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The Sobol method in sensitivity analysis for stochastic computer models

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Abstract

Sensitivity analysis often accompanies computer modeling to understand what are the important factors of a model of interest. In particular, Sobol indices, naturally estimated by Monte-Carlo sampling, permit to quantify the contribution of the inputs to the variability of the output. However, when the model is stochastic, the problem of carrying out a sensitivity analysis remains open. There is no unique definition of Sobol indices and their estimation is more difficult because a good balance between repetitions of the computer code and explorations of the input space must be found. The problem of performing a sensitivity analysis for stochastic computer models with the Sobol method is addressed. Two Sobol indices are considered, their estimators constructed and their asymptotic properties established. An optimal balance between repetitions and explorations is proposed under a limited computing budget. A two-stage procedure is built: the first stage permits to find the optimal balance and the second stage produces the Sobol estimates based on the balance obtained in the first stage. The procedure is asymptotically oracle and the optimal convergence rates are derived. The theoretical results are tested with numerical experiments.

Keywords: Sobol; sensitivity; stochastic; random; model; efficient.

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1 Introduction

Sensitivity analysis often accompanies computer modeling to understand what are the important factors of a model of interest [15, 16]. In particular, Sobol indices [18, 19] permit to quantify the contribution of the inputs to the variability of the output. The Sobol index S_j is defined as

$$(1) \quad S_j = \frac{\text{Var E}(f(X)|X_j)}{\text{Var } f(X)}, \quad j = 1, \dots, p,$$

where $Y = f(X)$ is the output of the computer model f evaluated at the input $X = (X_1, \dots, X_p)$. The larger S_j , the more X_j is important in the following sense: if $X_j = x_j$ were fixed, $\text{Var } Y$ would be reduced by at least $S_j \times 100\%$. As a consequence, the Sobol indices satisfy $S_1 + \dots + S_p \leq 1$, with equality in the absence of interaction effects, which we shall not account for in this paper.

The estimation of Sobol indices is naturally performed by Monte-Carlo sampling [6, 13, 18, 19], which permits to build estimators with statistical guarantees [4, 10]. Sobol indices for multivariate, functional outputs [3, 11] or functional inputs [8] have been proposed as well.

Computer models employed to simulate physical systems/natural phenomena are increasingly stochastic. That is, two runs of the computer with the same input may lead to two different outputs. Examples can be found in epidemiology [1, 2, 14, 17] or ecology [20].

It is still unclear how sensitivity analysis should be performed when the models are stochastic. First, there is no unique definition of Sobol indices [5]. Second, it is unclear how to account for noise in the inference. Monte-Carlo sampling with repetitions is natural, but what is a good balance between the number of repetitions and the number of explorations of the input space [20]? Having efficient estimators would permit to achieve the same level of precision but with less computations, an important practical issue. An approach based on meta-models has been proposed [12], but it is difficult to control the induced bias and the construction of the meta-model itself can be challenging.

The problem of efficient estimation of Sobol indices for stochastic computer models is addressed. Two definitions of Sobol indices are given. Their estimators, based on Monte-Carlo sampling with repetitions, are built and their asymptotic properties established. It is shown that, when the computing budget is fixed, an optimal number of repetitions can be defined and estimated. A two-stage procedure is given for efficiently estimating Sobol indices, the first stage serving to find the optimal number of repetitions that should be used in the Monte-Carlo experiment of the second stage.

This paper is organized as follows. The sensitivity indices and their estimators are defined in Section 2. The optimal number of repetitions is defined in Section 3, where an estimator is also given. In Section 4, a two-stage procedure is proposed that permit to efficiently estimate the sensitivity indices by exploiting the results of Section 2 and Section 3. Numerical experiments are provided in Section 5 to test and illustrate the theory. A discussion closes the paper. The proofs are given in Appendix A.

2 Stochastic sensitivity analysis

2.1 Definition of the sensitivity indices

In the case of a stochastic computer model, the output is

$$Y = f(X, Z),$$

where Z is an unobserved random element that represents the “noise” of the model. That is to say, even if $X = x$ is fixed, the output, distributed as $f(x, Z)$, exhibits a residual variability due to the randomness of Z . In all this paper, we assume that X and Z are independent. Note that f does *not* represent the computer model, as seen by the user. For the user, the computer model is not even a mapping, since to runs of the computer at the same input can lead to two different outputs. Here, f is any mapping that, together with X and Z , produces the output Y . The existence of Z and f such that $Y = f(X, Z)$ is assumed.

Two kinds of Sobol indices can be built.

Definition 1. *The Sobol indices of the first kind are defined as*

$$S'_j = \frac{\text{Var E}(f(X, Z)|X_j)}{\text{Var } f(X, Z)}$$

for $j = 1, \dots, p$.

Definition 2. *The Sobol indices of the second kind are defined as*

$$S''_j = \frac{\text{Var E}(E[f(X, Z)|X]|X_j)}{\text{Var E}[f(X, Z)|X]}$$

for $j = 1, \dots, p$.

The first index is built by substituting $f(X, Z)$ for $f(X)$ in (1). The second by substituting $E[f(X, Z)|X]$. Thus, the index of the first kind is a direct application of (1): one does *as if* Z were another input, even though it is not

observable. The index of the second kind is also an application of (1) but to the function $x \mapsto \mathbb{E}[f(x, Z)|X = x]$ with the noise smoothed out.

For estimation purposes, it is convenient to rewrite the indices as

$$(2) \quad S'_j = \frac{\mathbb{E}\mathbb{E}[f(X, Z)|X] \mathbb{E}[f(\tilde{X}_{-j}, Z)|\tilde{X}_{-j}] - (\mathbb{E}\mathbb{E}[f(X, Z)|X])^2}{\mathbb{E}\mathbb{E}[f(X, Z)^2|X] - (\mathbb{E}\mathbb{E}[f(X, Z)|X])^2}$$

and

$$(3) \quad S''_j = \frac{\mathbb{E}\mathbb{E}[f(X, Z)|X] \mathbb{E}[f(\tilde{X}_{-j}, Z)|\tilde{X}_{-j}] - (\mathbb{E}\mathbb{E}[f(X, Z)|X])^2}{\mathbb{E}\mathbb{E}[f(X, Z)|X]^2 - (\mathbb{E}\mathbb{E}[f(X, Z)|X])^2},$$

where $\tilde{X} = (\tilde{X}_1, \dots, \tilde{X}_p)$ is an independent copy of X and

$$\tilde{X}_{-j} = (\tilde{X}_1, \dots, \tilde{X}_{j-1}, X_j, \tilde{X}_{j+1}, \dots, \tilde{X}_p),$$

for $j = 1, \dots, p$. Note that S'_j and S''_j differ only by the lower left term. In particular, the upper left term is the same in both formula and is the only term that depends on j , and hence the only term that permits to discriminate between any two indices of the same kind. For this reason, it is called the discriminator and is denoted by D_j . Notice that $S'_j \leq S''_j$.

Example 1. Let $Y = aX_1 + cX_2h(Z)$, where X_1, X_2, Z are independent standard normal variables, a, c are real coefficients and h is a function such that $\mathbb{E}h(Z) = 0$. Then

$$S'_1 = \frac{a^2}{a^2 + c^2 \mathbb{E}h(Z)^2}, S'_2 = 0, S''_1 = 1 \text{ and } S''_2 = 0.$$

Example 1 illustrates that the two kinds of sensitivity indices measure different aspects of the sensitivity of a computer model. While the sensitivity indices of the first kind depend on the coefficients of the model, those of the second kind do not.

Example 2. Let $f(X_1, X_2, Z) = \sin(X_1) + a \sin(X_2)^2 + bZ^4 \sin(X_1)$, where X_1, X_2, Z are independent uniform random variables on $(-\pi, \pi)$ and a, b are real coefficients. The Sobol indices of the first kind are given by

$$S'_1 = \frac{b\pi^4/5 + b^2\pi^8/50 + 1/2}{a^2/8 + b\pi^4/5 + b^2\pi^8/18 + 1/2}$$

and

$$S'_2 = \frac{a^2/8}{a^2/8 + b\pi^4/5 + b^2\pi^8/18 + 1/2}.$$

The Sobol indices of the second kind are given by

$$S''_1 = \frac{b\pi^4/5 + b^2\pi^8/50 + 1/2}{(1 + b\pi^4/5)^2/2 + a^2/8}$$

and

$$S''_2 = \frac{a^2/8}{(1 + b\pi^4/5)^2/2 + a^2/8}.$$

The model in Example 2 with $a = 7$ and $b = 0.1$ was used to test sensitivity analysis methods based on meta-models [12]. When $Z = X_3$ is a controllable input, this model is a standard benchmark for deterministic models [6, 9]. Although, in the examples above, Z is a scalar, it is easy to build other examples in which Z is a random vector.

2.2 Inference

Estimation is based on Monte-Carlo sampling. The sampling scheme is given in Algorithm 1. The input space is explored n times and, for each exploration, the computer is run m times to smooth out the noise. Thus, the total number of calls to the computer is proportional to mn . Denote by $T = mn(p + 1)$ the total number of calls.

Algorithm 1 Generate a Monte-Carlo sample

```

for  $i = 1$  to  $n$  do
  draw two independent copies  $X^{(i)}, \tilde{X}^{(i)}$ 
  for  $j = 0, 1, \dots, p$  do
    for  $k = 1$  to  $m$  do
      run the computer model at  $\tilde{X}_{-j}^{(i)}$  to get an output  $Y_j^{(i,k)}$ 
    end for
  end for
end for

```

The data generated by the algorithm are

$$(Y_j^{(i,k)}, \tilde{X}_{-j}^{(i)}),$$

for $j = 0, 1, \dots, p$, $i = 1, \dots, n$ and $k = 1, \dots, m$, with the convention $\tilde{X}_{-0}^{(i)} = X^{(i)}$. By assumption, there are independent random elements $(Z_j^{(i,k)})$ such that

$$(4) \quad Y_j^{(i,k)} = f(\tilde{X}_{-j}^{(i)}, Z_j^{(i,k)}).$$

The estimators of the sensitivity indices are built by substituting empirical averages for expectations in (2) and (3), that is,

$$(5) \quad \hat{S}'_{j;n,m} = \frac{\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \frac{1}{m} \sum_{k'=1}^m Y_j^{(i,k')} - \left(\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \right)^2}{\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)2} - \left(\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \right)^2}$$

and

$$(6) \quad \hat{S}''_{j;n,m} = \frac{\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \frac{1}{m} \sum_{k'=1}^m Y_j^{(i,k')} - \left(\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \right)^2}{\frac{1}{n} \sum_{i=1}^n \left(\frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \right)^2 - \left(\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \right)^2}.$$

To our knowledge (personal communication), when faced with stochastic computer models, practitioners tend to use softwares for deterministic sensitivity analysis in which an average over repetitions is given to the program as a substitute for the value of the output. Thus, the second estimator is used in practice, albeit implicitly. The first estimator, to the best of our knowledge, was not formally defined. The second estimator appeared in [7], where it was studied only in the case $m = n$ (to the best of our understanding).

In (5) and (6), take $m = 1$ and assume $Y_j^{(i,1)} = f(\tilde{X}_{-j}^{(i)})$ instead of (4). Then the estimators reduce to those of Sobol [18, 19] in the deterministic case. In the later case, these estimators are sometimes called pick-freeze estimators [4].

In the rest of this paper, we assume that, for all x and all z ,

$$(7) \quad f(x, z) \leq F(x)$$

for some F with $\mathbb{E} F(X)^8 < \infty$. The existence of the bound F to control the stochastic part of the model is needed to apply Lindeberg-Feller's central limit theorem. The condition $\mathbb{E} F(X)^8 < \infty$ is the weakest moment condition needed to be able to apply classical central limit theorems to all of the estimators in this paper.

These conditions are verified for the model in Example 2. Indeed we have

$$f(X_1, X_2, Z) \leq \sin(X_1)(1 + |b|\pi^4) + a \sin(X_2)^2.$$

For the model in Example 1, it suffices to take

$$h(Z) = \begin{cases} -t & \text{if } Z \leq -t, \\ Z & \text{if } -t \leq Z \leq t, \\ t & \text{otherwise} \end{cases}$$

for some threshold $t > 0$.

We now establish asymptotic properties of the sensitivity estimators as the number of explorations goes to infinity. The number of repetitions can be fixed or go to infinity as well. In the later, $m = m_n$ is assumed to be a sequence growing with n . Denote by \mathbf{S}' (resp. \mathbf{S}'') the (column) vector with coordinates S'_j (resp. S''_j), $j = 1, \dots, p$, and denote by $\widehat{\mathbf{S}}'_{n,m}$ (resp. $\widehat{\mathbf{S}}''_{n,m}$) the vector with coordinates $\widehat{S}'_{j;n,m}$ (resp. $\widehat{S}''_{j;n,m}$).

Theorem 1. *Assume (7) holds and let $n \rightarrow \infty$. Then*

$$\sqrt{n} \left(\widehat{\mathbf{S}}''_{n,m} - \mathbf{S}'' \left[1 - \frac{\widehat{\mathbf{S}}'_{n,m} - \mathbf{S}'}{\mathbb{E} \text{Var}[f(X, Z)|X]} \right] \right) \xrightarrow{d} N(0, \Xi_m),$$

for some nonnegative matrix Ξ_m of size $2p \times 2p$. If $m = m_n \rightarrow \infty$ as $n \rightarrow \infty$, then, elementwise, $\Xi_m \rightarrow \Xi$ for some Ξ . Moreover, the convergence in distribution above still holds with Ξ in place of Ξ_m .

The result of Theorem 1 suggests that, when the number of explorations is large enough,

$$\widehat{\mathbf{S}}'_{n,m} \stackrel{d}{\approx} N(\mathbf{S}', \frac{1}{n} \Xi_{1m})$$

and

$$\widehat{\mathbf{S}}''_{n,m} \stackrel{d}{\approx} N \left(\mathbf{S}'' \left[1 + \frac{\mathbb{E} \text{Var}[f(X, Z)|X]}{\mathbb{E} \text{Var}[f(X, Z)|X] + m \text{Var} \mathbb{E}[f(X, Z)|X]} \right], \frac{1}{n} \Xi_{2m} \right)$$

for some variance-covariance matrices Ξ_{1m}, Ξ_{2m} of size $p \times p$ and for any m . Since Ξ_m has a limit, these approximations hold for m large as well. This permits to draw inferences about the Sobol indices for any number of repetitions.

When the number of repetitions is much smaller than the number of explorations, the sensitivity estimators of the second kind underestimate the corresponding Sobol indices. Fortunately, the bias is explicit and can be estimated in practice. Note that the bias is proportional to $\mathbb{E} \text{Var}[f(X, Z)|X]$, which is

zero whenever f actually does not depend on Z . This term is a noise term: it is expected to be large whenever the computer model is highly stochastic. When m grows, the bias diminishes but it could be that the sensitivity estimator is arbitrarily tightly concentrated around the wrong target. This phenomenon is avoided by choosing a number of repetitions much larger than the square root of the number of explorations, as stated in Corollary 1.

