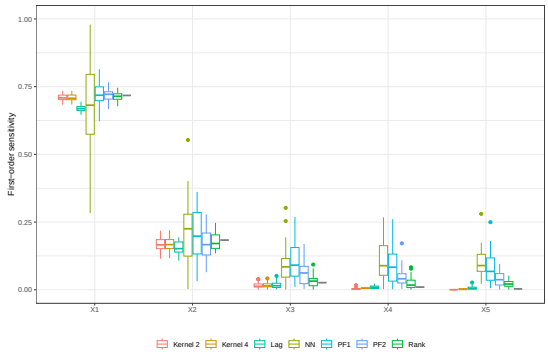


(b) $n = 1000$

Figure 4: Estimators for total-order indices of the Bratley function with $n = 500$ (left) and $n = 1000$ (right). The reference value is represented with a gray line.



(a) $n = 500$

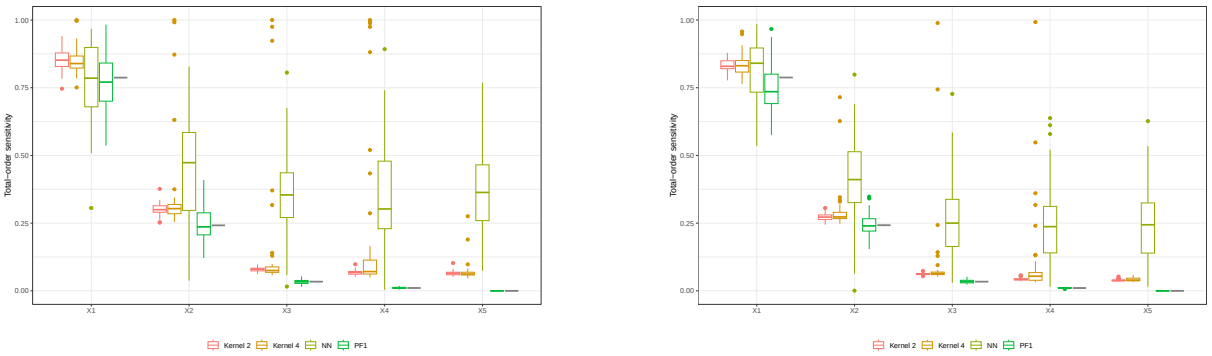


(b) $n = 1000$

Figure 5: Estimators for first-order indices of the g-Sobol function with $n = 500$ (left) and $n = 1000$ (right). The reference value is represented with a gray line.

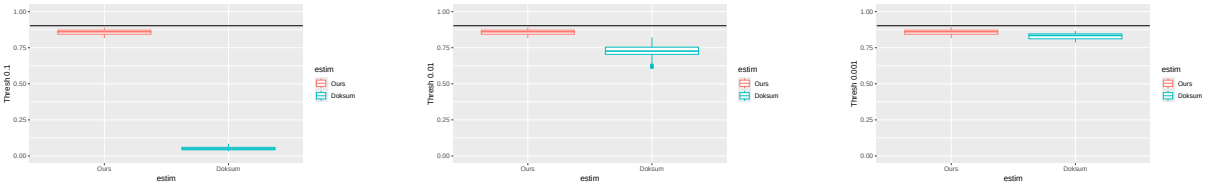
comparison with our estimator with a kernel of order 2 is given in Figure 7. When ϵ is equal to 10^{-3}, the performance of both estimators are similar. However in other cases, the bias of [13] can be very large. Since in practice such an estimation problem is unsupervised, the tuning of ϵ seems highly difficult and the non-robustness of the final estimator with respect to this parameter limits its practical use.

Additional material Extended numerical studies discussing numerical stability of high-order kernels can be found on the link `https://hal.science/hal-04052837`.



(a) $n = 500$ (b) $n = 1000$

Figure 6: Estimators for total-order indices of the g-Sobol function with $n = 500$ (left) and $n = 1000$ (right). The reference value is represented with a gray line.



(a) $\epsilon = 10^{-1}$ (b) $\epsilon = 10^{-2}$ (c) $\epsilon = 10^{-3}$

Figure 7: Comparison of our mirror-type estimator with the estimator of [13] for different values of ϵ. The reference value is represented with a gray line.

A Proof of the results

In the following, h_n is simply denoted by h and C is a deterministic and finite constant, the value of which is allowed to change between occurrences. Recall also that f_X is the density of X with respect to the Lebesgue measure. The regression function is denoted by m: $m(x) = \mathbb{E}[Y|X = x]$ and we introduce the function g defined by $g(x) = f_X(x)m(x)$. In addition, $\sigma^2(x)$ stands for $\mathrm{Var}(Y|X = x)$.

A.1 Proof of the preliminary results of Section 3.1

Now, recall that $\widehat{f}_{n,h,i}$ defined in (11) and $\widehat{m}_{n,h,i}$ defined in (7) are respectively the leave-one-out estimator of f_X based on $(X_1, \cdots, X_{i-1}, \cdots, X_{i+1}, \cdots, X_n)$ and the estimator of the regression function m based on the $(n-1)$-input/output sample $((X_1, Y_1), \cdots, (X_{i-1}, Y_{i-1}), \cdots, (X_{i+1}, Y_{i+1}), \cdots, (X_n, Y_n))$. Then, the leave-one-out estimator of g is naturally given by $\widehat{g}_{n,h,i} = \widehat{m}_{n,h,i}\widehat{f}_{n,h,i}$.

To lighten notation, we write m_i, σ_i^2, g_i, and f_i for $m(X_i)$, $\sigma^2(X_i)$, $g(X_i)$, and $f_X(X_i)$ respectively. Additionally, $\widehat{m}_i$, $\widehat{g}_i$, and $\widehat{f}_i$ denote $\widehat{m}_{n,h,i}(X_i)$, $\widehat{g}_{n,h,i}(X_i)$, and $\widehat{f}_{n,h,i}(X_i)$ respectively. By abuse of notation, we denote $\widehat{f}_{n,h,i}(x)$ and $\widehat{g}_{n,h,i}(x)$ by $\widehat{f}_i(x)$ and $\widehat{g}_i(x)$.

Proof of Lemma 3.1. The result can be deduced from the proof of the bound (8) in [2, Proposition 1] (see [2, Section 7.2.]) as the domain $[0,1]^d$ is compact. More precisely, one has

$$\mathbb{E}[\widehat{f}_{n,h,i}(x)] = \int_{[0,1]^d} K_h \circ A_x(x' - x) f_X(x') dx' = \int_{\mathcal{D}_x} K(u) f_X(x + hA_x^{-1}(u)) du$$

where the last display is obtained after the variable change $u = A_x(x' - x)/h$, using the fact that $|\det(A_x)| = 1$ and where $\mathcal{D}_x$ is the integration domain after the variable change. Now observe that the mirror property in (10) ensures that, if $0 < h \leqslant 1/2$ for all $i \in \{1, \cdots, d\}$, then $[0,1]^d \subset \mathcal{D}_x$ for all $x \in [0,1]^d$. Thus we have

$$\mathbb{E}[\widehat{f}_{n,h,i}(x)] - f_X(x) = \int_{[0,1]^d} K(u)(f_X(x + hA_x^{-1}(u)) - f_X(x)) du \tag{32}$$

since $\int_{[0,1]^d} K(u)du = 1$. If $\alpha \in (0,1)$, since $f_X \in \mathcal{C}^\alpha([0,1]^d)$, $\|K\|_\infty < \infty$ and $\|A_x^{-1}(u)\|_\infty \leqslant 1$, we conclude straightforwardly that

$$\left|\mathbb{E}[\widehat{f}_{n,h,i}(x)] - f_X(x)\right| \leqslant C_{f_X} h^\alpha \int_{[0,1]^d} \left\|A_x^{-1}(u)\right\|_\infty^\alpha |K(u)|\, du \leqslant Ch^\alpha.$$