Corollary 1. *Let $\sqrt{n}/m \rightarrow 0$. Then, under the assumptions of Theorem 1,*

$$\sqrt{n} \begin{pmatrix} \widehat{\mathbf{S}}'_{n,m} - \mathbf{S}' \\ \widehat{\mathbf{S}}''_{n,m} - \mathbf{S}'' \end{pmatrix} \xrightarrow{d} N(0, \Xi).$$

3 Balancing explorations and repetitions

Clearly, to get the best estimators, one should do as many explorations and repetitions as possible. However, in practice, each call to the computer model is costly and the budget is limited. Denote the total available budget by T and remember from Section 2 that $T = mn(p+1)$. Which, among all couples (m, n) that satisfy $T = mn(p+1)$, yields the best performance? The criterion often used to optimize statistical methods, the mean squared error, is intractable for Sobol estimators.

We propose to consider a more convenient criterion, given by

$$\text{MRE} = \mathbb{E} \sum_{j=1}^p |\widehat{R}_{j;n,m} - R_j|,$$

where R_j is the rank of D_j among D_1, \dots, D_p , that is, $R_j = \sum_{i=1}^p \mathbf{1}(D_i \leq D_j)$, and $\widehat{R}_{j;n,m}$ is an estimator of R_j . Recall that D_1, \dots, D_p , the upper-left terms in (2) and (3), determine the ranks of the sensitivity indices and that the ranks of the sensitivity indices of the first and of the second kind are the same. Thus, the MRE permits to find a unique solution to the balance problem for both kinds of sensitivity indices. The MRE is an error which is small when one succeeds in ranking the inputs of the computer model from the most to the least important. That is, one seeks the input which, if fixed, would lead to the greatest reduction of the output variance; then the second, etc. This is called *Factors Prioritisation* in [16, p. 52].

The MRE is more tractable than the MSE because it depends only on the discriminators, but it is still difficult to minimize it directly. Therefore, it is a bound of the MRE that is used to find an optimal balance between explorations and repetitions.

3.1 Defining an optimal number of repetitions

In what follows, the vector (X, \widetilde{X}) of size $2p$ is denoted by \mathbf{X} . Denote by $\widehat{D}_{j;n,m}$ the upper-left term in (5) and (6), the estimator of D_j . Let Y_j be a shorthand for $Y_j^{(1,1)} = f(\widetilde{X}_{-j}^{(1)}, Z_j^{(1,1)})$, $j = 0, 1, \dots, p$ and recall that $\widetilde{X}_{-0}^{(1)} = X^{(1)}$.

Proposition 1. Let $\widehat{R}_{j;n,m} = \sum_{i=1}^p \mathbf{1}(\widehat{D}_{i;n,m} \leq \widehat{D}_{j;n,m})$. Then

$$\begin{aligned} \mathbb{E} \sum_{j=1}^p |\widehat{R}_{j;n,m} - R_j| &\leq \frac{2(p-1)(p+1)^2}{\min_{j < j'} (|D_j - D_{j'}|^2) T} \\ &\quad \times \sum_{j=1}^p (m \operatorname{Var} \mathbb{E}[Y_0 Y_j | \mathbf{X}] \\ &\quad \quad + \mathbb{E}(\operatorname{Var}[Y_0 Y_j | \mathbf{X}] - \operatorname{Var}[Y_0 | \mathbf{X}] \operatorname{Var}[Y_j | \mathbf{X}]) \\ &\quad \quad + \frac{1}{m} \mathbb{E} \operatorname{Var}[Y_0 | \mathbf{X}] \operatorname{Var}[Y_j | \mathbf{X}]). \end{aligned}$$

This bound provides us with some insights. It is small when the Sobol indices are well separated and increases as the cube of the number of inputs. Denote $\sum_j \operatorname{Var} \mathbb{E}[Y_0 Y_j | \mathbf{X}]$ by ζ_1 , $\sum_j \mathbb{E}(\operatorname{Var}[Y_0 Y_j | \mathbf{X}] - \operatorname{Var}[Y_0 | \mathbf{X}] \operatorname{Var}[Y_j | \mathbf{X}])$ by ζ_2 and $\sum_j \mathbb{E} \operatorname{Var}[Y_0 | \mathbf{X}] \operatorname{Var}[Y_j | \mathbf{X}]$ by ζ_3 . Then $\zeta_l \geq 0$ for $l = 1, 2, 3$ and the bound is proportional to $n^{-1}(\zeta_1 + m^{-1}\zeta_2 + m^{-2}\zeta_3)$, which decreases as n increases or m increases. The function $T^{-1}(m\zeta_1 + \zeta_2 + m^{-1}\zeta_3)$ is a convex function of m and, forgetting at the moment that m is an integer, it is minimized at

$$(8) \quad m^* := \sqrt{\frac{\sum_{j=1}^p \mathbb{E} \operatorname{Var}[Y_0 | \mathbf{X}] \operatorname{Var}[Y_j | \mathbf{X}]}{\sum_{j=1}^p \operatorname{Var} \mathbb{E}[Y_0 Y_j | \mathbf{X}]}}.$$

The number m^* can be interpreted as a noise-to-signal ratio for ranking the Sobol indices. Indeed, recall that a variance can be decomposed into a variance of a conditional expectation and an expectation of a conditional variance, where the last represents a noise term and the former a signal term [16, p. 12]. The numerator in (8) is the noise term: if the computer model is deterministic, then the function $f(X, Z)$ does not in fact depend on Z , and the numerator is zero. The denominator is the signal term.

The *optimal number of repetitions* is naturally defined as the integer m^\dagger that minimizes the upper bound in Proposition 1 over all compatible integers, that is, over all integers m such that $T = mn(p+1)$. For instance, for $T = 300$ and $p = 2$, the set of compatible integers is $\{1, 2, 4, 5, 10, 20, 25, 50\}$. By convexity of the bound, the optimal number of repetitions is either the greatest compatible integer less than or equal to m^* , denoted by $\lfloor m^* \rfloor$, or the smallest compatible integer greater than or equal to m^* , denoted by $\lceil m^* \rceil$.

Proposition 2. The optimal number of repetitions m^\dagger is given according to the following three cases.

- (i) If $m^* \leq 1$ then $m^\dagger = 1$.
- (ii) If $m^* \geq T/(p+1)$ then $m^\dagger = T/(p+1)$.
- (iii) If $1 < m^* < T/(p+1)$ then

$$m^\dagger = \begin{cases} \lceil m^* \rceil & \text{if } \lfloor m^* \rfloor \lceil m^* \rceil \leq m^{*2} \\ \lfloor m^* \rfloor & \text{if } \lfloor m^* \rfloor \lceil m^* \rceil \geq m^{*2}. \end{cases}$$

Moreover, if $\lfloor m^* \rfloor = \lceil m^* \rceil = m^*$, then $m^* = m^\dagger$.

Provided that the Monte-Carlo experiment is large enough so that $m^* < T/(p+1)$, the noise-to-signal ratio m^* , and hence the optimal number of repetition m^\dagger , does *not* depend on the size of the experiment. For instance, if it happens that $m^* < 50$, then the optimal number of repetitions will be the same whether the size of the experiment is $T = 300$ or $T = 3000000$.

3.2 Estimation

The goal of this section is to build an estimator of the noise-to-signal ratio (8) based on the same outputs as those produced in Algorithm 1. In view of Proposition 2, this will yield immediately an estimator for the optimal number of repetitions.

Denote $\text{Var E}[Y_0 Y_j | \mathbf{X}]$ by $\zeta_{1,j}$, $\text{E}(\text{Var}[Y_0 Y_j | \mathbf{X}] - \text{Var}[Y_0 | \mathbf{X}] \text{Var}[Y_j | \mathbf{X}])$ by $\zeta_{2,j}$ and $\text{E Var}[Y_0 | \mathbf{X}] \text{Var}[Y_j | \mathbf{X}]$ by $\zeta_{3,j}$, $j = 1, \dots, p$. Then $m^* = \sqrt{\sum_{j=1}^p \zeta_{3,j} / \sum_{j=1}^p \zeta_{1,j}}$ and natural estimators for $\zeta_{1,j}$ and $\zeta_{3,j}$ can be built using the same principles as those that were used to build the sensitivity estimators. Thus, let

$$\begin{aligned} \hat{\zeta}_{3,j;n,m} &= \\ (9) \quad & \frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k_1=1}^m f(X^{(i)}, Z_0^{(i,k_1)})^2 \frac{1}{m} \sum_{k_2=1}^m f(\tilde{X}_{-j}^{(i)}, Z_j^{(i,k_2)})^2 \\ (10) \quad & + \frac{1}{n} \sum_{i=1}^n \left(\frac{1}{m} \sum_{k_1=1}^m f(X^{(i)}, Z_0^{(i,k_1)}) \right)^2 \left(\frac{1}{m} \sum_{k_2=1}^m f(\tilde{X}_{-j}^{(i)}, Z_j^{(i,k_2)}) \right)^2 \\ (11) \quad & - \frac{1}{n} \sum_{i=1}^n \left(\frac{1}{m} \sum_{k_1=1}^m f(X^{(i)}, Z_0^{(i,k_1)}) \right)^2 \frac{1}{m} \sum_{k_2=1}^m f(\tilde{X}_{-j}^{(i)}, Z_j^{(i,k_2)})^2 \\ (12) \quad & - \frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k_1=1}^m f(X^{(i)}, Z_0^{(i,k_1)})^2 \left(\frac{1}{m} \sum_{k_2=1}^m f(\tilde{X}_{-j}^{(i)}, Z_j^{(i,k_2)}) \right)^2, \end{aligned}$$

and

$$\begin{aligned} \hat{\zeta}_{1,j;n,m} &= \\ (13) \quad & \frac{1}{n} \sum_{i=1}^n \left(\frac{1}{m} \sum_{k=1}^m f(X^{(i)}, Z_0^{(i,k)}) f(\tilde{X}_{-j}^{(i)}, Z_j^{(i,k)}) \right)^2 \\ (14) \quad & - \left(\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m f(X^{(i)}, Z_0^{(i,k)}) f(\tilde{X}_{-j}^{(i)}, Z_j^{(i,k)}) \right)^2 \end{aligned}$$

so that m^* is estimated by

$$(15) \quad \hat{m}_{n,m}^* := \sqrt{\frac{\sum_{j=1}^p \hat{\zeta}_{3,j;n,m}}{\sum_{j=1}^p \hat{\zeta}_{1,j;n,m}}}.$$

It is easy to check that $\hat{\zeta}_{1,j;n,m} \geq 0$ and $\hat{\zeta}_{3,j;n,m} \geq 0$ so that $\hat{m}_{n,m}^* \geq 0$. Also, notice that for $m = 1$, we have $\hat{\zeta}_{3,j;n,1} = 0$, so that $\hat{m}_{n,1}^* = 0$. Asymptotic properties are given in Theorem 2.

Theorem 2. *Assume (7) holds and let $n \rightarrow \infty$ and $m \rightarrow \infty$. Then*

$$\sqrt{n} \left(\widehat{m}_{n,m}^* - \left[m^* + \frac{C + o(1)}{m} \right] \right) \rightarrow N(0, \sigma^2),$$

for some constant C and variance σ^2 .

The term $o(1)$ is a sequence of constants indexed by m that goes to zero as $m \rightarrow \infty$. The bias is subjected to the same phenomenon observed for the sensitivity estimators of the second kind: as shown in Corollary 2, it can be annihilated when the number of repetitions grow faster than the square root of the number of explorations.

Corollary 2. *Let $n \rightarrow \infty$ and $m \rightarrow \infty$ such that $\sqrt{n}/m \rightarrow 0$. Then, under the assumptions of Theorem 2, $\sqrt{n}(\widehat{m}_{n,m}^* - m^*) \rightarrow N(0, \sigma^2)$.*

Theorem 2 is useful to study the statistical performance of the procedure proposed in Section 4.

4 A two-stage procedure to estimate sensitivity indices

The goal is to estimate the sensitivity indices of Section 2 by using the results of Section 3. It is assumed that the total budget available is T . To estimate the sensitivity indices, the following procedure is natural.

1. Generate a Monte-Carlo sample to get an estimate of the optimal number of repetitions.
2. Use that estimate to generate another Monte-Carlo sample with which the sensitivity estimators are built.

Although simple, the above procedure raises some questions. The sum of the sizes of the two Monte-Carlo experiments must be T . Thus, the size of the second Monte-Carlo sample is smaller than it could have been if no share of the budget was spent to estimate the optimal number of repetitions. To what extent is the performance affected? How to calibrate the procedure? How should the budget be splitted? These questions are addressed.

4.1 The procedure

Assume that only $T = mn(p + 1)$ runs of the computer model are allowed. Choose integers K, m_0, n_0 such that $m_0 n_0 (p + 1) = K < T$. Algorithm 2 gives the details of the procedure.

The integer K is the share of the total budget T dedicated to the estimation of the optimal number of repetitions, which is performed in the first stage. The estimator is (15) with $m = m_0$ and $n = n_0$. In the second stage, the sensitivity indices are estimated with the remaining budget $T - K$. The estimators are (5) and (6) with $m = \widehat{m}_{K, m_0}^\dagger$ and n the integer satisfying $T - K = \widehat{m}_{K, m_0}^\dagger n(p + 1)$. (If this equation has no solution, take m near $\widehat{m}_{K, m_0}^\dagger$ such that the equation has a solution.) We allow for the case $K = 0$. That is, the sensitivity indices are

Algorithm 2 Estimate the sensitivity indices in a two-stage procedure

Stage 1. Generate a Monte-Carlo sample with K runs of the computer model, n_0 explorations and m_0 repetitions to get an estimate \hat{m}_{K,m_0}^\dagger of m^\dagger . If $K = 0$, simply return m_0 .

Stage 2. Generate a Monte-Carlo sample with $T - K$ runs and \hat{m}_{K,m_0}^\dagger repetitions to estimate the sensitivity indices.

estimated directly with $m = m_0$ based on the whole budget T . If, moreover, it happens accidentally that $m_0 = m^\dagger$, then the best performance is to be expected.

4.2 Theoretical analysis

As in Section 3, the statistical performance of the two-stage procedure is assessed with respect to the MRE. Remember that $\mathbf{X}^{(1)} = (X^{(1)}, \tilde{X}^{(1,1)})$, $Y_0^{(1,1)} = f(X^{(1)}, Z_0^{(1,1)})$ and $Y_j^{(1,1)} = f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)})$, $j = 1, \dots, p$, and the superscripts are dropped for convenience. Put

$$\begin{aligned} v(m) &= \frac{2(p-1)(p+1)^2}{\min_{j < j'} (|D_j - D_{j'}|^2)} \\ &\quad \times \sum_{j=1}^p (m \operatorname{Var} \mathbb{E}[Y_0 Y_j | \mathbf{X}] \\ &\quad \quad + \mathbb{E}(\operatorname{Var}[Y_0 Y_j | \mathbf{X}] - \operatorname{Var}[Y_0 | \mathbf{X}] \operatorname{Var}[Y_j | \mathbf{X}]) \\ &\quad \quad + \frac{1}{m} \mathbb{E} \operatorname{Var}[Y_0 | \mathbf{X}] \operatorname{Var}[Y_j | \mathbf{X}]) \end{aligned}$$

so that the MRE in Proposition 1 is $v(m)/T$. The function v is convex and, over all compatible integers m , attains a minimum at $m = m^\dagger$. Over the nonnegative reals, it attains minimum at $m = m^*$ and $v''(m^*)$, the second derivative, is positive.

Conditionally on Stage 1, the MRE obeys

$$\text{MRE} \leq \frac{1}{T-K} v(\hat{m}_{K,m_0}^\dagger).$$

This bound shall be compared to the least possible bound, given by $v(m^\dagger)/T$, which would be obtained by a hypothetical ‘‘oracle’’ who would know the true value of the optimal number of repetitions.

For the sake of simplicity, we shall work with the noise-to-signal ratio. This permits to avoid issues related to the fact that m^\dagger must be a compatible integer, while still providing useful insights.

Define the excess-of-variance by

$$\hat{E}_{K,m_0} = \frac{\frac{1}{T-K} v(\hat{m}_{K,m_0}^*) - \frac{1}{T} v(m^*)}{\frac{1}{T} v(m^*)},$$

where \hat{m}_{K,m_0}^* is the noise-to-signal ratio produced by Stage 1. The excess-of-variance, which is greater or equal to zero, is literally the excess of variance

incurred by our ignorance about m^* . Thus, if $K = 0$ and $m_0 = m^*$, then $\widehat{E}_{0,m^*} = 0$. The budget K is subject to a compromise: on the one hand it must be large enough to get a good estimate of the noise-to-signal ratio, but on the other hand it must be small enough to keep the remaining budget $T - K$ large enough. The excess-of-variance has an asymptotic expansion given in Lemma 1.

Lemma 1. *Assume that $K/T \rightarrow c/(c+1)$ for some $c \geq 0$ as $m_0 \rightarrow \infty$ and $n_0 \rightarrow \infty$. Take $\sigma > 0$, C and the $o(1)$ term from Theorem 2 and put $V_K = \sqrt{n_0}(\widehat{m}_{K,m_0}^* - [m^* + \{C + o(1)\}/m_0])/\sigma$, so that $V_K \xrightarrow{d} N(0, 1)$. Then*

$$\begin{aligned} \widehat{E}_{K,m_0} &= \frac{(c+1)v''(m^*)}{2v(m^*)} \left(\frac{C}{m_0} + \frac{\sigma V_K}{\sqrt{n_0}} \right)^2 \\ &\quad + \frac{K}{T-K} + o_P\left(\frac{1}{m_0^2}\right) + o_P\left(\frac{1}{m_0\sqrt{n_0}}\right) + o_P\left(\frac{1}{n_0}\right). \end{aligned}$$

At the first order of approximation, that is, when $n_0 \rightarrow \infty$ and $m_0 \rightarrow \infty$, the behavior of the excess-of-variance is controlled by the growth rate of K/T . Indeed, all terms in the asymptotic expansion vanish except possibly $K/(T-K) = (K/T)(1-K/T)^{-1}$. Since $K/(T-K) \rightarrow c$, it holds that $\widehat{E}_{K,m_0} \xrightarrow{P} c$. The case $c = 0$, which demands that $K/T \rightarrow 0$, is called the oracle property and is formally stated in Corollary 3.

Corollary 3. *Assume that $K/T \rightarrow 0$. Then, under the assumptions of Lemma 1, $\widehat{E}_{K,m_0} \xrightarrow{P} 0$.*

At the second order of approximation, that is, removing all the $o_P(\cdot)$ terms, we see that the error increases with the curvature of v at m^* . A high curvature means that even a small deviation of the noise-to-signal ratio estimate from its target can lead to a large error. It is also seen that the error depends on the asymptotic bias and variance of the noise-to-signal ratio estimator, the former being controlled by m_0 and the later by $\sqrt{n_0}$. Since m_0 and $\sqrt{n_0}$ are related by the equation $K = m_0 n_0 (p+1)$, this means that there is a tradeoff to find. It turns out that it is exactly when $\sqrt{n_0}$ and m_0 are proportional that the best rate of convergence can be achieved for the excess-of-variance.

To see this, take the term $(Cm_0^{-1} + \sigma V_K n_0^{-1/2})^2$ in the asymptotic expansion of Lemma 1. Assume $m_0 = n_0^{1/2+\beta}$, $-1/2 < \beta < \infty$, so that $\sqrt{n_0}/m_0$ goes to ∞ , 0 or 1 whether $\beta < 0$, $\beta > 0$ or $\beta = 0$. Since $m_0 n_0 (p+1) = K$, the taken term is written, up to a multiplicative constant,

$$\begin{cases} K^{-2/(3+2\beta)} (CK^{-2\beta/(3+2\beta)} + \sigma V_K)^2 & \text{if } \beta \geq 0, \\ K^{-2(1+2\beta)/(3+2\beta)} (C + \sigma V_K K^{2\beta/(3+2\beta)})^2 & \text{if } \beta \leq 0. \end{cases}$$

In both cases, the fastest rate of decrease toward zero is $K^{-2/3}$, attained for $\beta = 0$, meaning that m_0 is proportional to $\sqrt{n_0}$.

The above argument carries over to get the optimal rate for K . Let $K = T^\alpha$, $0 < \alpha \leq 1$. The rate $K^{-2/3}$ is then $T^{-2\alpha/3}$ and must be balanced with the term $K/(T-K) \sim T^{\alpha-1}$ in the asymptotic expansion. The sum of those two terms is

$$\begin{cases} T^{-2\alpha/3}(1 + T^{5\alpha/3-1}) & \text{if } 5\alpha/3 \leq 1, \\ T^{\alpha-1}(T^{-5\alpha/3+1} + 1) & \text{if } 5\alpha/3 \geq 1. \end{cases}$$

In both cases, the fastest rate of decrease is $T^{-2/5}$, attained for $\alpha = 3/5$.

These results are stated in Theorem 3, for which a formal proof is given in Appendix A.

Theorem 3. *Take $K = T^{3/5}$, $m_0 = T^{1/5}(p+1)^{-1/3}$ and $n_0 = T^{2/5}(p+1)^{-2/3}$. Then, under the assumptions of Lemma 1,*

$$T^{2/5}\widehat{E}_{K,m_0} \xrightarrow{d} \frac{v''(m^*)(p+1)^{2/3}(C + \sigma W)^2}{2v(m^*)},$$

where $W \sim N(0, 1)$. Moreover, if $|C| > 0$, then the rate $T^{2/5}$ is optimal: there exist no $\delta > 0$, $0 < \alpha \leq 1$, $-1/2 < \beta < \infty$ such that

$$T^{2/5+\delta}\widehat{E}_{K,m_0} = O_P(1)$$

with K proportional to T^α and m_0 proportional to $n_0^{1/2+\beta}$.

Theorem 3 give the answers to the questions raised at the beginning of this section, albeit in an asymptotic framework. Asymptotically, to get the best performance, the share of the budget to be spent in the first stage of Algorithm 2 should be of order $T^{3/5}$ and the number of repetitions of order $T^{1/5}$. This way, the excess-of-variance is guaranteed to vanish at the rate $T^{2/5}$, which is the optimal one.

Remark 1. *The coefficients α and β are not equally important. For instance, if $\beta \geq 0$ and $\alpha \geq 3/5$, the logarithm of the rate is of order $\log(T)(-2\alpha/(3+2\beta) + \alpha - 1)$. The gradient with respect to (α, β) at $(3/5, 0)$ is about $(1.67, -0.27)$. This means that a change in α is likely to have a greater effect on the performance than a change in β . In practice, this means that the choice of m_0 may not be important.*

5 Numerical illustrations

Two kinds of experiments are conducted.

In the direct experiments, the initial budget K is set to zero and various initial number of repetitions m_0 are tested. For each m_0 , the biases, variances and errors of the two kinds of sensitivity indices estimators are computed based on `nreplic` replications. This allows to see the effect of the number of repetitions on the sensitivity analysis.

In the calibration experiments, various calibration parameters (K, m_0) are tested to see their effect on the estimators. The results obtained can be compared with the results of the direct experiment.

Two models have been considered: the linear model with normal inputs and a randomized Ishigami model. These models have been chosen because the sensitivity indices are explicit and hence the performance of the estimators can easily be evaluated. For the linear model, the noise-to-signal ratio has been calculated in Appendix D.

5.1 Linear model

The model is of the form $Y = X_1 + \beta X_2 + \sigma Z$, where X_1, X_2, Z , are standard normal random variables and β, σ are real coefficients.

	2	5	10	20	40	$m_0 n_0$	40	20	10	5	2
3200	NA	0.25	0.28	0.23	0.24	NA	0.20	0.22	0.20	0.22	NA
1600	NA	0.16	0.16	0.11	NA	NA	NA	0.10	0.09	0.12	NA
800	0.16	0.15	0.09	0.08	NA	NA	NA	0.04	0.06	0.08	0.13
400	0.13	0.10	0.11	NA	NA	NA	NA	NA	0.08	0.08	0.08
200	0.11	0.11	0.10	NA	NA	NA	NA	NA	0.06	0.05	0.11
100	0.19	0.13	NA	NA	NA	NA	NA	NA	NA	0.05	0.08
50	0.18	0.08	NA	NA	NA	NA	NA	NA	NA	0.06	0.07

Table 1: MRE for various calibrations: $K/(p + 1) = 50, 100, 200, 400, 800, 1600, 3200$ and $m_0 = 2, 5, 10, 20, 40, \dots$. The greatest values depend on K and hence the values for n_0 have been given instead. For instance, for $K/(p + 1) = 200 = m_0 n_0$, the available MREs are for $m_0 = 2, 5, 10, 20, 40, 100$.

5.1.1 High noise context

Here $\beta = 1.2, \sigma = 4$, leading to a noise-to-signal ratio $m^* \approx 5.8$. The total budget is $T/(p + 1) = 4200$. The number of replication is 400.

The results of the direct experiment are given in Figure 1. While the squared bias of first kind is almost null, that of second kind is large for small m_0 . This is in accordance with Theorem 1, where it was noticed that the sensitivity estimators of the second kind suffer from a bias term that vanishes as $m_0 \rightarrow \infty$. The variances of both kinds are negligible with respect to the bias of second kind, which is the most important contributor to the MSE of second kind. In comparison, the MSE of first kind is quite small. The MRE is approximately convex with a peak at around 10 and increases linearly for large values of m_0 . This shape is that which was found in Proposition 1 for the upper bound, indicating that the bound is a good proxy for the MRE in this case. The MRE attains its minimum at $m_0 = 10$, close enough to 5.8, the number predicted by the theory.

The results of the calibration experiment is given in Table 1, Table 2 and Table 3. A heat-map in Figure 2 is given to help the reader to see the ‘‘spatial’’ pattern of the errors. We see that the lowest MREs, around 6-8%, are reached for m_0 of the same order or larger than n_0 and $K/(p + 1)$ less than 800, which is around 1/5 of the total budget. By comparing Table 1 with Figure 1 (c), we see that a MRE of 6-8% is close to the optimal performance. Happily, it appears that a large spectrum of calibration parameters $(K/(p + 1), m_0)$ yield low errors.

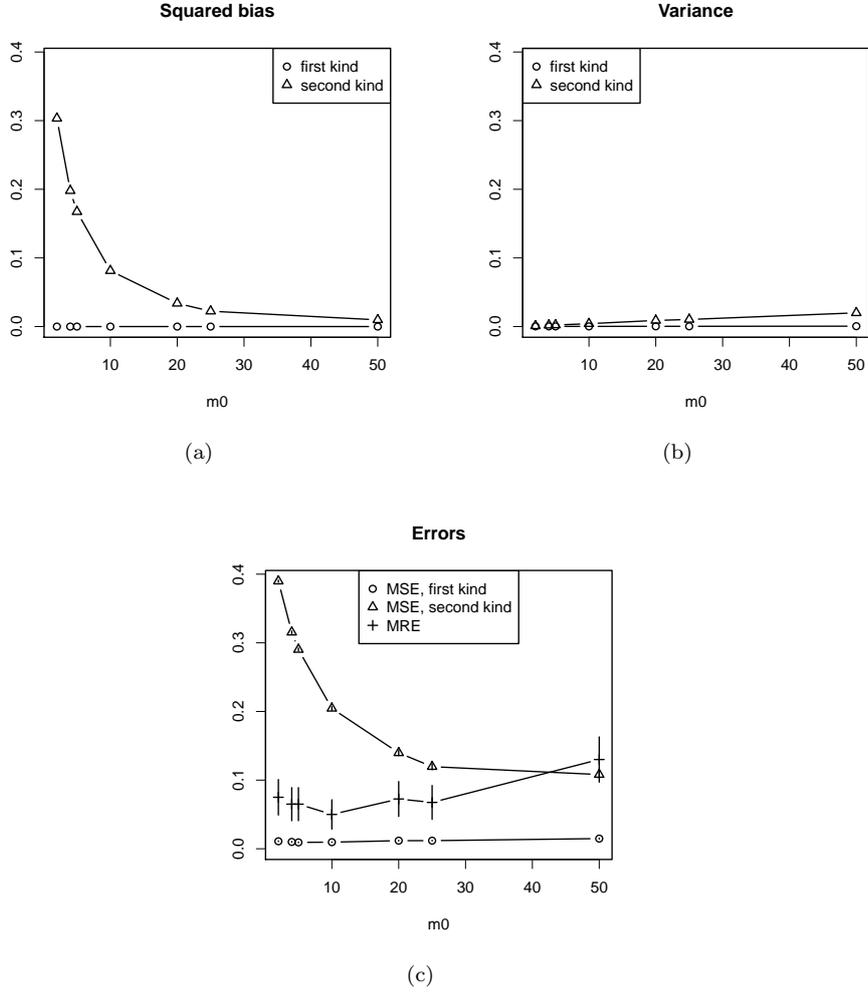


Figure 1: Sum of squared biases (a), sum of variances (b) and errors (c) of the sensitivity indices estimators. In (c) 95% confidence intervals were calculated.

	2	5	10	20	40	m_0	n_0	40	20	10	5	2
3200	NA	0.02	0.02	0.02	0.02	NA	NA	0.02	0.02	0.02	0.02	NA
1600	NA	0.01	0.01	0.01	0.01	NA	NA	NA	0.01	0.01	0.01	NA
800	0.01	0.01	0.01	0.01	0.01	NA	NA	NA	0.01	0.01	0.01	0.01
400	0.01	0.01	0.01	NA	NA	NA	NA	NA	NA	0.01	0.01	0.01
200	0.01	0.01	0.01	NA	NA	NA	NA	NA	NA	0.01	0.01	0.01
100	0.01	0.01	NA	NA	NA	NA	NA	NA	NA	NA	0.01	0.01
50	0.01	0.01	NA	NA	NA	NA	NA	NA	NA	NA	0.01	0.01

Table 2: MSE of the first kind for various calibrations. See Table 1 for the legend.