Now, for $\alpha \geqslant 1$, observe that, still due to the mirror property in (10), $0 < h \leqslant 1/2$ for all $i \in \{1, \cdots, d\}$ ensures that $x + hA_x^{-1}(u) \in [0,1]^d$ for all $x \in [0,1]^d$ and for all $u \in [0,1]^d$. Thus the term in (32) can be handled with a Taylor expansion of f_X (see, e.g., [6, Theorem 5.4]). More precisely, by a multivariate Taylor expansion, since f_X is $\mathcal{C}^\alpha([0,1]^d)$, we get:

$$f_X(x + uh) - f_X(x) = \sum_{1 \leqslant |\beta| < \lfloor\alpha\rfloor} \frac{h^{|\beta|}}{\beta\,!} u^\beta \frac{\partial^\beta f_X}{\partial x^\beta}(x) + h^{\lfloor\alpha\rfloor} \sum_{|\beta| = \lfloor\alpha\rfloor} R_\beta(x + uh) u^\beta$$

with

$$R_\beta(x+uh) = \frac{\lfloor\alpha\rfloor}{\beta!}\int_0^1 (1-t)^{\lfloor\alpha\rfloor-1}\frac{\partial^\beta f_X}{\partial x^\beta}(x+tuh)\,dt.$$

Then, recalling that $(A_x^{-1}(u))^\beta = (A_x^{-1}(u)_1)^{\beta_1}\dots(A_x^{-1}(u)_d)^{\beta_d}$, we have

$$\begin{aligned}\mathbb{E}[\widehat{f}_{n,h,i}(x)] - f_X(x) &= \sum_{1\leqslant|\beta|<\lfloor\alpha\rfloor}\frac{h^{|\beta|}}{\beta\,!}\Big(\int_{[0,1]^d}(A_x^{-1}(u))^\beta K(u)du\Big)\frac{\partial^\beta f_X}{\partial x^\beta}(x)\\ &\qquad + h^{\lfloor\alpha\rfloor}\sum_{|\beta|=\lfloor\alpha\rfloor}\int_{[0,1]^d}(A_x^{-1}(u))^\beta K(u)R_\beta(x+hA_x^{-1}(u))du\\ &= \lfloor\alpha\rfloor h^{\lfloor\alpha\rfloor}\sum_{|\beta|=\lfloor\alpha\rfloor}\frac{1}{\beta!}\int_{[0,1]^d}(A_x^{-1}(u))^\beta K(u)\int_0^1(1-t)^{\lfloor\alpha\rfloor-1}\frac{\partial^\beta f_X}{\partial x^\beta}(x+thA_x^{-1}(u))\,dtdu\end{aligned}$$

using the fact that $(A_x^{-1}(u))^\beta$ is polynomial in $(u_1,\dots,u_d)$ of degree β and K is of order $(\lfloor\alpha\rfloor+1)$. Now, using again that K is of order $(\lfloor\alpha\rfloor+1)$, we get

$$\begin{aligned}\mathbb{E}[\widehat{f}_{n,h,i}(x)] - f_X(x) = \lfloor\alpha\rfloor h^{\lfloor\alpha\rfloor}\sum_{|\beta|=\lfloor\alpha\rfloor}\frac{1}{\beta!}\int_{[0,1]^d}(A_x^{-1}(u))^\beta K(u)\\ \int_0^1(1-t)^{\lfloor\alpha\rfloor-1}\Big(\frac{\partial^\beta f_X}{\partial x^\beta}(x+thA_x^{-1}(u)) - \frac{\partial^\beta f_X}{\partial x^\beta}(x)\Big)\,dtdu.\end{aligned}$$

Then, using (4) since $f_X\in\mathcal{C}^\alpha([0,1]^d)$, one gets

$$\Big|\frac{\partial^\beta f_X}{\partial x^\beta}(x+thA_x^{-1}(u)) - \frac{\partial^\beta f_X}{\partial x^\beta}(x)\Big| \leqslant C_{f_X}(ht\|A_x^{-1}(u)\|_\infty)^{\alpha-\lfloor\alpha\rfloor}$$

for all $u\in[0,1]^d$, $x\in[0,1]^d$, $t\in[0,1]$, $h\in(0,\infty)$, and $\beta\in\mathbb{N}^d$ such that $|\beta|=\lfloor\alpha\rfloor$. Then,

$$\begin{aligned}&|\mathbb{E}[\widehat{f}_{n,h,i}(x)] - f_X(x)|\\ &\leqslant C_{f_X}\lfloor\alpha\rfloor h^\alpha\Big(\sum_{|\beta|=\lfloor\alpha\rfloor}\frac{1}{\beta!}\Big)\Big(\int_{[0,1]^d}\|A_x^{-1}(u)\|_\infty^\beta\|A_x^{-1}(u)\|_\infty^{\alpha-\lfloor\alpha\rfloor}|K(u)|du\Big)\Big(\int_0^1(1-t)^{\lfloor\alpha\rfloor-1}t^{\alpha-\lfloor\alpha\rfloor}dt\Big)\\ &= Ch^\alpha\Big(\sum_{|\beta|=\lfloor\alpha\rfloor}\frac{1}{\beta!}\Big)\Big(\int_{[0,1]^d}|K(u)|du\Big)\Big(\int_0^1(1-t)^{\lfloor\alpha\rfloor-1}t^{\alpha-\lfloor\alpha\rfloor}dt\Big)\leqslant Ch^\alpha\end{aligned}$$

since $\|A_x^{-1}(u)\|_\infty^\beta\leqslant 1$ and $\|K\|_\infty<\infty$. □

Proof of Lemma 3.2. For $u\subset\{1,\dots,d\}$, let $\sim u = \{1,\dots,d\}\setminus u$. For $x\in[0,1]^d$,

$$\begin{aligned}(n-1)\widehat{f}_{n,h,i}(x) &= \sum_{j\neq i}\prod_{\substack{1\leqslant k\leqslant d\text{ s.t.}\\ x_k\in[0,1/2]}}k_h(X_{k,j}-x_k)\prod_{\substack{1\leqslant k\leqslant d\text{ s.t.}\\ x_k\in(1/2,1]}}k_h(x_k-X_{k,j})\\ &= \sum_{j\neq i}\sum_{u\subseteq\{1,\dots,d\}}\prod_{k\in u}\mathbb{1}_{[0,1/2]}(x_k)k_h(X_{k,j}-x_k)\prod_{k\in\sim u}\mathbb{1}_{(1/2,1]}(x_k)k_h(x_k-X_{k,j})\\ &=: \sum_{j\neq i}K_{h,x}^*(X_j).\end{aligned}$$

Arguing as in [33, Section 5.1.2] and since the class of functions $\mathcal{F}$ defined by (13) is a uniformly bounded VC-class of functions by $(\mathcal{A}\mathbf{8})$, we can say that the class

$$\mathcal{F}^* = \{K^*_{h,x},\ h > 0, x \in [0,1]^d\}$$

is also a uniformly bounded VC-class of functions. Thus it follows from a particular case of [23, Corollary 13] that the bound in (14) holds with probability $1 - \delta_n$. □

Proof of Corollary 3.4. First, by Lemmas 3.1 and 3.2, we get

$$\begin{aligned}\left\|\widehat{f}_{n,h,i} - f_X\right\|^2_\infty &\leqslant 2\left\|\widehat{f}_{n,h,i} - \mathbb{E}\left[\widehat{f}_{n,h,i}\right]\right\|^2_\infty + 2\left\|\mathbb{E}\left[\widehat{f}_{n,h,i}\right] - f_X\right\|^2_\infty \\ &= O_{\mathbb{P}}\Big(h^{2\alpha} + \frac{\left(\log(\frac{1}{h_n})\right)_+ + \log(\frac{2}{\delta_n})}{nh_n^d}\Big) = o_{\mathbb{P}}(n^{-1/2})\end{aligned}$$

as soon as $nh^{2d} \to \infty$ and $nh^{4\alpha} \to 0$ by considering, e.g., $\delta_n = 1/n$. Since the input space $[0,1]^d$ is compact by Assumption $(\mathcal{A}\mathbf{1})$, one concludes that (15) holds.
Moreover, for all $i \in \{1, \cdots, d\}$, as $\widehat{f}_{n,h,i}(x) = f_X(x) + \widehat{f}_{n,h,i}(x) - f_X(x)$, and from Assumption $(\mathcal{A}\mathbf{2})$, we get with probability $1 - 1/\delta_n$ and for n large enough:

$$\inf_{x\in[0,1]^d}\left|\widehat{f}_{n,h,i}(x)\right| \geqslant \delta - C\left(h^{2\alpha} + \frac{\left(\log(\frac{1}{h_n})\right)_+ + \log(\frac{2}{\delta_n})}{nh_n^d}\right)$$

for some positive constant C. This last quantity is nonnegative as soon as n is large enough when $nh^d \to \infty$ and $h^\alpha \to 0$ by considering, e.g., $\delta_n = 1/n$. □

We also state Lemma A.1 below as a preliminary result for the proof of Theorem 4.1.

Lemma A.1. *Under Assumptions* $(\mathcal{A}\mathbf{1})$, $(\mathcal{A}\mathbf{5})$, $(\mathcal{A}\mathbf{6})$, *and* $(\mathcal{A}\mathbf{8})$, *one has, for all* $i \in \{1, \cdots, d\}$,

$$\mathbb{E}\Big[\int_{[0,1]^d}(\widehat{g}_{n,h,i}(x) - g(x))^2 dx\Big] = o(n^{-1/2}) \tag{33}$$

as soon as $nh^{2d} \to \infty$, *and* $nh^{4\alpha} \to 0$.

Proof of Lemma A.1. Similarly as for density estimation, we prove that

$$\left\|\mathbb{E}\left[\widehat{g}_{n,h,1}\right] - g\right\|_\infty = O(h^\alpha) \tag{34}$$

and that there exists some constant $C > 0$ such that, with probability $1 - \delta_n$,

$$\left\|\widehat{g}_{n,h,1} - \mathbb{E}\left[\widehat{g}_{n,h,1}\right]\right\|_\infty \leqslant C\left(\frac{\log(\frac{1}{h}) + \log(\frac{2}{\delta_n})}{nh^d}\right). \tag{35}$$

Then, we deduce (33) as soon as $nh^d \to \infty$ and $h^\alpha \to 0$ by considering, e.g., $\delta_n = 1/n$. Now, to prove (34), observe that

$$\mathbb{E}[\widehat{g}_{n,h,1}(x)] = \int_{[0,1]^d} K_h \circ A_x(x' - x)g(x')dx'.$$

Then, (34) comes following the same lines as in the proof of (21) since $g \in \mathcal{C}^\alpha([0,1]^d)$.

As for the proof of (35), one has, for all $i \in \{1, \cdots, d\}$,

$$(n-1)\widehat{g}_{n,h,i}(x) = \sum_{j \neq i} Y_j \prod_{\substack{1 \leqslant k \leqslant d \text{ s.t.} \\ x_k \in [0,1/2]}} k_h(X_{k,j} - x_k) \prod_{\substack{1 \leqslant k \leqslant d \text{ s.t.} \\ x_k \in (1/2,1]}} k_h(x_k - X_{k,j})$$

$$= \sum_{j \neq i} Y_j \sum_{u \subseteq \{1,\ldots,d\}} \prod_{k \in u} \mathbb{1}_{[0,1/2]}(x_k) k_h(X_{k,j} - x_k) \prod_{k \in \sim u} \mathbb{1}_{(1/2,1]}(x_k) k_h(x_k - X_{k,j})$$

$$= O\Big(\sum_{j \neq i} K^*_{h,x}(X_j)\Big).$$

We conclude as in the proof of Lemma 3.2. □

A.2 Proof of the preliminary results of Section 3.2

Now, recall that $\widetilde{f}_{n,h,i}$ defined in (17) and $\widetilde{g}_{n,h,i}$ defined in 18 are the leave-one-out estimators of f_X and g respectively based on the $(n-1)$-input/output sample $((X_1, Y_1), \cdots, (X_{i-1}, Y_{i-1}), \cdots, (X_{i+1}, Y_{i+1}), \cdots, (X_n, Y_n))$. Then, the estimator of the regression function m is naturally given by $\widetilde{m}_{n,h,i} = \widetilde{g}_{n,h,i}/\widetilde{f}_{n,h,i}$.

Proof of Lemma 3.5. It follows the same lines as in the proof of Lemma 3.1. We consider the case $x \in [0, 1/2]^d$. The remaining cases can be deduced by symmetry. Let $\mathcal{A} := \{k \in \{1, \ldots, d\} : x_k \leqslant h\}$. For all $k \in \{1, \cdots, d\}$ and all $t_k \in [0, 1]$,

$$\widetilde{k}_h(M^1(t_k) - x_k) = \widetilde{k}_h(2 - t_k - x_k) = 0$$

as $\widetilde{k}$ is supported on $[-1, 1]$ and $h < 1/2$. In addition, for all $k \in \{1, \cdots, d\} \setminus \mathcal{A}$ and all $t_k \in [0, 1]$,

$$\widetilde{k}_h(M^{-1}(t_k) - x_k) = \widetilde{k}_h(-t_k - x_k) = 0.$$

For any subset $\mathcal{B} \subset \mathcal{A}$, define $x_{\mathcal{B}}$ such that $x_{\mathcal{B},k} = x_k = M^0(x_k)$ if $k \notin \mathcal{B}$ and $x_{\mathcal{B},k} = -x_k = M^{-1}(x_k)$ if $k \in \mathcal{B}$. Then, the expected value of $\widetilde{f}_{n,h,i}(x)$ can be written as:

$$\begin{aligned}\mathbb{E}[\widetilde{f}_{n,h,i}(x)] &= \sum_{\mathcal{B} \subset \mathcal{A}} \int_{[0,1]^d} \prod_{k \in \mathcal{B}} \widetilde{k}_h(-z_k - x_k) \prod_{k \notin \mathcal{B}} \widetilde{k}_h(z_k - x_k) f_X(z) dz \\ &= \sum_{\mathcal{B} \subset \mathcal{A}} \int_{\mathcal{X}_{\mathcal{B}}} \prod_{k=1}^{d} \widetilde{k}(u_k) f_X(z_{\mathcal{B}}) du = \sum_{\mathcal{B} \subset \mathcal{A}} \int_{\mathcal{X}_{\mathcal{B}}} \widetilde{K}(u) f_X(z_{\mathcal{B}}) du\end{aligned}$$

with

$$z_{\mathcal{B},k} = \begin{cases} -x_k - u_k h, & k \in \mathcal{B} \\ x_k + u_k h, & k \notin \mathcal{B} \end{cases} \text{ and } \mathcal{X}_{\mathcal{B},k} = \begin{cases} \{u_k \in [-1, 1) : -x_k - u_k h \in [0, 1]\}, & k \in \mathcal{B} \\ \{u_k \in [-1, 1) : x_k + u_k h \in [0, 1]\}, & k \notin \mathcal{B} \end{cases}$$

(recalling that the support of $\widetilde{K}$ is $[-1, 1]^d$) and $\mathcal{X}_{\mathcal{B}} = \prod_{k=1}^{d} \mathcal{X}_{\mathcal{B},k}$. Note that $(\mathcal{X}_{\mathcal{B}})_{\mathcal{B} \subset \mathcal{A}}$ forms a partition of $[-1, 1)^d$. Indeed, one has

$$\mathcal{X}_{\mathcal{B}} = \prod_{k=1}^{d} \mathcal{X}_{\mathcal{B},k} = \prod_{k \in \mathcal{B}} [-1, -\frac{x_k}{h}) \prod_{k \in \mathcal{A} \setminus \mathcal{B}} [-\frac{x_k}{h}, 1) \prod_{k \in \{1, \cdots, d\} \setminus \mathcal{A}} [-1, 1).$$

Let us now define f_X^{MI} on $[-1,2]^d$ such that, for all $y \in [-1,2]^d$,

$$f_X^{\mathrm{MI}}(y) = f_X(y^{\mathrm{MI}}) \quad \text{where} \quad y_k^{\mathrm{MI}} = \begin{cases} -y_k & \text{if } y_k \in [-1,0] \\ y_k & \text{if } y_k \in [0,1] \\ 2-y_k & \text{if } y_k \in [1,2] \end{cases}.$$