	2	5	10	20	40	:m0 n0:	40	20	10	5	2
3200	NA	0.39	0.39	0.32	0.32	NA	0.31	0.28	0.27	0.25	NA
1600	NA	0.40	0.39	0.32	NA	NA	NA	0.29	0.27	0.25	NA
800	0.44	0.40	0.39	0.33	NA	NA	NA	0.31	0.28	0.25	0.20
400	0.44	0.40	0.39	NA	NA	NA	NA	NA	0.30	0.27	0.21
200	0.44	0.41	0.38	NA	NA	NA	NA	NA	0.33	0.29	0.21
100	0.44	0.40	NA	NA	NA	NA	NA	NA	NA	0.32	0.24
50	0.44	0.40	NA	NA	NA	NA	NA	NA	NA	0.36	0.26

Table 3: MSE of the second kind for various calibrations. See Table 1 for the legend.

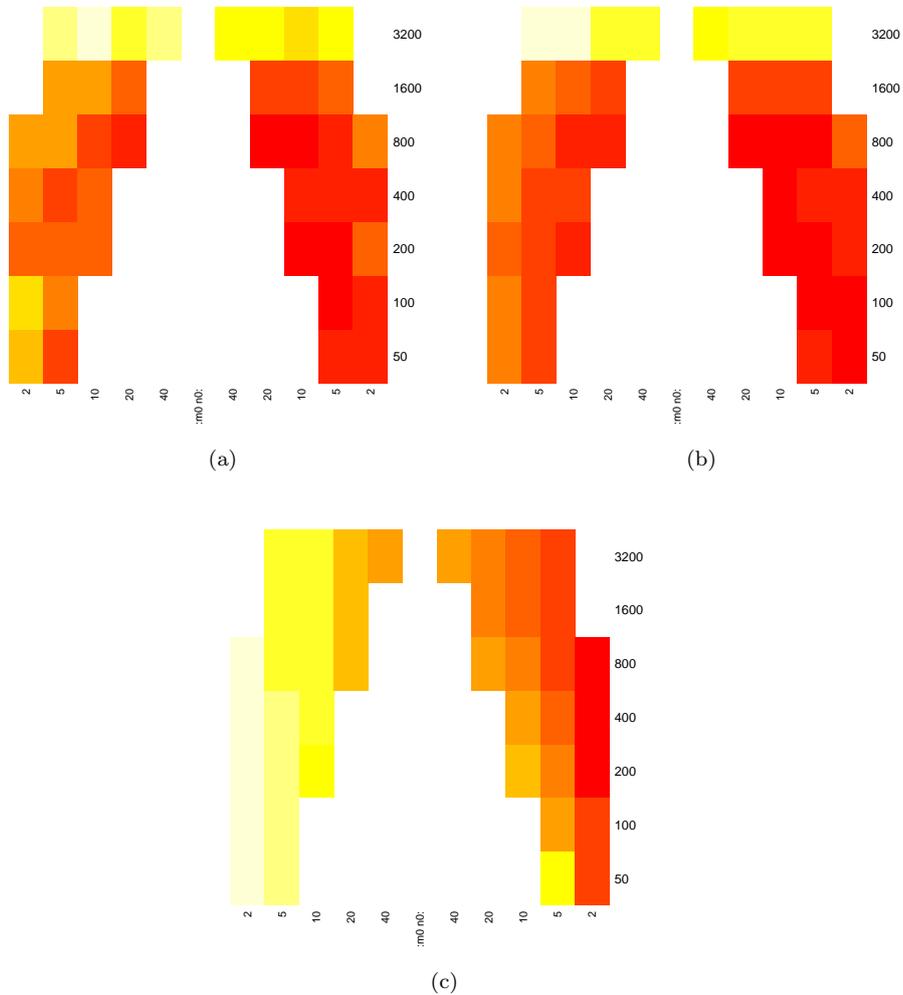


Figure 2: Heat-map corresponding to Table 1, Table 2 and Table 3.

5.1.2 Low noise context

Here $\beta = 1.2, \sigma = 0.9$, leading to a noise-to-signal ratio $m^* = 1$. The total budget is $T/(p+1) = 500$. The number of replication is 200.

The results for the squared biases, the variances and the errors are given in Figure 3. The squared biases of both kinds are negligible with respect to the variances, which contribute the most to the MSE of both kinds. The MRE is small when m_0 is small and its optimal value is reached for the smallest m_0 . This agrees with the calculated value $m^* = 1$.

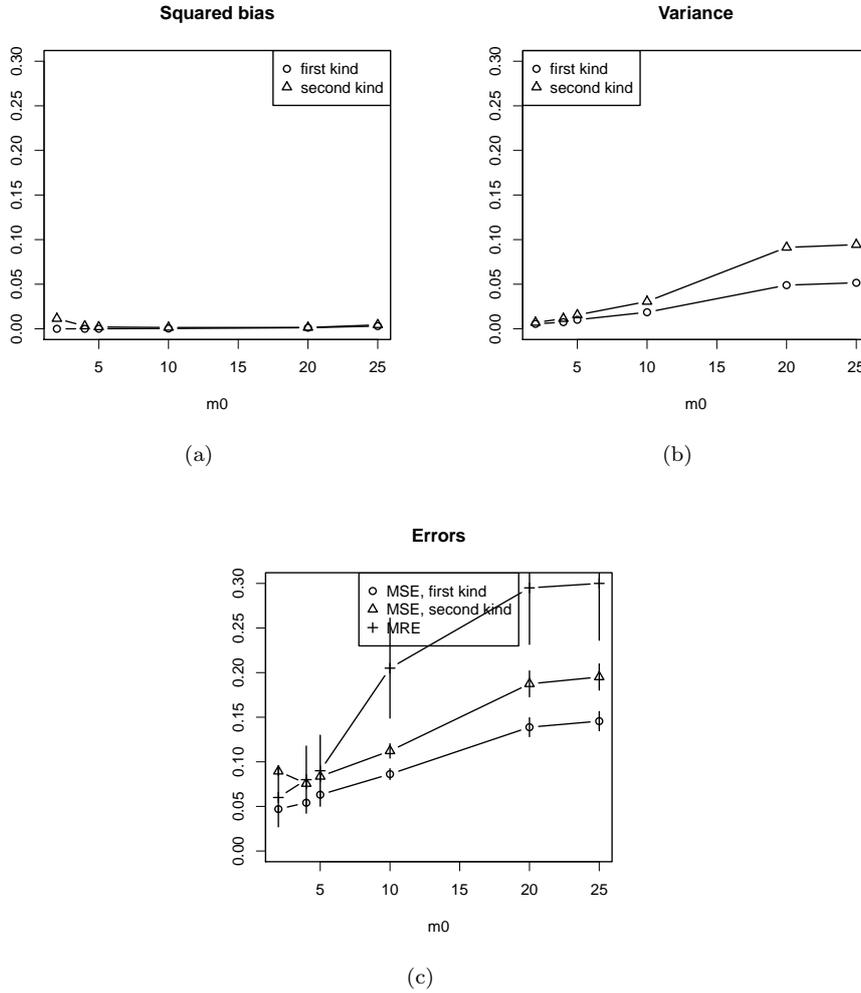


Figure 3: Sum of squared biases (a), sum of variances (b) and errors (c) of the sensitivity indices estimators. In (c) 95% confidence intervals were calculated.

The results of the calibration experiment is given in Table 4, Table 5 and Table 6. A heat-map in Figure 4 is given to help the reader to see the “spatial” pattern of the errors. Let us look at the MREs. As in the high-noise context, a large spectrum of calibration parameters ($K/(p+1), m_0$) yield low errors, of

	2	5	10	20	:m0 n0:	20	10	5	2
400	0.18	0.14	0.20	NA	NA	NA	0.20	0.20	0.18
200	0.03	0.02	0.04	NA	NA	NA	0.04	0.06	0.06
100	0.06	0.02	NA	NA	NA	NA	NA	0.04	0.04
50	0.02	0.01	NA	NA	NA	NA	NA	0.02	0.04
25	NA	NA	NA	NA	NA	NA	NA	NA	NA

Table 4: MRE for various calibrations.

	2	5	10	20	:m0 n0:	20	10	5	2
400	0.09	0.08	0.08	NA	NA	NA	0.09	0.08	0.11
200	0.05	0.05	0.04	NA	NA	NA	0.05	0.04	0.06
100	0.04	0.04	NA	NA	NA	NA	NA	0.04	0.05
50	0.04	0.04	NA	NA	NA	NA	NA	0.04	0.04
25	NA	NA	NA	NA	NA	NA	NA	NA	NA

Table 5: MSE of the first kind for various calibrations.

order 1-6% for $K/(p+1) \leq 200$. This is close to the optimal performance in Figure 3 (c).

	2	5	10	20	:m0 n0:	20	10	5	2
400	0.15	0.15	0.15	NA	NA	NA	0.16	0.16	0.98
200	0.14	0.14	0.13	NA	NA	NA	0.13	0.13	0.13
100	0.14	0.13	NA	NA	NA	NA	NA	0.13	0.13
50	0.13	0.13	NA	NA	NA	NA	NA	0.13	0.12
25	NA	NA	NA	NA	NA	NA	NA	NA	NA

Table 6: MSE of the second kind for various calibrations.

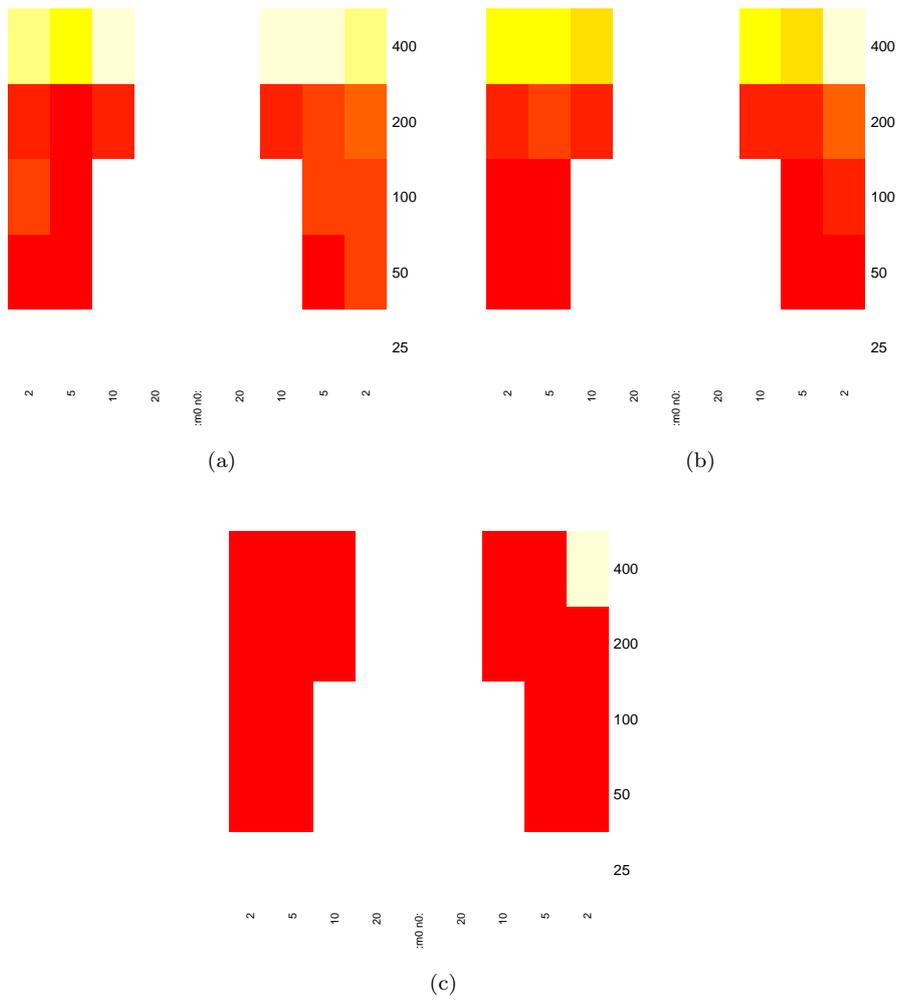


Figure 4: Heat-map corresponding to Table 4, Table 5 and Table 6.

5.2 The Ishigami model

The model is $Y = \sin(X_1) + \beta \sin(X_2)^2 + \sigma Z^4 \sin(X_1)$, where $\beta = 7$, $\sigma = 0.1$, $X_1, X_2, Z \sim \mathcal{U}(-\pi, \pi)$. This is the Ishigami model, a benchmark model in the sensitivity analysis literature [6, 12]. The total budget is $T/(p+1) = 500$ and the number of replications is `nreplic` = 200.

The results of the direct experiment are given in Figure 5. The plots are similar to the linear model in the low noise context: the bias is negligible with respect to the variance which increases as m_0 increases. The MSEs and the MRE follow the same pattern as the variances. Since the Ishigami is nonlinear, the noise-to-signal ratio is cumbersome to calculate explicitly but Figure 5 (c) suggests it must be one or two.

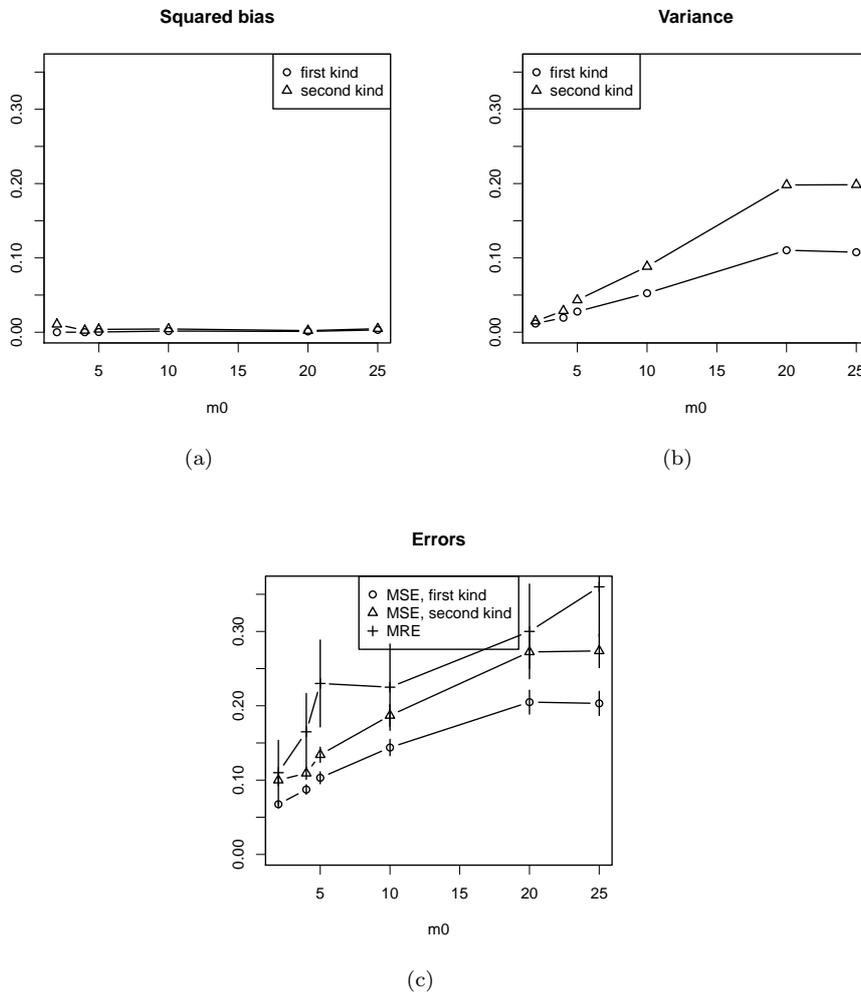


Figure 5: Sum of squared biases (a), sum of variances (b) and errors (c) of the sensitivity indices estimators. In (c) 95% confidence intervals were calculated.