Then, for all $x \in [0,1]^d$ and $a \in \{-1,0,1\}^d$, $f_X^{\mathrm{MI}}(M^a(x)) = f_X(x)$ and similarly, for any $\mathcal{B} \subset \mathcal{A}$, $f_X^{\mathrm{MI}}(x_{\mathcal{B}}) = f_X(x)$. Now, since $f_X^{\mathrm{MI}} = f_X$ on $[0,1]^d$ and for any $u \in \mathcal{X}_{\mathcal{B}}$, $f_X^{\mathrm{MI}}(z_{\mathcal{B}}) = f_X(z_{\mathcal{B}})$, we have

$$\mathbb{E}[\widetilde{f}_{n,h,i}(x)] = \sum_{\mathcal{B}\subset\mathcal{A}} \int_{\mathcal{X}_{\mathcal{B}}} \widetilde{K}(u) f_X^{\mathrm{MI}}(z_{\mathcal{B}}) du = \sum_{\mathcal{B}\subset\mathcal{A}} \int_{\mathcal{X}'_{\mathcal{B}}} \widetilde{K}(v) f_X^{\mathrm{MI}}(z_{\mathcal{B}}) dv \tag{36}$$

using the variable change $v = u_{\mathcal{B}}$, the symmetry of $\widetilde{K}$ and with

$$\mathcal{X}'_{\mathcal{B},k} = \begin{cases} \{v_k \in [-1,1) \,:\, -x_k + v_k h \in [0,1]\}, & k \in \mathcal{B} \\ \{v_k \in [-1,1) \,:\, x_k + v_k h \in [0,1]\}, & k \notin \mathcal{B} \end{cases}.$$

In addition, since $\int_{[-1,1]^d} \widetilde{K}(u)du = 1$, $(\mathcal{X}'_{\mathcal{B}})_{\mathcal{B}\subset\mathcal{A}}$ forms also a partition of $[-1,1)^d$, and $f_X^{\mathrm{MI}}(x_{\mathcal{B}}) = f_X(x)$, one has

$$f_X(x) = f_X(x) \int_{[-1,1]^d} \widetilde{K}(u)du = \sum_{\mathcal{B}\subset\mathcal{A}} \int_{\mathcal{X}'_{\mathcal{B}}} \widetilde{K}(u) f_X(x) du = \sum_{\mathcal{B}\subset\mathcal{A}} \int_{\mathcal{X}'_{\mathcal{B}}} \widetilde{K}(u) f_X^{\mathrm{MI}}(x_{\mathcal{B}}) du\,. \tag{37}$$

From (36) and (37), we deduce

$$\mathbb{E}[\widetilde{f}_{n,h,i}(x)] - f_X(x) = \sum_{\mathcal{B}\subset\mathcal{A}} \int_{\mathcal{X}'_{\mathcal{B}}} \widetilde{K}(u) \Big(f_X^{\mathrm{MI}}(x_{\mathcal{B}} + vh) - f_X^{\mathrm{MI}}(x_{\mathcal{B}}) \Big) dv.$$

By construction and since Assumption $(\mathcal{A}'\mathbf{4})$ is satisfied (in particular derivatives up to order $\lfloor\alpha\rfloor$ vanish near the boundary), f_X^{MI} has derivatives up to order $\lfloor\alpha\rfloor$. Then, f_X^{MI} belongs to $\mathcal{C}^\alpha([-1,2]^d)$ with $C_{f_X^{\mathrm{MI}}} = 3C_{f_X}$. Thus, proceeding as in the proof of Lemma 3.1 we write:

$$f_X^{\mathrm{MI}}(x_{\mathcal{B}} + uh) - f_X^{\mathrm{MI}}(x_{\mathcal{B}}) = \sum_{1\leqslant|\beta|<\lfloor\alpha\rfloor} \frac{h^{|\beta|}}{\beta\,!} u^\beta \frac{\partial^\beta f_X^{\mathrm{MI}}}{\partial x^\beta}(x_{\mathcal{B}}) + h^{\lfloor\alpha\rfloor} \sum_{|\beta|=\lfloor\alpha\rfloor} R_\beta(x_{\mathcal{B}} + uh) u^\beta \tag{38}$$

with

$$R_\beta(x_{\mathcal{B}} + uh) = \frac{\lfloor\alpha\rfloor}{\beta!} \int_0^1 (1-t)^{\lfloor\alpha\rfloor - 1} \frac{\partial^\beta f_X^{\mathrm{MI}}}{\partial x^\beta}(x_{\mathcal{B}} + tuh)\, dt. \tag{39}$$

Then, with similar arguments as in the proof of Lemma 3.1, together with Assumptions $(\mathcal{A}'\mathbf{4})$ and $(\mathcal{A}'\mathbf{5})$ and the fact that $(\mathcal{X}'_{\mathcal{B}})_{\mathcal{B}\subset\mathcal{A}}$ forms a partition of $[-1,1)^d$, we get

$$\begin{aligned}
&|\mathbb{E}[\widetilde{f}_{n,h,i}(x)] - f_X(x)| \\
&\quad\leqslant 3C_{f_X}\lfloor\alpha\rfloor h^\alpha \Big(\sum_{|\beta|=\lfloor\alpha\rfloor} \frac{1}{\beta!} \Big) \Big(\int_0^1 (1-t)^{\lfloor\alpha\rfloor-1} t^{\alpha-\lfloor\alpha\rfloor} dt \Big) \Big(\sum_{\mathcal{B}\subset\mathcal{A}} \int_{\mathcal{X}'_{\mathcal{B}}} |u|^\alpha |\widetilde{K}(u)| du \Big) \\
&\quad\leqslant 3C_{f_X}\lfloor\alpha\rfloor h^\alpha \Big(\sum_{|\beta|=\lfloor\alpha\rfloor} \frac{1}{\beta!} \Big) \Big(\int_0^1 (1-t)^{\lfloor\alpha\rfloor-1} t^{\alpha-\lfloor\alpha\rfloor} dt \Big) \Big(\int_{[-1,1]^d} |\widetilde{K}(u)| du \Big) = Ch^\alpha. \quad \square
\end{aligned}$$

We also state Lemma A.2 below as a preliminary result to the proof of Theorem 4.2.

Lemma A.2. *Let $\alpha > 0$. Under Assumptions* $(\mathcal{A}\mathbf{1})$, $(\mathcal{A}\mathbf{5})$, $(\mathcal{A}'\mathbf{5})$, *and* $(\mathcal{A}\mathbf{8})$, *one has, for all $i \in \{1, \cdots, d\}$,*

$$\mathbb{E}\Big[\int (\widetilde{g}_{n,h,i}(x) - g(x))^2 dx\Big] = o(n^{-1/2}) \tag{40}$$

as soon as $nh^{2d} \to \infty$, and $nh^{4\alpha} \to 0$.

Proof of Lemma A.2. The proof follows similar lines as the one of Lemma A.1. Recall that for $x \in [0,1]^d$, $g(x) = f_X(x)m(x)$. We extend m as m^{MI} on $[-1,2]^d$ as follows. For all $y \in [-1,2]^d$, $m^{\mathrm{MI}}(y) = m(y^{\mathrm{MI}})$ with y^{MI} defined in the proof of Lemma 3.5. Then, for all $x \in [0,1]^d$ and $a \in \{-1,0,1\}^d$, $m^{\mathrm{MI}}(M^a(x)) = m(x)$ and similarly, for any $\mathcal{B} \subset \mathcal{A}$, $m^{\mathrm{MI}}(x_{\mathcal{B}}) = m(x)$. We introduce the function $g^{\mathrm{MI}}(x) = f_X^{\mathrm{MI}}(x)m^{\mathrm{MI}}(x)$. We also introduce the intermediate function $\widetilde{g}^{\mathrm{MI}}(x) = f_X^{\mathrm{MI}}(x)m(x)$. Now following the proof of Lemma A.1, we get, for all $x \in [0,1]^d$,

$$\mathbb{E}[\widetilde{g}_{n,h,i}(x)] - g(x) = \sum_{\mathcal{B}\subset\mathcal{A}} \int_{\mathcal{X}'_{\mathcal{B}}} \widetilde{K}(u)\Big(g^{\mathrm{MI}}(x_{\mathcal{B}} + uh) - g^{\mathrm{MI}}(x_{\mathcal{B}})\Big)du\,.$$

Now,

$$\begin{aligned} g^{\mathrm{MI}}(x_{\mathcal{B}} + uh) - g^{\mathrm{MI}}(x_{\mathcal{B}}) &= g^{\mathrm{MI}}(x_{\mathcal{B}} + uh) - \widetilde{g}^{\mathrm{MI}}(x_{\mathcal{B}} + uh) + \widetilde{g}^{\mathrm{MI}}(x_{\mathcal{B}} + uh) - \widetilde{g}^{\mathrm{MI}}(x_{\mathcal{B}}) \\ &\quad + \widetilde{g}^{\mathrm{MI}}(x_{\mathcal{B}} + uh) - \widetilde{g}^{\mathrm{MI}}(x_{\mathcal{B}}) + \widetilde{g}^{\mathrm{MI}}(x_{\mathcal{B}}) - g^{\mathrm{MI}}(x_{\mathcal{B}}) \\ &= f_X^{\mathrm{MI}}(x_{\mathcal{B}} + uh)\Big(m^{\mathrm{MI}}(x_{\mathcal{B}} + uh) - m(x_{\mathcal{B}} + uh)\Big) \\ &\quad + \widetilde{g}^{\mathrm{MI}}(x_{\mathcal{B}} + uh) - \widetilde{g}^{\mathrm{MI}}(x_{\mathcal{B}}) + f_X^{\mathrm{MI}}(x_{\mathcal{B}})\Big(m(x_{\mathcal{B}}) - m^{\mathrm{MI}}(x_{\mathcal{B}})\Big)\,. \end{aligned}$$

Now by definition, we have $m^{\mathrm{MI}}(x_{\mathcal{B}} + uh) = m(x_{\mathcal{B}} + uh)$ and $m^{\mathrm{MI}}(x_{\mathcal{B}}) = m(x_{\mathcal{B}})$. Thus we have $g^{\mathrm{MI}}(x_{\mathcal{B}}+uh) - g^{\mathrm{MI}}(x_{\mathcal{B}}) = \widetilde{g}^{\mathrm{MI}}(x_{\mathcal{B}}+uh) - \widetilde{g}^{\mathrm{MI}}(x_{\mathcal{B}})$. As f_X^{MI} and m belong to $\mathcal{C}^\alpha([-1,2]^d)$ from Assumptions $(\mathcal{A}'\mathbf{4})$ and $(\mathcal{A}\mathbf{5})$, the function $\widetilde{g}^{\mathrm{MI}}$ also belongs to $\mathcal{C}^\alpha([-1,2]^d)$. Then, mimicking (38) and (39), we obtain for any $y \in \mathcal{Y}$,

$$\widetilde{g}^{\mathrm{MI}}(x_{\mathcal{B}} + uh) - \widetilde{g}^{\mathrm{MI}}(x_{\mathcal{B}}) = \sum_{1 \leqslant |\beta| < \lfloor\alpha\rfloor} \frac{h^{|\beta|}}{\beta\,!} u^\beta \frac{\partial^\beta \widetilde{g}^{\mathrm{MI}}}{\partial x^\beta}(x_{\mathcal{B}}) + h^{\lfloor\alpha\rfloor} \sum_{|\beta| = \lfloor\alpha\rfloor} R_\beta(x_{\mathcal{B}} + uh) u^\beta$$

with

$$R_\beta(x_{\mathcal{B}} + uh) = \frac{\lfloor\alpha\rfloor}{\beta!} \int_0^1 (1-t)^{\lfloor\alpha\rfloor - 1} \frac{\partial^\beta \widetilde{g}^{\mathrm{MI}}}{\partial x^\beta}(x_{\mathcal{B}} + tuh)\, dt.$$

Then, we conclude with similar arguments as in the proof of Lemma 3.1. From Assumption $(\mathcal{A}'\mathbf{5})$ and as $(\mathcal{X}'_{\mathcal{B}})_{\mathcal{B}\subset\mathcal{A}}$ forms a partition of $[-1,1)^d$, we have

$$\sum_{\mathcal{B}\subset\mathcal{A}} \int_{\mathcal{X}'_{\mathcal{B}}} \widetilde{K}(u) \sum_{|\beta| = \lfloor\alpha\rfloor} u^\beta du = \int_{-1}^1 \Big(\sum_{|\beta| = \lfloor\alpha\rfloor} u^\beta\Big)\widetilde{K}(u)du = 0\,.$$

Thus

$$\begin{aligned}\mathbb{E}[\widetilde{g}_{n,h,i}(x)] - g(x) &= \sum_{\mathcal{B}\subset\mathcal{A}} \int_{\mathcal{X}'_{\mathcal{B}}} \widetilde{K}(u)\Big(g^{\mathrm{MI}}(x_{\mathcal{B}}+uh) - g^{\mathrm{MI}}(x_{\mathcal{B}})\Big)du \\ &= \sum_{\mathcal{B}\subset\mathcal{A}} \int_{\mathcal{X}'_{\mathcal{B}}} \widetilde{K}(u) h^{\lfloor\alpha\rfloor} \sum_{|\beta|=\lfloor\alpha\rfloor} R_\beta(x_{\mathcal{B}}+uh)u^\beta du \\ &= \sum_{\mathcal{B}\subset\mathcal{A}} \int_{\mathcal{X}'_{\mathcal{B}}} \widetilde{K}(u) h^{\lfloor\alpha\rfloor} \sum_{|\beta|=\lfloor\alpha\rfloor} \tfrac{\lfloor\alpha\rfloor}{\beta!} \\ &\qquad \int_0^1 (1-t)^{\lfloor\alpha\rfloor-1}\Big(\tfrac{\partial^\beta \widetilde{g}^{\mathrm{MI}}}{\partial x^\beta}(x_{\mathcal{B}}+tuh) - \tfrac{\partial^\beta \widetilde{g}^{\mathrm{MI}}}{\partial x^\beta}(x_{\mathcal{B}})\Big)dtu^\beta du\,.\end{aligned}$$

Now, using (4) since $\widetilde{g}^{\mathrm{MI}} \in \mathcal{C}^\alpha([0,1]^d)$, we have

$$\left|\frac{\partial^\beta \widetilde{g}^{\mathrm{MI}}}{\partial x^\beta}(x_{\mathcal{B}}+tuh) - \frac{\partial^\beta \widetilde{g}^{\mathrm{MI}}}{\partial x^\beta}(x_{\mathcal{B}})\right| \leqslant C(ht\|u\|_\infty)^{\alpha-\lfloor\alpha\rfloor} \leqslant Ch^{\alpha-\lfloor\alpha\rfloor}$$

for all $u \in [0,1]^d$, $x \in [0,1]^d$, $t \in [0,1]$, $h \in (0,\infty)$, and $\beta \in \mathbb{N}^d$ such that $|\beta| = \lfloor\alpha\rfloor$. We hence conclude that $\mathbb{E}[\widetilde{g}_{n,h,i}(x)] - g(x) \leqslant Ch^\alpha$. □

A.3 Proof of Theorems 4.1 and 4.2

Proof of Theorem 4.1. Following the same lines as in the proof of Theorem 2.1 in [13], we aim at proving that

$$\widehat{T}_{n,h} - \mathbb{E}[\mathbb{E}[Y|X]^2] = \frac{1}{n}\sum_{i=1}^n (2Y_i - m_i)m_i - \mathbb{E}[\mathbb{E}[Y|X]^2] + o_{\mathbb{P}}(n^{-1/2}). \tag{41}$$

The conclusion of Theorem 4.1 will then follow directly applying the standard central limit theorem for the sum of i.i.d. random variables to the right-hand side of the previous display together with Slutsky's lemma.
To establish (41), we compute

$$\begin{aligned}\widehat{T}_{n,h} - \frac{1}{n}\sum_{i=1}^n (2Y_i - m_i)m_i &= \frac{1}{n}\sum_{i=1}^n \Big[(2Y_i - \widehat{m}_i)\widehat{m}_i - (2Y_i - m_i)m_i\Big] \\ &= \frac{1}{n}\sum_{i=1}^n \Big[2Y_i(\widehat{m}_i - m_i) + m_i^2 - \widehat{m}_i^2\Big] \\ &= \frac{1}{n}\sum_{i=1}^n \Big[2(Y_i - m_i)(\widehat{m}_i - m_i) - (\widehat{m}_i - m_i)^2\Big] \\ &=: I_1 - I_2.\end{aligned}$$