The results of the calibration experiment are given in Table 7, Table 8 and

	2	5	10	20	m_0	n_0	20	10	5	2
400	0.20	0.28	0.22	NA	NA	NA	NA	0.28	0.26	0.24
200	0.14	0.10	0.11	NA	NA	NA	NA	0.12	0.11	0.12
100	0.08	0.12	NA	NA	NA	NA	NA	NA	0.10	0.11
50	0.07	0.04	NA	NA	NA	NA	NA	NA	0.08	0.06
25	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA

Table 7: MRE for various calibrations.

	2	5	10	20	m_0	n_0	20	10	5	2
400	0.13	0.12	0.12	NA	NA	NA	NA	0.13	0.12	0.13
200	0.07	0.08	0.07	NA	NA	NA	NA	0.07	0.07	0.08
100	0.06	0.06	NA	NA	NA	NA	NA	NA	0.06	0.07
50	0.06	0.06	NA	NA	NA	NA	NA	NA	0.06	0.06
25	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA

Table 8: MSE of the first kind for various calibrations.

Table 9. A heat-map is given in Figure 6 to see the “spatial” pattern of the errors. For the MRE, $K/(p + 1) = 50$ yields the lowest errors, of order 4-8%. As seen in Figure 5 (c), this corresponds to the optimal performance.

5.3 Summary of the numerical experiments

It was confirmed that the sensitivity estimators of the second kind, that arising from the attempt to smooth out the output of the computer model, are biased, especially in a high noise when the number of repetitions is small. The variance tends to increase when the number of repetitions increases because, since the budget is fixed, this means that the number of explorations decreases. It was observed two behaviors for the MRE curves: it is an increasing function of the number of repetitions when the model has low noise and it has a U shape when the model is noisy. The minimum was attained near the values predicted by the theory and yielded near optimal performance. The Ishigami model appears to be close to the linear model with low noise in that the MRE exhibit the same behavior in both cases. The two-stage procedure of Section 4 seems to be robust to the choice of the calibration parameters. Indeed, many values of K and m_0 yielded a performance close to the optimum. This is in agreement with Remark 1.

	2	5	10	20	m_0	n_0	20	10	5	2
400	0.17	0.17	0.17	NA	NA	NA	NA	0.17	0.17	0.17
200	0.13	0.14	0.14	NA	NA	NA	NA	0.14	0.14	0.13
100	0.14	0.13	NA	NA	NA	NA	NA	NA	0.14	0.13
50	0.13	0.13	NA	NA	NA	NA	NA	NA	0.14	0.13
25	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA

Table 9: MSE of the second kind for various calibrations.

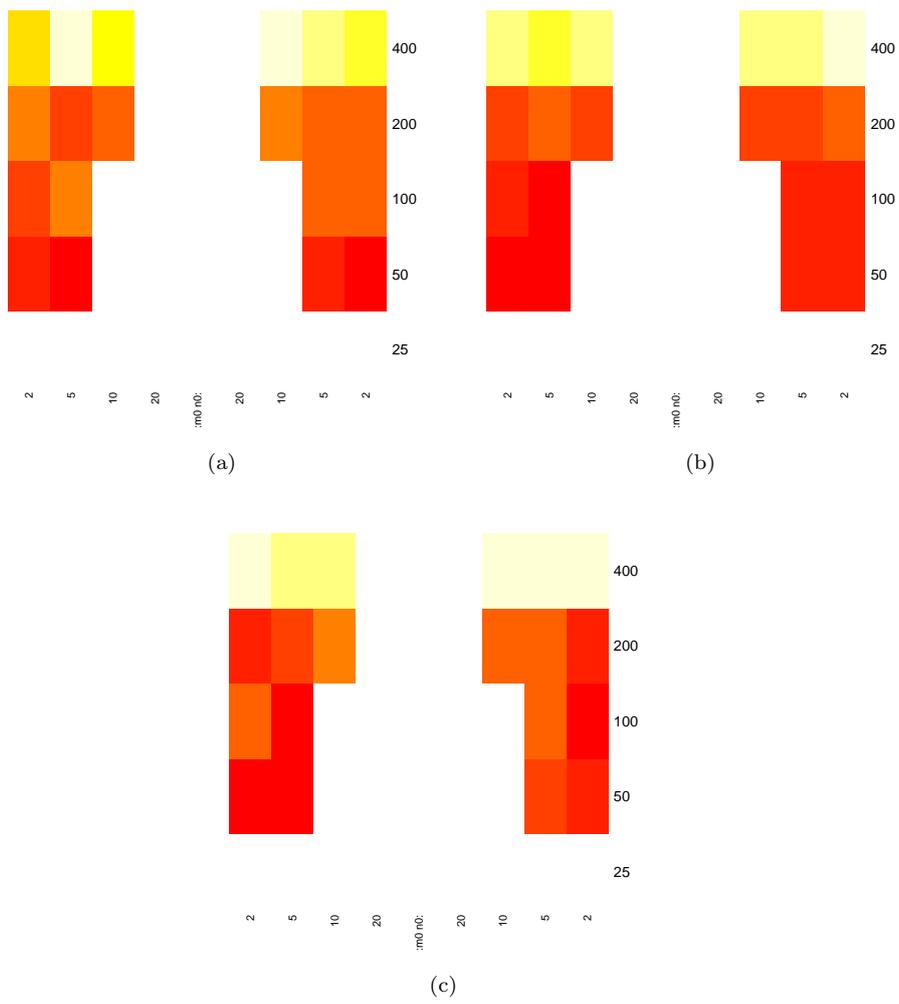


Figure 6: Heat-map corresponding to Table 7, Table 8 and Table 9.

6 Discussion

We have considered two sensitivity indices for stochastic models. Asymptotic normality of the estimators, which depend both on the number of explorations and the number of repetitions, has been established, and it was noticed that the second kind, that which arises from smoothing out the computer model, suffers from a bias term which vanishes only when the number of repetitions goes to infinity.

Assuming a fixed computing budget, a definition of the optimal number of repetitions has been proposed and an estimator has been built. The optimal number of repetitions minimizes an upper-bound of the MRE, and this has been exploited in a two-stage procedure to efficiently estimate the sensitivity indices. The procedure is simple: in the first stage the optimal number of repetitions is estimated and plugged into the sensitivity estimators in the second stage.

Although a share of the total budget must be sacrificed in the first stage, we have shown that the proposed procedure is asymptotically oracle, that is, performs as well as the hypothetical procedure in which the optimal number of repetitions would be known. The optimal convergence rates have been given. To test the procedure, simulation experiments were conducted, where the bias of the sensitivity estimator of the second kind was confirmed. The two-stage procedure appeared to be robust to the choice of the tuning parameters K and m_0 and yielded a performance close to the optimum.

Research questions remain open. First, the sensitivity estimators of the two stages could be aggregated to build estimators with a lower variance. Second, higher-order Sobol indices could be studied in the light of the theory introduced in this paper. Third, it would be interesting to look for other optimality criteria or Monte-Carlo sampling schemes. Finally, the obtained results could be extended to the multivariate case, that in which the output is a multivariate vector.

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A Proofs

Proof of Theorem 1

The proof is based on the results in Appendix B. The Sobol estimators in (5) and (6) are made of empirical averages of the form (20) and (21) with $L = 2$ and coefficients

$$\xi_{1;m,i}^{\text{UL}} \simeq \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \end{pmatrix}, \dots, \xi_{p;m,i}^{\text{UL}} \simeq \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 1 \end{pmatrix}$$

for the upper left (UL) terms,

$$\xi_{m,i}^{\text{UR}} \simeq \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \end{pmatrix}$$

for the upper right (UR) term,

$$\xi_{m,i}^{\prime\text{LL}} \simeq \begin{pmatrix} 2 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \end{pmatrix}$$

for the lower left (LL) term of $\widehat{S}_{j;n,m}'$ and

$$\xi_{m,i}^{\prime\prime\text{LL}} \simeq \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 1 & 0 & \cdots & 0 \end{pmatrix}$$

for the lower left (LL) term of $\widehat{S}_{j;n,m}''$ (see Appendix B). Therefore, denoting by

$$\boldsymbol{\xi}_{m,i} := (\xi_{1;m,i}^{\text{UL}}, \dots, \xi_{p;m,i}^{\text{UL}}, \xi_{m,i}^{\text{UR}}, \xi_{m,i}^{\prime\text{LL}}, \xi_{m,i}^{\prime\prime\text{LL}})$$

the corresponding summands, Lemma 3 in Appendix B yields

$$\sqrt{n} \left(\frac{1}{n} \sum_{i=1}^n \boldsymbol{\xi}_{m,i} - \mathbb{E} \boldsymbol{\xi}_{m,1} \right) \xrightarrow{d} N(0, \Sigma_m),$$

for some nonnegative matrix Σ_m of size $p+3$, where the expectation is given by

$$\mathbb{E} \boldsymbol{\xi}_{m,1} = \begin{pmatrix} \mathbb{E} \mathbb{E}[f(X, Z)|X] \mathbb{E}[f(\widetilde{X}_{-1}, Z)|\widetilde{X}_{-1}] \\ \vdots \\ \mathbb{E} \mathbb{E}[f(X, Z)|X] \mathbb{E}[f(\widetilde{X}_{-p}, Z)|\widetilde{X}_{-p}] \\ \mathbb{E} f(X, Z) \\ \mathbb{E} f(X, Z)^2 \\ \mathbb{E} \mathbb{E}[f(X, Z)|X]^2 + \frac{\mathbb{E} \text{Var}[f(X, Z)|X]}{m} \end{pmatrix}.$$

(Some calculations are carried out in Appendix C.) Define the function

$$s(x_1, \dots, x_p, x_{p+1}, x_{p+2}, x_{p+3}) = \left(\frac{x_1 - x_{p+1}^2}{x_{p+2} - x_{p+1}^2}, \dots, \frac{x_p - x_{p+1}^2}{x_{p+2} - x_{p+1}^2}, \frac{x_1 - x_{p+1}^2}{x_{p+3} - x_{p+1}^2}, \dots, \frac{x_p - x_{p+1}^2}{x_{p+3} - x_{p+1}^2} \right).$$

Then clearly

$$s(n^{-1} \sum_{i=1}^n \boldsymbol{\xi}_{m,i}) = \begin{pmatrix} \widehat{\mathbf{S}}'_{m,n} \\ \widehat{\mathbf{S}}''_{m,n} \end{pmatrix}$$

and

$$s(\mathbb{E} \boldsymbol{\xi}_{m,1}) = \begin{pmatrix} \mathbf{S}' \\ \mathbf{S}'' \left[1 - \frac{\mathbb{E} \text{Var}[f(X,Z)|X]}{\mathbb{E} \text{Var}[f(X,Z)|X] + m \text{Var} \mathbb{E}[f(X,Z)|X]} \right] \end{pmatrix}.$$

The result follows by the delta-method.

If $m = m_n \rightarrow \infty$, Lemma 3 still holds with the variance-covariance matrix replaced by its limit.

Proof of Proposition 1

Assume without loss of generality that $D_1 < \dots < D_p$. We first prove the following Lemma. For convenience, the subscripts n and m are left out.

Lemma 2. *Let $i < j$. Then*

$$P(\widehat{D}_i - \widehat{D}_j \geq 0) \leq \frac{\text{Var} \widehat{D}_i + \text{Var} \widehat{D}_j}{\frac{1}{2}|D_i - D_j|^2}.$$

Proof. We have

$$\begin{aligned} P(\widehat{D}_i - \widehat{D}_j \geq 0) &\leq P(|\widehat{D}_i - D_i| + |\widehat{D}_j - D_j| \geq D_j - D_i) \\ &\leq P(|\widehat{D}_i - D_i|^2 + |\widehat{D}_j - D_j|^2 \geq \frac{1}{2}|D_j - D_i|^2) \end{aligned}$$

and the claim follows from Markov's inequality.

We now prove Proposition 1. Recall that $D_1 < \dots < D_p$. We have

$$\begin{aligned} \sum_{i=1}^p \mathbb{E} |\widehat{R}_i - R_i| &= \sum_{i=1}^p \sum_{j=1}^p \mathbb{E} |\mathbf{1}(\widehat{D}_j \leq \widehat{D}_i) - \mathbf{1}(D_j \leq D_i)| \\ &\leq \sum_{i=1}^p \sum_{j \neq i} \frac{\text{Var} \widehat{D}_i + \text{Var} \widehat{D}_j}{\frac{1}{2}|D_i - D_j|^2} \\ &\leq \frac{2(p-1)(p+1)}{\min_{j < j'} |D_j - D_{j'}|^2} \sum_{i=1}^p \text{Var} \widehat{D}_i, \end{aligned}$$

where the first inequality holds by Lemma 2 and because

$$\mathbb{E} |\mathbf{1}(\widehat{D}_j \leq \widehat{D}_i) - \mathbf{1}(D_j \leq D_i)| = \begin{cases} \mathbb{E} |\mathbf{1}(\widehat{D}_j > \widehat{D}_i)| & \text{if } j < i, \\ 0 & \text{if } j = i, \\ \mathbb{E} |\mathbf{1}(\widehat{D}_j \leq \widehat{D}_i)| & \text{if } j > i. \end{cases}$$

It remains to calculate the variances. But this is done in Lemma 6 in Appendix C, where it is found that

$$\begin{aligned} \text{Var} \widehat{D}_j &= \frac{1}{n} \{ \text{Var} \mathbb{E}[Y_0 Y_j | \mathbf{X}] + \frac{1}{m} (\mathbb{E} \text{Var}[Y_0 Y_j | \mathbf{X}] - \text{Var}[Y_0 | \mathbf{X}] \text{Var}[Y_j | \mathbf{X}]) \\ &\quad + \frac{1}{m^2} \mathbb{E} \text{Var}[Y_0 | \mathbf{X}] \text{Var}[Y_j | \mathbf{X}] \}. \end{aligned}$$

Proof of Proposition 2

Denote by $f(m)$ the upper-bound in Proposition 1. By convexity of the function f , if $m^* \leq 1$, then $f(1) \leq f(m)$ for all (compatible) integers m and hence $m^\dagger = 1$. Likewise, if $m^* \geq T/(p+1)$, then $f(T/(p+1)) \leq f(m)$ for all m and hence $m^\dagger = T/(p+1)$. For (iii), note that m^\dagger must be either $\lfloor m \rfloor^*$ or $\lceil m \rceil^*$. Since $\lfloor m \rfloor^* \leq \lceil m \rceil^*$, $f(\lfloor m \rfloor^*) \geq f(\lceil m \rceil^*)$ is equivalent to $\lfloor m \rfloor^* \lceil m \rceil^* \leq m^{*2}$.

Proof of Theorem 2

We want to show

$$\sqrt{n} \left(\sqrt{\frac{\sum_{j=1}^p \widehat{\zeta}_{3,j}}{\sum_{j=1}^p \widehat{\zeta}_{1,j}}} - \left[m^* + \frac{C}{m} + o\left(\frac{1}{m}\right) \right] \right) \rightarrow N(0, \sigma^2),$$

for some C and $\sigma \geq 0$, as $n \rightarrow \infty$, $m = m_n \rightarrow \infty$. In view of (9)–(14), the estimators $\widehat{\zeta}_{3,j}$ and $\widehat{\zeta}_{1,j}$ can be expressed in terms of estimators of the form (20) and (21), namely,

$$\begin{aligned} \widehat{\zeta}_{3,j} &= \frac{1}{n} \sum_{i=1}^n \xi_{j;m,i}^{(9)} + \xi_{j;m,i}^{(10)} - \xi_{j;m,i}^{(11)} - \xi_{j;m,i}^{(12)}, \quad \text{and,} \\ \widehat{\zeta}_{1,j} &= \frac{1}{n} \sum_{i=1}^n \xi_{j;m,i}^{(13)} - \left(\frac{1}{n} \sum_{i=1}^n \xi_{j;m,i}^{(14)} \right)^2, \end{aligned}$$

where $\xi_{j;m,i}^{(e)}$, $j = 1, \dots, p$, $e = 9, \dots, 14$, are all of the form (21), that is, they are all elements of the set $\mathcal{E}_{m,i}(4)$, introduced in Appendix B. Their coefficients are given by

$$\widehat{\xi}_{j;m,i}^{(9)} \simeq \begin{pmatrix} 2 & 0 \\ 0 & 2 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \widehat{\xi}_{j;m,i}^{(10)} \simeq \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{pmatrix}, \widehat{\xi}_{j;m,i}^{(11)} \simeq \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 2 \\ 0 & 0 \end{pmatrix}, \widehat{\xi}_{j;m,i}^{(12)} \simeq \begin{pmatrix} 2 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 0 \end{pmatrix},$$

and

$$\widehat{\xi}_{j;m,i}^{(13)} \simeq \begin{pmatrix} 1 & 1 \\ 1 & 1 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \widehat{\xi}_{j;m,i}^{(14)} \simeq \begin{pmatrix} 1 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

Stack all the estimators in a vector $\boldsymbol{\xi}_{m,i}$ of size $6p$, that is, $\boldsymbol{\xi}_{m,i} = (\boldsymbol{\xi}_{1;m,i}^\top, \dots, \boldsymbol{\xi}_{p;m,i}^\top)^\top$, where $\boldsymbol{\xi}_{j;m,i} = (\xi_{j;m,i}^{(9)}, \dots, \xi_{j;m,i}^{(14)})^\top$ for $j = 1, \dots, p$. Let $\bar{\boldsymbol{\xi}} = n^{-1} \sum_{i=1}^n \boldsymbol{\xi}_{m,i}$. Since, for each element of $\mathcal{E}_{m,i}(4)$, the sum of the coefficients is less than four, the condition in Lemma 3 in Appendix B is fulfilled because we assumed $f(X, Z) \leq F(X)$ with $E F(X)^8 < \infty$. Therefore,

$$\sqrt{n}(\bar{\boldsymbol{\xi}} - E \boldsymbol{\xi}_{m,1}) \rightarrow N(0, \Sigma),$$

for some variance-covariance matrix Σ of size $6p \times 6p$. A delta-method will yield the result. Let $\mathbf{x}_j = (x_j^{(9)}, \dots, x_j^{(14)})$, $j = 1, \dots, p$, and

$$s(\mathbf{x}_1, \dots, \mathbf{x}_p) = \sqrt{\frac{\sum_{j=1}^p x_j^{(9)} + x_j^{(10)} - x_j^{(11)} - x_j^{(12)}}{\sum_{j=1}^p x_j^{(13)} - x_j^{(14)2}}},$$

so that $s(\bar{\boldsymbol{\xi}}) = \hat{m}^*$. Denote $\mathbb{E} \boldsymbol{\xi}_{m,1}$ by $\boldsymbol{\theta}_m$ for simplicity. A Taylor expansion of s around $\mathbb{E} \boldsymbol{\xi}_{m,1}$ yields

$$\sqrt{n}(\hat{m}^* - s(\boldsymbol{\theta}_m)) = \sqrt{n}(\bar{\boldsymbol{\xi}} - \boldsymbol{\theta}_m)^\top \dot{s}(\boldsymbol{\theta}_m) + \frac{1}{2}(\bar{\boldsymbol{\xi}} - \boldsymbol{\theta}_m)^\top \ddot{s}_{n,m} \sqrt{n}(\bar{\boldsymbol{\xi}} - \boldsymbol{\theta}_m),$$

where $\ddot{s}_{n,m}$ is the Hessian matrix of s at a point between $\bar{\boldsymbol{\xi}}$ and $\boldsymbol{\theta}_m$. The second order term is $o_P(1)$ by Cauchy-Schwartz's inequality, the continuity of \ddot{s} , and the fact that $\sqrt{n}(\bar{\boldsymbol{\xi}} - \boldsymbol{\theta}_m) = O_P(1)$. By Proposition 3 in Appendix B, there exists $\boldsymbol{\theta}$ such that $\boldsymbol{\theta}_m \rightarrow \boldsymbol{\theta}$ and hence the first order term goes to $N(0, \dot{s}^\top \Sigma \dot{s})$, where \dot{s} is the gradient of s at $\boldsymbol{\theta}$.

The image of $\boldsymbol{\theta}_m$ by s is not m^* but the discrepancy can be controlled when $m \rightarrow \infty$. Elementary calculations show that

$$\mathbb{E} \boldsymbol{\xi}_{j;m,1} = \mathbb{E} \underbrace{\begin{pmatrix} Y_0^{(1,1)2} Y_j^{(1,1)2} \\ Y_0^{(1,1)} Y_0^{(1,2)} Y_j^{(1,1)} Y_j^{(1,2)} \\ Y_0^{(1,1)} Y_0^{(1,2)} Y_j^{(1,1)2} \\ Y_j^{(1,1)} Y_j^{(1,2)} Y_0^{(1,1)2} \\ Y_0^{(1,1)} Y_0^{(1,2)} Y_j^{(1,1)} Y_j^{(1,2)} \\ Y_j^{(1,1)} Y_0^{(1,1)} \end{pmatrix}}_{\boldsymbol{\theta}_j} + \frac{\mathbf{C}_j}{m} + o\left(\frac{1}{m}\right)$$

for some constant $\mathbf{C}_j \in \mathbf{R}^p$. It can be checked that $s(\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_p) = m^*$. Thus, for some constant C ,

$$\begin{aligned} \sqrt{n}(\hat{m}^* - s(\boldsymbol{\theta}_m)) &= \sqrt{n}(\hat{m}^* - s(\boldsymbol{\theta})) - (\boldsymbol{\theta}_m - \boldsymbol{\theta})^\top \dot{s} + o(\|\boldsymbol{\theta}_m - \boldsymbol{\theta}\|) \\ &= \sqrt{n}(\hat{m}^* - [m^* + C/m + o(1/m)]), \end{aligned}$$

and hence the proof is complete with $\sigma^2 = \dot{s}^\top \Sigma \dot{s}$.

Proof of Corollary 2

With the same notations as those of the proof of Theorem 2, if $\sqrt{n}/m \rightarrow 0$, then $\sqrt{n}(\hat{m}^* - m^*) = \sqrt{n}(\hat{m}^* - s(\boldsymbol{\theta}_m)) + O(\sqrt{n}/m) \rightarrow N(0, \sigma^2)$. The proof is complete.

Proof of Lemma 1

Denote $m^* + (C + o(1))/m_0$ by m_K^* . We have the following Taylor expansions:

$$(16) \quad v(m_K^*) = v(m^*) + \frac{1}{2}(m_K^* - m^*)^2 v''(\bar{m}_K^*),$$

$$(17) \quad v(\hat{m}_K^*) = v(m_K^*) + (\hat{m}_K^* - m_K^*) v'(m_K^*) + \frac{1}{2}(\hat{m}_K^* - m_K^*)^2 v''(\tilde{m}_K^*),$$

where \tilde{m}_K^* is between \hat{m}_K^* and m_K^* , \bar{m}_K^* is between m_K^* and m^* . By using (17), we get

$$(18) \quad \hat{E}_K = E_K + \frac{(\hat{m}_K^* - m_K^*)v'(m_K^*)T}{(T - K)v(m^*)} + \frac{(\hat{m}_K^* - m_K^*)^2 v''(\tilde{m}_K^*)T}{2(T - K)v(m^*)},$$

where

$$E_K = \frac{\frac{1}{T-K}v(m_K^*) - \frac{1}{T}v(m^*)}{\frac{1}{T}v(m^*)}.$$

Let us find asymptotic expansions for the three terms in the right-hand side of (18). Since v'' is continuous, \tilde{m}_K^* goes to m^* in probability and $T/(T - K) \rightarrow c + 1$ as $n_0 \rightarrow \infty$ and $m_0 \rightarrow \infty$, the third term satisfies

$$\frac{(\hat{m}_K^* - m_K^*)^2 v''(\tilde{m}_K^*)T}{2(T - K)v(m^*)} = \frac{(c + 1)\sigma^2 V_K^2 v''(m^*)}{2v(m^*)n_0} + o_P\left(\frac{1}{n_0}\right).$$

For the second term, use Taylor's expansion of v' at m^* to get

$$\frac{(\hat{m}_K^* - m_K^*)v'(m_K^*)T}{(T - K)v(m^*)} = \frac{(c + 1)Cv''(m^*)\sigma V_K}{v(m^*)m_0\sqrt{n_0}} + o_P\left(\frac{1}{m_0\sqrt{n_0}}\right).$$

Finally, using (16), we get

$$\begin{aligned} E_K &= \frac{T[v(m_K^*) - v(m^*)] + Kv(m^*)}{(T - K)v(m^*)} \\ &= \frac{Tv''(\bar{m}_K)(m_K^* - m^*)^2}{2(T - K)v(m^*)} + \frac{K}{T - K} \\ &= \frac{(c + 1)v''(m^*)C^2}{2v(m^*)m_0^2} + \frac{K}{T - K} + o_P\left(\frac{1}{m_0^2}\right). \end{aligned}$$

The proof is complete.

Proof of Theorem 3

With the given choice for K , m_0 and n_0 , the rates m_0^{-2} , $m_0^{-1}n_0^{-1/2}$ and n_0^{-1} are all equal to $T^{-2/5}(p + 1)^{2/3}$. The formula in Lemma 1 simplifies to

$$\begin{aligned} T^{2/5}\hat{E}_{K,m_0} &= \frac{v''(m^*)(p + 1)^{2/3}(C + \sigma V_K)^2}{2v(m^*)} + o_P(1) \\ &\xrightarrow{d} \frac{v''(m^*)(p + 1)^{2/3}(C + \sigma W)^2}{2v(m^*)}, \end{aligned}$$

where $W \sim N(0, 1)$. The proof of the first statement is complete.

Let us prove by contradiction that the rate $T^{2/5}$ is optimal. Suppose there are $\delta > 0$, $0 < \alpha \leq 1$ and $-1/2 < \beta < \infty$ such that

$$T^{2/5+\delta}\hat{E}_{K,m_0} = O_P(1)$$

with $K \propto T^\alpha$ and $m_0 \propto n_0^{1/2+\beta}$, where \propto denotes proportionality. There are three cases to consider: $\sqrt{n_0}/m_0 \rightarrow c' > 0$, $\sqrt{n_0}/m_0 \rightarrow 0$ or $\sqrt{n_0}/m_0 \rightarrow \infty$.

Note that K/T must converge, and recall that the limit is denoted by $c/(c+1) \geq 0$. Note also that

$$m_0^2 \propto T^{\frac{2\alpha(1+2\beta)}{3+2\beta}}, m_0\sqrt{n_0} \propto T^{2\alpha(1+\beta)/(3+2\beta)} \quad \text{and} \quad n_0 \propto T^{2\alpha/(3+2\beta)}.$$

Put $A = (c+1)v''(m^*)/v(m^*)$.

If $\sqrt{n_0}/m_0 \rightarrow c' > 0$ then $\beta = 0$ and, by Lemma 1, we have

$$(19) \quad T^{2/5+\delta} \widehat{E}_{K,m_0} = \frac{T^{2/5+\delta}}{m_0\sqrt{n_0}} U_K^2 + \frac{T^{2/5+\delta} K}{T-K},$$

where (U_K^2) is sequence of random variables such that

$$U_K^2 \xrightarrow{d} \frac{A}{2} \left(\sqrt{c'} C + \frac{1}{\sqrt{c'}} \sigma W \right)^2,$$

for some $W \sim N(0,1)$. Since both terms in the right hand side of (19) are positive and U_K^2 goes to a positive random variable, we must have

$$\frac{2}{5} + \delta - \frac{2\alpha(1+\beta)}{3+2\beta} \leq 0 \quad \text{and} \quad \frac{2}{5} + \delta + \alpha - 1 \leq 0.$$

But this leads to a contradiction because the first inequality implies that the second is false.

If $\sqrt{n_0}/m_0 \rightarrow 0$, then $\beta > 0$ and

$$T^{2/5+\delta} \widehat{E}_{K,m_0} = \frac{T^{2/5+\delta}}{n_0} U_K^2 + T^{2/5+\delta} \frac{K}{T-K}$$

with

$$U_K^2 \xrightarrow{d} \frac{A\sigma^2 W^2}{2}.$$

We proceed as before. We must have

$$\frac{2}{5} + \delta - \frac{2\alpha}{3+2\beta} \leq 0 \quad \text{and} \quad \frac{2}{5} + \delta + \alpha - 1 \leq 0.$$

But the first inequality implies that the second is false.

If $\sqrt{n_0}/m_0 \rightarrow \infty$, then $-1/2 < \beta < 0$ and

$$T^{2/5+\delta} \widehat{E}_{K,m_0} = \frac{T^{2/5+\delta}}{m_0^2} U_K^2 + T^{2/5+\delta} \frac{K}{T-K}$$

with

$$U_K^2 \xrightarrow{d} \frac{AC^2}{2}.$$

Again, we must have

$$\frac{2}{5} + \delta - \frac{2\alpha(1+2\beta)}{(3+2\beta)} \leq 0 \quad \text{and} \quad \frac{2}{5} + \delta + \alpha - 1 \leq 0,$$

where the first inequality implies the second is false. The proof of the second statement is complete.