Study of I_1 Since

$$\widehat{m}_i - m_i = \frac{\widehat{g}_i - \widehat{f}_i m_i}{f_i} + \frac{(f_i - \widehat{f}_i)(\widehat{g}_i - \widehat{f}_i m_i)}{f_i \widehat{f}_i},$$

I_1 rewrites as the sum of two terms I_{11} and I_{12} with

$$\begin{aligned} I_{11} &= \frac{2}{n}\sum_{i=1}^{n}(Y_i - m_i)\frac{\widehat{g}_i - \widehat{f}_i m_i}{f_i} \\ &= \frac{2}{n(n-1)}\sum_{i=1}^{n}\sum_{\substack{j=1,\\ j\neq i}}^{n}(Y_i - m_i)(Y_j - m_i)\frac{K_h \circ A_{X_i}(X_j - X_i)}{f_i} \\ &= \frac{2}{n(n-1)}\sum_{i=1}^{n}\sum_{\substack{j=1,\\ j\neq i}}^{n}\varepsilon_i(\varepsilon_j + m_j - m_i)\frac{K_h \circ A_{X_i}(U_{ij})}{f_i} \end{aligned}$$

denoting the residual $Y_i - m_i$ by ε_i and the difference $X_j - X_i$ by U_{ij}. Conditioning by $X^{(n)} = (X_1, \cdots, X_n)$ and using independence, we deduce that

$$\begin{aligned} \mathbb{E}[I_{11}] &= 2\mathbb{E}\Big[\varepsilon_1(\varepsilon_2 + m_2 - m_1)\frac{K_h \circ A_{X_1}(U_{12})}{f_i}\Big] \\ &= 2\mathbb{E}\Big[\mathbb{E}[\varepsilon_1|X_1](\mathbb{E}[\varepsilon_2|X_2] + m_2 - m_1)\frac{K_h \circ A_{X_1}(U_{12})}{f_i}\Big] \end{aligned}$$

that cancels since $E[\varepsilon_1|X_1] = 0$ while $\mathbb{E}[I_{11}^2]$ equals

$$\frac{4}{n^2(n-1)^2}\sum_{i,k=1}^{n}\sum_{\substack{j,\ell=1,\\ j\neq i,\\ \ell\neq k}}^{n}\mathbb{E}\Big[\varepsilon_i\varepsilon_k(\varepsilon_j + m_j - m_i)(\varepsilon_\ell + m_\ell - m_k)\frac{K_h \circ A_{X_i}(U_{ij})}{f_i}\frac{K_h \circ A_{X_k}(U_{k\ell})}{f_k}\Big]$$

$$\begin{aligned} &= \frac{4}{n^2(n-1)^2}\sum_{i=1}^{n}\sum_{\substack{j=1,\\ j\neq i}}^{n}\mathbb{E}\Big[\varepsilon_i^2(\varepsilon_j + m_j - m_i)^2\frac{(K_h \circ A_{X_i}(U_{ij}))^2}{f_i^2}\Big] \\ &\quad + \frac{4}{n^2(n-1)^2}\sum_{i=1}^{n}\sum_{\substack{j=1,\\ j\neq i}}^{n}\mathbb{E}\Big[\varepsilon_i\varepsilon_j(\varepsilon_j + m_j - m_i)(\varepsilon_i + m_i - m_j)\frac{K_h \circ A_{X_i}(U_{ij})}{f_i}\frac{K_h \circ A_{X_j}(U_{ji})}{f_j}\Big]. \end{aligned}$$

Conditioning by $X^{(n)} = (X_1, \cdots, X_n)$ once again leads to

$$\begin{aligned} \mathbb{E}[\varepsilon_i^2(\varepsilon_j + m_j - m_i)^2|X^{(n)}] &= \mathbb{E}[\varepsilon_i^2\varepsilon_j^2|X^{(n)}] + 2\mathbb{E}[\varepsilon_i^2\varepsilon_j(m_j - m_i)|X^{(n)}] + \mathbb{E}[\varepsilon_i^2(m_j - m_i)^2|X^{(n)}] \\ &= \mathbb{E}[\varepsilon_i^2|X_i]\mathbb{E}[\varepsilon_j^2|X_j] + 2(m_j - m_i)\mathbb{E}[\varepsilon_i^2|X_i]\mathbb{E}[\varepsilon_j|X_j] + (m_j - m_i)^2\mathbb{E}[\varepsilon_i^2|X_i] \\ &= \sigma_i^2\sigma_j^2 + (m_j - m_i)^2\sigma_i^2 \end{aligned}$$

and

$$\begin{aligned} &\mathbb{E}[\varepsilon_i\varepsilon_j(\varepsilon_j + m_j - m_i)(\varepsilon_i + m_i - m_j)|X^{(n)}] \\ &= \mathbb{E}[\varepsilon_i^2\varepsilon_j^2|X^{(n)}] + (m_j - m_i)\mathbb{E}[\varepsilon_i^2\varepsilon_j|X^{(n)}] + (m_i - m_j)\mathbb{E}[\varepsilon_j^2\varepsilon_i|X^{(n)}] - (m_j - m_i)^2\mathbb{E}[\varepsilon_i\varepsilon_j|X^{(n)}] \\ &= \sigma_i^2\sigma_j^2. \end{aligned}$$

Hence

$$\begin{aligned} \mathbb{E}[I_{11}^2] &= \frac{4}{n^2(n-1)^2}\sum_{i=1}^{n}\sum_{\substack{j=1,\\ j\neq i}}^{n}\mathbb{E}\Big[(\sigma_i^2\sigma_j^2 + (m_j - m_i)^2\sigma_i^2)\frac{(K_h \circ A_{X_i}(U_{ij}))^2}{f_i^2}\Big] \\ &\quad + \frac{4}{n^2(n-1)^2}\sum_{i=1}^{n}\sum_{\substack{j=1,\\ j\neq i}}^{n}\mathbb{E}\Big[\sigma_i^2\sigma_j^2\frac{K_h \circ A_{X_i}(U_{ij})}{f_i}\frac{K_h \circ A_{X_j}(U_{ji})}{f_j}\Big]. \end{aligned}$$

By Assumptions $(\mathcal{A}\mathbf{2})$, $(\mathcal{A}\mathbf{3})$, $(\mathcal{A}\mathbf{6})$, and the fact that m is bounded from above, we conclude that

$$\mathbb{E}[I_{11}^2] = O\Big(\frac{1}{n^2h^{2d}}\Big) = o\Big(\frac{1}{n}\Big)$$

since $nh^{2d} \to \infty$ by assumption.
Let us turn to the computation of I_{12} defined as follows

$$I_{12} = \frac{2}{n}\sum_{i=1}^{n}(Y_i - m_i)\frac{(f_i - \widehat{f}_i)(\widehat{g}_i - \widehat{f}_i m_i)}{f_i\widehat{f}_i}.$$