B A unified treatment of the asymptotics

All estimators in this paper have a common form, given by

$$(20) \quad \frac{1}{n} \sum_{i=1}^n \xi_{m,i},$$

with

$$(21) \quad \xi_{m,i} = \prod_{l=1}^L \frac{1}{m} \sum_{k=1}^m \prod_{j=0}^p Y_j^{(i,k)b_{j;l}},$$

where $Y_0^{(i,k)} = Y^{(i,k)} = f(X^{(i)}, Z_0^{(i,k)})$, $Y_j^{(i,k)} = f(\tilde{X}_{-j}^{(i)}, Z_j^{(i,k)})$ for $j = 1, \dots, p$, and $b_{j;l}$, $j = 0, \dots, p$, $l = 1, \dots, L$, are nonnegative coefficients. The coefficients are arranged in a matrix $(b_{j;l})$ with L rows and $p+1$ columns, where $b_{j;l}$ is the element in the l th row and $(j+1)$ th column. This way, all estimators of the form (20) and (21), or, equivalently, all summands (21), can be identified with a matrix. For instance, we have

$$\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \frac{1}{m} \sum_{k'=1}^m Y_j^{(i,k')} \simeq \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \end{pmatrix},$$

where the non-null columns are the first and the $(j+1)$ th ones. This identity is reduced to

$$\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \frac{1}{m} \sum_{k'=1}^m Y_j^{(i,k')} \simeq \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

where it is implicitly understood that we have taken the first and $(j+1)$ th columns only, the remaining columns being zero. Note that the identification of an estimator to a matrix is done up to permutations between the rows. Thus, we also have

$$\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \frac{1}{m} \sum_{k'=1}^m Y_j^{(i,k')} \simeq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \simeq \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Proceeding the same way, we get

$$\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \simeq \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)2} \simeq \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}$$

and

$$\frac{1}{n} \sum_{i=1}^n \left(\frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \right)^2 \simeq \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}.$$

The above matrices can always be completed with rows full of zeros whenever the dimensions of the matrices need to match (mainly for comparison purposes).

For each n , the random variables $\xi_{m,1}, \dots, \xi_{m,n}$ are independent and identically distributed. Denote by $\mathcal{E}_{m,i}(L)$ the set of all summands (21). In other words, $\mathcal{E}_{m,i}(L)$ is the set of all nonnegative matrices of size $L \times (p+1)$. This set has useful properties, gathered in Proposition 3 for subsequent use.

Proposition 3. Let $L \geq 0$ and take $(b_{j;l}) \simeq \xi \in \mathcal{E}_{m,i}(L)$. The following statements are true.

(i) If $(b'_{j;l}) \simeq \xi' \in \mathcal{E}_{m,i}(L)$, then

$$\xi \xi' \simeq \begin{pmatrix} b_{0;1} & \cdots & b_{p;1} \\ \vdots & & \vdots \\ b_{0;L} & \cdots & b_{p;L} \\ b'_{0;1} & \cdots & b'_{p;1} \\ \vdots & & \vdots \\ b'_{0;L} & \cdots & b'_{p;L} \end{pmatrix}$$

belongs to $\mathcal{E}_{m,i}(2L)$.

(ii) There exists a real θ such that $\mathbb{E} \xi \rightarrow \theta$ whenever $m = m_n \rightarrow \infty$ as $n \rightarrow \infty$.

(iii) Under the assumption $f(X, Z) \leq F(X)$ for all X and Z , it holds that

$$|\xi| \leq \left(\bigvee_{j=0}^p F_j(\mathbf{X}^{(i)}) \right)^{\sum_{j=0}^p \sum_{l=1}^L b_{j;l}},$$

where $F_j(\mathbf{X}^{(i)})$ is $F(X^{(i)}) \vee 1$ if $j = 0$ and $F(\tilde{X}_{-j}^{(i)}) \vee 1$ if $j \geq 1$.

Proof. The proof of (i) is trivial. Let us prove (ii). Put

$$a(k_1, \dots, k_L) = \mathbb{E} \prod_{l=1}^L \prod_{j=0}^p Y_j^{(1, k_l) b_{j;l}}.$$

Then

$$(22) \quad \mathbb{E} \xi = \frac{1}{m^L} \sum_{(k_1, \dots, k_L) \in \{1, \dots, m\}^L} a(k_1, \dots, k_L).$$

This sum can be decomposed into a finite number of sub-sums such that each sub-sum has a polynomial number of equal terms. The first sub-sum is built as follows. Take (k_1, \dots, k_L) all distinct and $m \geq L$. Let $\mathbf{X}^{(1)} = (X^{(1)}, \tilde{X}^{(1)})$ and $\mathbf{Z}^{(1,k)} = (Z_0^{(1,k)}, Z_1^{(1,k)}, \dots, Z_p^{(1,k)})$ for $k = 1, \dots, m$. Since $\mathbf{X}^{(1)}$ and $\{\mathbf{Z}^{(1,k)}, k = 1, \dots, m\}$ are independent, and since the law of $(\mathbf{Z}^{(1,k_1)}, \dots, \mathbf{Z}^{(1,k_L)})$ is invariant through any permutation of (k_1, \dots, k_L) , the corresponding coefficients $a(k_1, \dots, k_L)$ are all equal. Thus, by summing over all permutations of (k_1, \dots, k_L) for distinct k_1, \dots, k_L , we get that the sub-sum is

$$m(m-1) \cdots (m-L+1) a(1, \dots, L).$$

For the second sub-sum, take (k_1, \dots, k_L) such that exactly two of the indices are equal. The same arguments can be used to get a polynomial in m with degree at most L . Go on until all the sub-sums are calculated. An example is given in the proof of Lemma 5 in Appendix C. The result is a polynomial in m with degree at most L , and hence, divided by m^L , the expectation in (22) must converge to some constant (possibly zero).

To prove (iii), simply remember that, by assumption, $|Y_j^{(1,k)}| \leq F(X^{(1)})$ and $|Y_j^{(1,k)}| \leq F(\tilde{X}_{-j}^{(1)})$ for all k and all j . \square

Lemma 3. Take $\xi_{m,i}^{(I)} \simeq (b_{j;l}^{(I)})$, $I = 1, \dots, N$ in $\mathcal{E}_{m,i}(L)$ for $i = 1, 2, \dots$ and $m = 1, 2, \dots$. Assume

$$\mathbb{E} F(X^{(1)})^2 \sum_{j=0}^p \sum_{l=1}^L b_{j;l}^{(I)} < \infty$$

for all $I = 1, \dots, N$. Let $n \rightarrow \infty$. Then

$$\sqrt{n} \left[\frac{1}{n} \sum_{i=1}^n \xi_{m,i}^{(1)} - \mathbb{E} \xi_{m,1}^{(1)}, \dots, \frac{1}{n} \sum_{i=1}^n \xi_{m,i}^{(N)} - \mathbb{E} \xi_{m,1}^{(N)} \right] \xrightarrow{d} N(0, \Sigma_m),$$

where Σ_m is the variance-covariance matrix of $\boldsymbol{\xi}_{m,i} = (\xi_{m,i}^{(1)}, \dots, \xi_{m,i}^{(N)})$. If $m = m_n \rightarrow \infty$, then $\Sigma_m \rightarrow \Sigma$ elementwise for some variance-covariance matrix Σ and the convergence in distribution still holds with Σ in place of Σ_m .

Proof. For any $I = 1, \dots, N$, by Proposition 3 (i), $\xi_{m,i}^{(I)2}$ belongs to $\mathcal{E}_{m,i}(2L)$ and has coefficients

$$\xi_{m,i}^{(I)2} \simeq \begin{pmatrix} b_{0;1} & \cdots & b_{p;1} \\ \vdots & & \vdots \\ b_{0;L} & \cdots & b_{p;L} \\ b_{0;1} & \cdots & b_{p;1} \\ \vdots & & \vdots \\ b_{0;L} & \cdots & b_{p;L} \end{pmatrix}.$$

Thus, denoting $\sum_{j=0}^p \sum_{l=1}^L b_{j;l}$ by β , Proposition 3 (iii) yields

$$\mathbb{E} \xi_{m,1}^{(I)2} = \mathbb{E} \bigvee_{j=0}^p F_j(\mathbf{X}^{(1)})^{2\beta} \leq (p+1) \mathbb{E} \left(1 \vee F(X^{(1)}) \right)^{2\beta},$$

which is finite by assumption. Therefore, Σ_m exists and we can apply the central limit theorem, which concludes the proof for m fixed.

Let $m = m_n \rightarrow \infty$. According to Lindeberg-Feller's central limit theorem (see e.g. [21]), it suffices to show

(i) for all $\epsilon > 0$,

$$\sum_{i=1}^n \mathbb{E} \left\| \frac{1}{\sqrt{n}} \boldsymbol{\xi}_{m_n,i} \right\|^2 \mathbf{1} \left\{ \left\| \frac{1}{\sqrt{n}} \boldsymbol{\xi}_{m_n,i} \right\| > \epsilon \right\} \rightarrow 0,$$

and

(ii) there exists Σ such that

$$\sum_{i=1}^n \text{Cov} \left(\frac{1}{\sqrt{n}} \boldsymbol{\xi}_{m_n,i} \right) \rightarrow \Sigma.$$

Let us show (i). We have

$$\begin{aligned} \sum_{i=1}^n \mathbb{E} \left\| \frac{\boldsymbol{\xi}_{m_n,i}}{\sqrt{n}} \right\|^2 \mathbf{1} \{ \|\boldsymbol{\xi}_{m_n,i}\| > \sqrt{n}\epsilon \} &= \mathbb{E} \|\boldsymbol{\xi}_{m_n,1}\|^2 \mathbf{1} \{ \|\boldsymbol{\xi}_{m_n,1}\| > \sqrt{n}\epsilon \} \\ &= \mathbb{E} \sum_{I=1}^N \xi_{m_n,1}^{(I)2} \mathbf{1} \{ \|\boldsymbol{\xi}_{m_n,1}\| > \sqrt{n}\epsilon \}. \end{aligned}$$

Write $\mathbf{X} = (X^{(1)}, \tilde{X}^{(1)})$. By Proposition 3 (iii), there exists an integrable function $G(\mathbf{X})$ such that

$$\mathbb{E} \left(\xi_{m_n,1}^{(I)2} \mathbf{1}_{\{\|\boldsymbol{\xi}_{m_n,1}\| > \sqrt{n}\epsilon\}} | \mathbf{X} \right) \leq G(\mathbf{X}) P(\|\boldsymbol{\xi}_{m_n,1}\| > \sqrt{n}\epsilon | \mathbf{X}).$$

By Proposition 3 (ii) and Chebyshev's inequality, the upper bound goes to zero and is dominated by $G(\mathbf{X})$, which is integrable. Thus, we can apply the dominated convergence theorem to complete the proof.

Let us show that (ii) holds. We have $\sum_{i=1}^n \text{Cov}(\boldsymbol{\xi}_{m_n,i}/\sqrt{n}) = \text{Cov}(\boldsymbol{\xi}_{m_n,1})$. The element (I, J) in this matrix is given by $\mathbb{E} \xi_{m_n,1}^{(I)} \xi_{m_n,1}^{(J)} - \mathbb{E} \xi_{m_n,1}^{(I)} \mathbb{E} \xi_{m_n,1}^{(J)}$. But since $\xi_{m_n,1}^{(I)} \xi_{m_n,1}^{(J)} \in \mathcal{E}$, the limit of $\text{Cov} \boldsymbol{\xi}_{m_n,1}$ exists and is finite. The proof is complete. \square

C Explicit moment calculations

Explicit moment calculations are given for the summands in the proof of Theorem 1. In this section, $\mathbb{E} f(X, Z)$ and $\mathbb{E} \mathbb{E}[f(X, Z) | X]^2$ are denoted by μ and D , respectively. Recall that the upper-left term in (2) and (3) is denoted by D_j . The moments are given in Lemma 4 and Lemma 5. The variances and covariances are given in Lemma 6. Let $\mathbf{X} = (X^{(1)}, \tilde{X}^{(1)})$. Whenever there is a superscript \mathbf{X} added to the expectation symbol \mathbb{E} or the variance symbol Var , this means that these operators are to be understood conditionally on \mathbf{X} . An integral with respect to $P(d\mathbf{x})$ means that we integrate with respect to the law of \mathbf{X} .

Lemma 4 (Moments of order 1). *The moments of order 1 are given by*

$$\begin{aligned} \mathbb{E} \xi_{m1}^{UL} &= D_j, \\ \mathbb{E} \xi_{m1}^{UR} &= \mu, \\ \mathbb{E} \xi_{m1}^{\prime LL} &= \frac{1}{m} \mathbb{E} \text{Var}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) + D. \end{aligned}$$

Proof. One has

$$\begin{aligned} \mathbb{E} \xi_{m1}^{UL} &= \frac{1}{m^2} \sum_{k,k'} \mathbb{E} f(X^{(1)}, Z^{(1,k)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,k')}) \\ &= \frac{1}{m^2} \sum_{k,k'} \int \mathbb{E} f(x, Z^{(1,k)}) f(\tilde{x}_{-j}, Z_j^{(1,k')}) P(d\mathbf{x}) \\ &= \mathbb{E} f(X^{(1)}, Z^{(1,1)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \\ &= D_j, \end{aligned}$$

where the integral is taken with respect to the law of $\mathbf{x} = (x, \tilde{x})$, and,

$$\begin{aligned} \mathbb{E} \xi_{m1}^{\prime LL} &= \frac{1}{m^2} \sum_{k,k'} \mathbb{E} f(X^{(1)}, Z^{(1,k)}) f(X^{(1)}, Z^{(1,k')})^2 \\ &= \frac{1}{m} \mathbb{E} \text{Var}^{\mathbf{X}} f(X, Z) + \mathbb{E} (\mathbb{E}^{\mathbf{X}} f(X, Z))^2 \\ &= \frac{1}{m} \mathbb{E} \text{Var}^{\mathbf{X}} f(X, Z) + D. \end{aligned}$$