By (16) and since $\widehat{g}_1$ does not depend on Y_1,

$$\begin{aligned}
|\mathbb{E}[I_{12}]| &\leqslant \frac{C}{n}\sum_{i=1}^{n}\mathbb{E}_{\substack{X_1,\cdots,X_n\\Y_1,\cdots,Y_n}}\Big[|\varepsilon_i|\frac{|f_i - \widehat{f}_i|(|g_i - \widehat{g}_i| + |f_i - \widehat{f}_i||m_i|)}{f_i}\Big]\\
&= C\ \mathbb{E}_{\substack{X_1,\cdots,X_n\\Y_1,\cdots,Y_n}}\Big[|\varepsilon_1|\frac{|f_1 - \widehat{f}_1|(|g_1 - \widehat{g}_1| + |f_1 - \widehat{f}_1||m_1|)}{f_1}\Big]\\
&= C\ \mathbb{E}_{X_1,\cdots,X_n}\Big[\frac{|f_1 - \widehat{f}_1|}{f_1}\mathbb{E}_{Y_1,\cdots,Y_n}[|\varepsilon_1|(|g_1 - \widehat{g}_1| + |f_1 - \widehat{f}_1||m_1|)|X^{(n)}]\Big]\\
&= C\ \mathbb{E}_{X_1,\cdots,X_n}\Big[\frac{|f_1 - \widehat{f}_1|}{f_1}\mathbb{E}_{Y_1}[|\varepsilon_1||X_1](\mathbb{E}_{Y_2,\cdots,Y_n}[|g_1 - \widehat{g}_1||X^{(n)}] + |f_1 - \widehat{f}_1||m_1|)\Big]\\
&\leqslant C\ \mathbb{E}_{X_1,\cdots,X_n}\Big[\frac{|f_1 - \widehat{f}_1|}{f_1}\sigma_1(\mathbb{E}_{Y_2,\cdots,Y_n}[|g_1 - \widehat{g}_1||X^{(n)}] + |f_1 - \widehat{f}_1||m_1|)\Big]\\
&= C\ \mathbb{E}_{\substack{X_1,\cdots,X_n\\Y_2,\cdots,Y_n}}\Big[\frac{|f_1 - \widehat{f}_1|}{f_1}\sigma_1(|g_1 - \widehat{g}_1| + |f_1 - \widehat{f}_1||m_1|)\Big]\\
&= C\ \mathbb{E}_{\substack{X_2,\cdots,X_n\\Y_2,\cdots,Y_n}}\Big[\int_{[0,1]^d}|f_X(x) - \widehat{f}_{n,h,1}(x)|\sigma(x)(|g(x) - \widehat{g}_{n,h,1}(x)| + |f_X(x) - \widehat{f}_{n,h,1}(x)||m(x)|)dx\Big]\\
&\leqslant C\ \mathbb{E}_{\substack{X_2,\cdots,X_n\\Y_2,\cdots,Y_n}}\Big[\int_{[0,1]^d}|f_X(x) - \widehat{f}_{n,h,1}(x)||g(x) - \widehat{g}_{n,h,1}(x)|dx\Big]\\
&\quad + C\ \mathbb{E}_{\substack{X_2,\cdots,X_n\\Y_2,\cdots,Y_n}}\Big[\int_{[0,1]^d}|f_X(x) - \widehat{f}_{n,h,1}(x)||f_X(x) - \widehat{f}_{n,h,1}(x)||m(x)|)dx\Big].
\end{aligned}$$

By applying twice Cauchy-Schwartz inequality, the first term is bounded from above by

$$\begin{aligned}
&C\ \mathbb{E}_{\substack{X_2,\cdots,X_n\\Y_2,\cdots,Y_n}}\Big[\Big(\int_{[0,1]^d}(f_X(x) - \widehat{f}_{n,h,1}(x))^2dx\Big)^{1/2}\Big(\int_{[0,1]^d}(g(x) - \widehat{g}_{n,h,1}(x))^2dx\Big)^{1/2}\Big]\\
&\quad\leqslant C\ \mathbb{E}_{\substack{X_2,\cdots,X_n\\Y_2,\cdots,Y_n}}\Big[\int_{[0,1]^d}(f_X(x) - \widehat{f}_{n,h,1}(x))^2dx\Big]^{1/2}\mathbb{E}_{\substack{X_2,\cdots,X_n\\Y_2,\cdots,Y_n}}\Big[\int_{[0,1]^d}(g(x) - \widehat{g}_{n,h,1}(x))^2dx\Big]^{1/2}\\
&\quad= o(n^{-1/2})
\end{aligned}$$

using (15) and (33) while the second term is $o(n^{-1/2})$.

Study of I_2 Recall that

$$I_2 = \frac{1}{n}\sum_{i=1}^{n}(\widehat{m}_i - m_i)^2 = \frac{1}{n}\sum_{i=1}^{n}\frac{(\widehat{g}_i - \widehat{f}_i m_i)^2}{\widehat{f}_i^2} = O_{\mathbb{P}}\Big(\frac{1}{n}\sum_{i=1}^{n}(\widehat{g}_i - \widehat{f}_i m_i)^2\Big)$$

by (16). Then,

$$\begin{aligned}
\mathbb{E}[I_2] &\leqslant C\ \mathbb{E}_{\substack{X_2,\cdots,X_n\\Y_2,\cdots,Y_n}}\Big[\int_{[0,1]^d}(\widehat{g}_{n,h,i}(x)-\widehat{f}_{n,h,i}(x)m(x))^2 f_X(x)dx\Big]\\
&= C\ \mathbb{E}_{\substack{X_2,\cdots,X_n\\Y_2,\cdots,Y_n}}\Big[\int_{[0,1]^d}[(\widehat{g}_{n,h,i}(x)-g(x))+(f_X(x)m(x)-\widehat{f}_{n,h,i}(x)m(x))]^2 f_X(x)dx\Big]\\
&\leqslant C\ \mathbb{E}_{\substack{X_2,\cdots,X_n\\Y_2,\cdots,Y_n}}\Big[\int_{[0,1]^d}(\widehat{g}_{n,h,i}(x)-g(x))^2 f_X(x)dx\Big] + C\ \mathbb{E}\Big[\int_{[0,1]^d}(\widehat{f}_{n,h,i}(x)-f(x))^2 m(x)^2 f_X(x)dx\Big]\\
&= o(n^{-1/2})
\end{aligned}$$

as f_X is continuous thus bounded on $[0,1]^d$, as m is also bounded on $[0,1]^d$ (recall that it follows from the boundedness of σ^2) and from the results stated in (15) and (33). □

Proof of Theorem 4.2. The proof is similar as the proof of Theorem 4.1 except that for any $i \neq j$, $K_h \circ A_{X_i}(U_{ij})$ is replaced by $\sum_{a\in\{-1,0,1\}^d}\prod_{k=1}^d K_h(M^{a_k}(X_{k,j})-X_i)$. □

A.4 Proof of the remaining results

Proof of Proposition 4.3. We denote by P the distribution of (X,Y) and we introduce

$$\psi(P) = \mathbb{E}[\mathbb{E}[Y|X]^2].$$

The influence efficient function of ψ at P, as stated in [13], is given by $\widetilde{\psi}_P(x,y) = (2y - m(x))m(x) - \mathbb{E}[Ym(X)]$ (see [24] for explicit computations). Moreover, we deduce from (41) that

$$\widehat{T}_{n,h} = \psi(P) + \frac{1}{n}\sum_{i=1}^n \widetilde{\psi}_P(X_i,Y_i) + o_{\mathbb{P}}(n^{-1/2})$$

and, by [42, Condition (25.22)], $\widehat{T}_{n,h}$ is asymptotically efficient. The same holds true for $\widetilde{T}_{n,h}$. □

Proof of Corollary 4.4. In view of the definition of the asymptotic efficiency (see, e.g., [42, Lemma 25.23] or [24, Definition 2.4], the asymptotic efficiency ensures the asymptotic normality. Thus we only need to prove the asymptotic efficiency. To do so, it suffices to use the asymptotic efficiency of $\widehat{T}_{n,h}$ and $\widetilde{T}_{n,h}$ in Proposition 4.3, the asymptotic efficiency of the empirical mean $\overline{Y_n}$ and the empirical variance $\overline{Y_n^2}$ (see, e.g., [22]) together with the efficiency in product space [42, Theorem 25.50] to conclude to the joint asymptotic efficiency of $(\widehat{T}_{n,h}, \overline{Y_n}, \overline{Y_n^2})$ and $(\widetilde{T}_{n,h}, \overline{Y_n}, \overline{Y_n^2})$. Finally, we follow the same lines as in the proof of [22, Proposition 2.5] using the efficiency and delta method [42, Theorem 25.47] to get the required result. It remains to perform easy computations to get the expression of the asymptotic variance

$$\begin{aligned}
\sigma^2 &= \frac{1}{\mathrm{Var}(Y)^2}(4(\mathrm{Var}(Yg_1(X)) - 2\mathrm{Cov}(Yg_1(X),Y)\mathbb{E}[Y] + \mathbb{E}[Y]^2\mathrm{Var}(Y))\\
&+ 4S^X(2\mathrm{Cov}(Yg_1(X),Y)\mathbb{E}[Y] - \mathrm{Cov}(Yg_1(X),Y^2) - 2\mathbb{E}[Y]^2\mathrm{Var}(Y) + \mathbb{E}[Y]\mathrm{Cov}(Y,Y^2))\\
&+ (S^X)^2(4\mathbb{E}[Y]^2\mathrm{Var}(Y) - 4\mathbb{E}[Y]\mathrm{Cov}(Y,Y^2) + \mathrm{Var}(Y^2))).
\end{aligned}$$

□

Proof of Corollary 4.5. It suffices to apply [42, Theorem 25.50]. □

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References

[1] A. Antoniadis. Analysis of variance on function spaces. Statistics: A Journal of Theoretical and Applied Statistics, 15(1):59–71, 1984.

[2] K. Bertin, N. Klutchnikoff, J. R. Léon, and C. Prieur. Adaptive density estimation on bounded domains under mixing conditions. Electronic Journal of Statistics, 14(1):2198 – 2237, 2020.

[3] P. J. Bickel, C. A. Klaassen, P. J. Bickel, Y. Ritov, J. Klaassen, J. A. Wellner, and Y. Ritov. Efficient and adaptive estimation for semiparametric models, volume 4. Springer, 1993.

[4] B. Broto, F. Bachoc, and M. Depecker. Variance reduction for estimation of shapley effects and adaptation to unknown input distribution. SIAM/ASA Journal on Uncertainty Quantification, 8(2):693–716, 2020.

[5] S. Chatterjee. A new coefficient of correlation. Journal of the American Statistical Association, pages 1–26, 2020.

[6] R. Coleman. Calculus on normed vector spaces. Springer Science & Business Media, 2012.

[7] S. Da Veiga and F. Gamboa. Efficient estimation of sensitivity indices. Journal of Nonparametric Statistics, 25(3):573–595, 2013.

[8] S. Da Veiga, F. Gamboa, B. Iooss, and C. Prieur. Basics and Trends in Sensitivity Analysis: Theory and Practice in R. SIAM, 2021.

[9] S. Da Veiga, F. Wahl, and F. Gamboa. Local polynomial estimation for sensitivity analysis on models with correlated inputs. Technometrics, 51(4):452–463, 2009.

[10] L. Devroye, P. G. Ferrario, L. Györfi, and H. Walk. Strong universal consistent estimate of the minimum mean squared error. Empirical Inference: Festschrift in Honor of Vladimir N. Vapnik, pages 143–160, 2013.

[11] L. Devroye, L. Györfi, G. Lugosi, and H. Walk. A nearest neighbor estimate of the residual variance. Electronic Journal of Statistics, 12(1):1752–1778, 2018.

[12] L. Devroye, D. Schäfer, L. Györfi, and H. Walk. The estimation problem of minimum mean squared error. Statistics & Decisions, 21(1):15–28, 2003.

[13] K. Doksum and A. Samarov. Nonparametric estimation of global functionals and a measure of the explanatory power of covariates in regression. The Annals of Statistics, pages 1443–1473, 1995.

[14] F. Gamboa, P. Gremaud, T. Klein, and A. Lagnoux. Global sensitivity analysis: A novel generation of mighty estimators based on rank statistics. Bernoulli, 28(4):2345–2374, 2022.

[15] F. Gamboa, A. Janon, T. Klein, A. Lagnoux, and C. Prieur. Statistical inference for Sobol Pick-Freeze Monte Carlo method. Statistics, 50(4):881–902, 2016.

[16] F. Gamboa, T. Klein, A. Lagnoux, and P. Rochet. Erratum to "Global Sensitivity Analysis: a new generation of mighty estimators based on rank statistics".

[17] L. Gilquin, E. Arnaud, C. Prieur, and A. Janon. Making the best use of permutations to compute sensitivity indices with replicated orthogonal arrays. Reliability Engineering & System Safety, 187:28–39, 2019.

[18] L. Györfi and H. Walk. On the asymptotic normality of an estimate of a regression functional. J. Mach. Learn. Res., 16:1863–1877, 2015.

[19] B. E. Hansen. Exact mean integrated squared error of higher order kernel estimators. Econometric Theory, 21(6):1031–1057, 2005.

[20] M. B. Heredia, C. Prieur, and N. Eckert. Nonparametric estimation of aggregated sobol'indices: application to a depth averaged snow avalanche model. Reliability Engineering & System Safety, 212:107422, 2021.

[21] W. Hoeffding. A class of statistics with asymptotically normal distribution. Ann. Math. Statistics, 19:293–325, 1948.

[22] A. Janon, T. Klein, A. Lagnoux, M. Nodet, and C. Prieur. Asymptotic normality and efficiency of two Sobol index estimators. ESAIM: Probability and Statistics, 18:342–364, 1 2014.

[23] J. Kim, J. Shin, A. Rinaldo, and L. Wasserman. Uniform convergence rate of the kernel density estimator adaptive to intrinsic volume dimension. In International Conference on Machine Learning, pages 3398–3407. PMLR, 2019.

[24] T. Klein, A. Lagnoux, and P. Rochet. Efficient influence functions for Sobol' indices under two designs of experiments. Work in progress, 2024.

[25] T. Klein and P. Rochet. Efficiency of the averaged rank-based estimator for first order sobol' index inference. Statistics & Probability Letters, 207:110015, 2024.

[26] E. Liitiäinen, F. Corona, and A. Lendasse. On nonparametric residual variance estimation. Neural Processing Letters, 28:155–167, 2008.

[27] E. Liitiäinen, F. Corona, and A. Lendasse. Residual variance estimation using a nearest neighbor statistic. Journal of Multivariate Analysis, 101(4):811–823, 2010.

[28] H. Liu, L. Wasserman, and J. Lafferty. Exponential concentration for mutual information estimation with application to forests. Advances in Neural Information Processing Systems, 25, 2012.

[29] W. K. Newey, F. Hsieh, and J. Robins. Undersmoothing and bias corrected functional estimation. 1998.

[30] K. Pearson. On the partial correlation ratio. Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character, 91(632):492–498, 1915.

[31] J. Pfanzagl. Lecture notes in statistics. Contributions to a general asymptotic statistical theory, 13:11–15, 1982.

[32] E. Plischke and E. Borgonovo. Fighting the curse of sparsity: Probabilistic sensitivity measures from cumulative distribution functions. Risk Analysis, 40(12):2639–2660, 2020.

[33] L. Pujol. Nonparametric estimation of a multivariate density under Kullback-Leibler loss with ISDE. arXiv preprint arXiv:2205.03199, 2022.

[34] S. Razavi, A. Jakeman, A. Saltelli, C. Prieur, B. Iooss, E. Borgonovo, E. Plischke, S. Lo Piano, T. Iwanaga, W. Becker, S. Tarantola, J. H. Guillaume, J. Jakeman, H. Gupta, N. Melillo, G. Rabitti, V. Chabridon, Q. Duan, X. Sun, S. Smith, R. Sheikholeslami, N. Hosseini, M. Asadzadeh, A. Puy, S. Kucherenko, and H. Maier. The Future of Sensitivity Analysis: An essential discipline for systems modeling and policy support. Environmental Modelling and Software, 137:104954, Mar. 2021.

[35] A. Saltelli, K. Chan, and E. Scott. Sensitivity analysis. Wiley Series in Probability and Statistics. John Wiley & Sons, Ltd., Chichester, 2000.

[36] I. M. Sobol'. Sensitivity estimates for nonlinear mathematical models. Math. Modeling Comput. Experiment, 1(4):407–414 (1995), 1993.

[37] I. M. Sobol'. Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates. Mathematics and Computers in Simulation, 55(1-3):271–280, 2001.

[38] M. Solís. Non-parametric estimation of the first-order Sobol' indices with bootstrap bandwidth. Communications in Statistics-Simulation and Computation, 50(9):2497–2512, 2021.

[39] B. Sudret. Global sensitivity analysis using polynomial chaos expansions. Reliability Engineering & System Safety, 93(7):964–979, 2008.

[40] J.-Y. Tissot and C. Prieur. A randomized orthogonal array-based procedure for the estimation of first-and second-order sobol'indices. Journal of Statistical Computation and Simulation, 85(7):1358–1381, 2015.

[41] A. B. Tsybakov and A. B. Tsybakov. Nonparametric estimators. Introduction to Nonparametric Estimation, pages 1–76, 2009.

[42] A. W. van der Vaart. Asymptotic statistics, volume 3 of Cambridge Series in Statistical and Probabilistic Mathematics. Cambridge University Press, Cambridge, 1998.