The proof for ξ_{m1}^{UR} is similar. \square

Lemma 5 (Moments of order 2). *The moments of order 2 are given by*

$$\begin{aligned}
\mathbb{E} \xi_{m1}^{(UL)2} &= \text{Var} \mathbb{E}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) + D_j^2 \\
&\quad + \frac{1}{m} [\mathbb{E} \text{Var}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \\
&\quad - \text{Var}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) \text{Var}^{\mathbf{X}} f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)})] \\
&\quad + \frac{1}{m^2} \mathbb{E} \text{Var}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) \text{Var}^{\mathbf{X}} f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}), \\
\mathbb{E} \xi_{m1}^{(UR)2} &= \frac{1}{m} \mathbb{E} \text{Var}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) + \mathbb{E} (\mathbb{E}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}))^2, \\
\mathbb{E} \xi_{m1}^{\prime(LL)2} &= \frac{m(m-1)(m-2)(m-3)}{m^4} \\
&\quad \mathbb{E} f(X^{(1)}, Z^{(1,1)}) f(X^{(1)}, Z^{(1,2)}) f(X^{(1)}, Z^{(1,3)}) f(X^{(1)}, Z^{(1,4)}) \\
&\quad + \frac{\binom{4}{2} m(m-1)(m-2)}{m^4} \mathbb{E} f(X^{(1)}, Z^{(1,1)})^2 f(X^{(1)}, Z^{(1,2)}) f(X^{(1)}, Z^{(1,3)}) \\
&\quad + \frac{\binom{4}{3} m(m-1)}{m^4} \mathbb{E} f(X^{(1)}, Z^{(1,1)})^3 f(X^{(1)}, Z^{(1,2)}) \\
&\quad + \frac{m}{m^4} \mathbb{E} f(X^{(1)}, Z^{(1,1)})^4 \\
&\quad + \frac{\binom{4}{2} m(m-1)/2}{m^4} \mathbb{E} f(X^{(1)}, Z^{(1,1)})^2 f(X^{(1)}, Z^{(1,2)})^2
\end{aligned}$$

Proof. Let us first deal with ξ_{m1}^{UL} . We have

$$\mathbb{E} \xi_{m1}^{(\text{UL})2} = \frac{1}{m^4} \sum_{k_1, k_2, k_3, k_4} \mathbb{E} f(X^{(1)}, Z^{(1, k_1)}) f(X^{(1)}, Z^{(1, k_2)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1, k_3)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1, k_4)})$$

where, in the sum, the indices run over $1, \dots, m$. We split the sum into four parts. The first contains the $m^2(m-1)^2$ terms that satisfy $k_1 \neq k_3$ and $k_2 \neq k_4$. In this part, all the terms are equal to

$$(\text{term 1}) \quad \mathbb{E} \left(\mathbb{E}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \right)^2.$$

The second part contains the $m^2(m-1)$ terms that satisfy $k_1 \neq k_3$ and $k_2 = k_4$ and that are equal to

$$(\text{term 2}) \quad \mathbb{E} f(X^{(1)}, Z^{(1,1)}) f(X^{(1)}, Z^{(1,2)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)})^2.$$

The third part contains the $m^2(m-1)$ terms that satisfy $k_1 = k_3$ and $k_2 \neq k_4$ and that are equal to

$$(\text{term 3}) \quad \mathbb{E} f(X^{(1)}, Z^{(1,1)})^2 f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,2)}).$$

Finally, the fourth part contains the m^2 terms that satisfy $k_1 = k_4$ and $k_2 = k_4$ and are equal to

$$(\text{term 4}) \quad \mathbb{E} f(X^{(1)}, Z^{(1,1)})^2 f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)})^2.$$

(One can see that the number of terms is m^4 .) Thus,

$$\begin{aligned} \mathbb{E} \xi_{m1}^{(\text{UL})2} &= (\text{term 1}) \\ &+ \frac{1}{m} [(\text{term 2}) + (\text{term 3}) - 2(\text{term 1})] \\ &+ \frac{1}{m^2} [(\text{term 1}) - (\text{term 2}) - (\text{term 3}) + (\text{term 4})]. \end{aligned}$$

Furthermore, $[(\text{term 1}) - (\text{term 2}) - (\text{term 3}) + (\text{term 4})]$ is equal to

$$\begin{aligned} &\int \left(\mathbb{E}^{\mathbf{X}} f(x, Z) f(\tilde{x}_{-j}, Z_j) \right)^2 \\ &\quad - \mathbb{E}^{\mathbf{X}} f(x, Z^{(1,1)}) f(x, Z^{(1,2)}) f(\tilde{x}_{-j}, Z_j^{(1,1)})^2 \\ &\quad - \mathbb{E}^{\mathbf{X}} f(x, Z^{(1,1)})^2 f(\tilde{x}_{-j}, Z_j^{(1,1)}) f(\tilde{x}_{-j}, Z_j^{(1,2)}) \\ &\quad + \mathbb{E}^{\mathbf{X}} f(x, Z^{(1,1)})^2 f(\tilde{x}_{-j}, Z_j^{(1,1)})^2 dP(\mathbf{x}) \\ &= \int \left(\mathbb{E}^{\mathbf{X}} f(x, Z) \right)^2 \left(\mathbb{E}^{\mathbf{X}} f(\tilde{x}_{-j}, Z_j) \right)^2 \\ &\quad - \left(\mathbb{E}^{\mathbf{X}} f(x, Z) \right)^2 \mathbb{E}^{\mathbf{X}} f(\tilde{x}_{-j}, Z_j)^2 \\ &\quad - \mathbb{E}^{\mathbf{X}} f(x, Z)^2 \left(\mathbb{E}^{\mathbf{X}} f(\tilde{x}_{-j}, Z_j) \right)^2 \\ &\quad + \mathbb{E}^{\mathbf{X}} f(x, Z)^2 \mathbb{E}^{\mathbf{X}} f(\tilde{x}_{-j}, Z_j)^2 dP(\mathbf{x}) \\ &= \int \text{Var}^{\mathbf{X}} f(X, Z) \text{Var}^{\mathbf{X}} f(\tilde{X}_{-j}, Z_j) dP(\mathbf{x}). \end{aligned}$$

Likewise, we find that $[(\text{term 2}) + (\text{term 3}) - 2(\text{term 1})]$ is equal to

$$\mathbb{E} \text{Var}^{\mathbf{X}} f(X, Z) f(\tilde{X}_{-j}, Z_j) - \text{Var}^{\mathbf{X}} f(X, Z) \text{Var}^{\mathbf{X}} f(\tilde{X}_{-j}, Z_j),$$

and term 1 is $\text{Var} \mathbb{E}^{\mathbf{X}} f(X, Z) f(\tilde{X}_{-j}, \tilde{Z}) + D_j^2$.

We now deal with $\xi_{m1}^{\prime\prime\text{LL}}$. We have

$$\mathbb{E} \xi_{m1}^{\prime\prime\text{LL}2} = \frac{1}{m^4} \sum_{k_1, k_2, k_3, k_4} \mathbb{E} f(X^{(1)}, Z^{(1, k_1)}) f(X^{(1)}, Z^{(1, k_2)}) f(X^{(1)}, Z^{(1, k_3)}) f(X^{(1)}, Z^{(1, k_4)}).$$

The sum is split into five parts. The first part consists of the $m(m-1)(m-2)(m-3)$ terms with different indices; those terms are equal to

$$\mathbb{E} f(X^{(1)}, Z^{(1,1)}) f(X^{(1)}, Z^{(1,2)}) f(X^{(1)}, Z^{(1,3)}) f(X^{(1)}, Z^{(1,4)}).$$

The second part consists of the $\binom{4}{2} m(m-1)(m-2)$ terms with exactly two equal indices; those terms are equal to

$$\mathbb{E} f(X^{(1)}, Z^{(1,1)})^2 f(X^{(1)}, Z^{(1,2)}) f(X^{(1)}, Z^{(1,3)}).$$

The third part consists of the $\binom{4}{3} m(m-1)$ terms with exactly three equal indices; those terms are equal to

$$\mathbb{E} f(X^{(1)}, Z^{(1,1)})^3 f(X^{(1)}, Z^{(1,2)}).$$

The fourth part consists of the m terms with exactly four equal indices; those terms are equal to

$$\mathbb{E} f(X^{(1)}, Z^{(1,1)})^4.$$

The fifth and last part consists of the $\binom{4}{2}m(m-1)/2$ terms with exactly two pairs of equal indices; those terms are equal to

$$\mathbb{E} f(X^{(1)}, Z^{(1,1)})^2 f(X^{(1)}, Z^{(1,2)})^2.$$

(One can check that the total number of terms is m^4 .) \square

Lemma 6 (Variances and covariances).

(i)

$$\begin{aligned} \text{Var } \xi_{m1}^{UL} &= \text{Var } \mathbb{E}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \\ &+ \frac{1}{m} [\mathbb{E} \text{Var}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) - \text{Var}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) \text{Var}^{\mathbf{X}} f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)})] \\ &+ \frac{1}{m^2} \mathbb{E} \text{Var}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) \text{Var}^{\mathbf{X}} f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}), \end{aligned}$$

(ii)

$$\begin{aligned} \text{Cov}(\xi_{m1}^{UL}, \xi_{m1}^{UR}) &= \frac{m-1}{m} \mathbb{E} f(X^{(1)}, Z^{(1,1)}) f(X^{(1)}, Z^{(1,2)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \\ &+ \frac{1}{m} \mathbb{E} f(X^{(1)}, Z^{(1,1)})^2 f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) - D_j \mu \end{aligned}$$

(iii)

$$\text{Cov}(\xi_{m1}^{UL}, f(X, Z)^2) = \frac{1}{m} \mathbb{E} f(X^{(1)}, Z^{(1,1)})^3 f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)})$$

(iii)

$$+ \frac{m-1}{m} \mathbb{E} f(X^{(1)}, Z^{(1,1)})^2 f(X^{(1)}, Z^{(1,2)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) - D_j \kappa$$

(iv)

$$\text{Var } \xi_{m1}^{UR} = \frac{1}{m} \text{Var } f(X, Z)$$

(v)

$$\begin{aligned} \text{Cov}(\xi_{m1}^{UR}, f(X, Z)^2) &= \frac{1}{m} f(X, Z)^3 \\ &+ \frac{m-1}{m} \mathbb{E} f(X^{(1)}, Z^{(1,1)})^2 f(X^{(1)}, Z^{(1,2)}) - \mu \kappa \end{aligned}$$

(vi)

$$\begin{aligned} \text{Cov}(\xi_{m_n1}^{UL}, \xi_{m_n1}^{ULL}) &= \frac{m}{m^3} \mathbb{E} f(X^{(1)}, Z^{(1,1)})^3 f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \\ &+ \frac{3m(m-1)}{m^3} \mathbb{E} f(X^{(1)}, Z^{(1,1)})^2 f(X^{(1)}, Z^{(1,2)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \\ &+ \frac{m(m-1)(m-2)}{m^3} \mathbb{E} f(X^{(1)}, Z^{(1,1)}) f(X^{(1)}, Z^{(1,2)}) \\ &f(X^{(1)}, Z^{(1,3)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \\ &- \mathbb{E} f(X^{(1)}, Z^{(1,1)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \\ &\left\{ \frac{1}{m} \mathbb{E} f(X^{(1)}, Z^{(1,1)})^2 + \frac{m-1}{m} \mathbb{E} f(X^{(1)}, Z^{(1,1)}) f(X^{(1)}, Z^{(1,2)}) \right\} \end{aligned}$$

Proof. The proof follows from direct calculations. \square

D Calculations for the linear model

Lemma 7. *Suppose that $f(X, Z) = \beta_0 + \beta_{p+1}Z + \sum_{j=1}^p \beta_j X_j$ where $X = (X_1, \dots, X_p), Z_k, \tilde{Z}_{ik}$ are independent, $\mathbb{E} X_j = \mathbb{E} Z = 0$, $\mathbb{E} X_j^2 = \mathbb{E} Z^2 = 1$, $\mathbb{E} X_j^3 = 0$, $\mathbb{E} X_j^4 = 3$. Then the squared optimal number of repetitions is given by*

$$(m_i^*)^2 = \frac{\beta_{p+1}^4}{(\beta_0 + \beta_i)^2 - 2\beta_0^4 + (\sum_{j=0}^p \beta_j^2)^2}$$

and the discriminator (the upper-left term in (2) and (3)) is

$$\beta_0^2 + \beta_i^2.$$

Proof. We have

$$m_i^* = \frac{A_i + B_i + C_i + D_i}{E_i},$$

with

$$\begin{aligned} A_i &= \mathbb{E} f(X, Z_1)^2 f(\tilde{X}_{-i}, \tilde{Z}_{i1})^2 \\ B_i &= \mathbb{E} f(X, Z_1) f(\tilde{X}_{-i}, \tilde{Z}_{i1}) f(X, Z_2) f(\tilde{X}_{-i}, \tilde{Z}_{i2}) \\ C_i &= -\mathbb{E} f(X, Z_1)^2 f(\tilde{X}_{-i}, \tilde{Z}_{i1}) f(\tilde{X}_{-i}, \tilde{Z}_{i2}) \\ D_i &= -\mathbb{E} f(\tilde{X}_{-i}, \tilde{Z}_{i1})^2 f(X, Z_1) f(X, Z_2) \\ E_i &= B - [\mathbb{E} f(X, Z_1) f(\tilde{X}_{-i}, \tilde{Z}_{i1})]^2 \end{aligned}$$

where $X = (X_1, \dots, X_p), Z_k, \tilde{Z}_{ik}$ are independent, $\mathbb{E} X_j = \mathbb{E} Z = 0$, $\mathbb{E} X_j^2 = \mathbb{E} Z^2 = 1$, $\mathbb{E} X_j^3 = 0$, $\mathbb{E} X_j^4 = 3$. We deal with the case

$$f(X, Z) = \beta_0 + \beta_{p+1}Z + \sum_{j=1}^p \beta_j X_j.$$

We calculate the terms one by one as follows. We have

$$(A_{j1}) \quad A_j = \mathbb{E} \left(\beta_0 + \sum_{j=1}^p \beta_j X_j \right)^2 \left(\beta_0 + \beta_i X_i + \sum_{j:1 \leq j \neq i} \beta_j \tilde{X}_j \right)^2$$

$$(A_{j2}) \quad + \left(\beta_0 + \sum_{j=1}^p \beta_j X_j \right)^2 \beta_{p+1}^2 \tilde{Z}_{i1}^2 + \beta_{p+1}^4 Z_1^2 \tilde{Z}_{i1}^2$$

$$(A_{j3}) \quad + \beta_{p+1}^2 Z_1^2 \left(\beta_0 + \beta_i X_i + \sum_{j:1 \leq j \neq i} \beta_j \tilde{X}_j \right)^2,$$

where $\mathbb{E} (A2) = \beta_{p+1}^4 + \beta_{p+1}^2 \sum_{j=0}^p \beta_j^2$, $\mathbb{E} (A3) = \beta_{p+1}^2 \sum_{j=0}^p \beta_j^2$. Elementary but somewhat tedious calculations yield

$$\mathbb{E} (A1) = \beta_0^4 + 3\beta_i^4 + 6\beta_0^2 \beta_i^2 + 2(\beta_0^2 + \beta_i^2) \sum_{j:1 \leq j \neq i} \beta_j^2 + \left(\sum_{j:1 \leq j \neq i} \beta_j^2 \right)^2.$$

Similar calculations show that $B_j = A_{j1}$, $C_j = -A_{j1} - A_{j3}$, $D_j = -A_{j1} - A_{j3}$, $E_j = A_{j1} - (\beta_0^2 + \beta_i^2)^2$. Thus,

$$(m_i^*)^2 = \frac{\beta_{p+1}^4}{(\beta_0 + \beta_i)^2 - 2\beta_0^4 + (\sum_{j=0}^p \beta_j^2)^2}.$$

□