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1 **A TRADEOFF BETWEEN EXPLORATIONS AND REPETITIONS**
2 **FOR ESTIMATORS OF TWO GLOBAL SENSITIVITY INDICES IN**
3 **STOCHASTIC MODELS INDUCED BY PROBABILITY MEASURES***

4 GILDAS MAZO[†]

5 **Abstract.** Sobol sensitivity indices assess how the output of a given mathematical model is
6 sensitive to its inputs. If the model is stochastic then it cannot be represented as a function of the
7 inputs, thus raising questions as how to do a sensitivity analysis in those models. Practitioners have
8 been using an approach that exploits the availability of methods for deterministic models. For each
9 input, the stochastic model is repeated and the outputs are averaged. These averages are seen as
10 if they came from a deterministic model and hence Sobol's method can be used. We show that
11 the estimator so obtained is asymptotically biased if the number of repetitions goes to infinity too
12 slowly. With limited computational resources, the number of repetitions of the stochastic model
13 and the number of explorations of the input space cannot be large together and hence some balance
14 must be found. We find the pair of numbers that minimizes a bound on some rank-based error
15 criterion, penalizing bad rankings of the inputs' sensitivities. Also, under minimal distributional
16 assumptions, we derive a functional relationship between the output, the input and some random
17 noise; the Sobol-Hoeffding decomposition can be applied to it to define a new sensitivity index, which
18 asymptotically is estimated without bias even though the number of repetitions remains fixed. The
19 theory is illustrated on numerical experiments.

20 **Key words.** asymptotic normality, Sobol indices, tradeoff, sensitivity analysis, stochastic model.

21 **AMS subject classifications.** 62G20, 60H99, 65C05

22 **1. Introduction.** The goal of sensitivity analysis is to assess how the output of
23 a given physical or mathematical model is sensitive to its inputs [26, 27]. Classically,
24 the model of interest is deterministic. To each input there corresponds an output
25 given by the model. Thus, in this case, the model is in fact a function, say f . To
26 assess the sensitivity of the model to its inputs, the probabilistic/statistical framework
27 is often employed. One draws at random a large number of inputs and observe how
28 the corresponding outputs vary. From a statistical perspective, at each draw, one
29 observes a random pair (X, Y) such that $Y = f(X)$, where $X = (X_1, \dots, X_p)$ is the
30 input vector and Y is the output.

31 Sobol's idea [29, 30] was to notice that, if X_1, \dots, X_p are drawn independently
32 then $f(X)$ can be decomposed into a sum of lower-dimensional functions and that this
33 decomposition can be used to allocate the variance of the output to the individual
34 components of the decomposition. More precisely, we have

35 (1.1)
$$f(X) - f_0 = f_1(X_1) + \dots + f_p(X_p)$$

36
$$+ f_{1,2}(X_1, X_2) + \dots + f_{p-1,p}(X_{p-1}, X_p)$$

37
$$+ \dots + f_{1,\dots,p}(X_1, \dots, X_p),$$

39 where $f_0 = E f(X)$, $f_j(X_j) = E(f(X) - f_0 | X_j)$, $j = 1, \dots, p$, and $f_{1,2}, \dots, f_{1,\dots,p}$
40 are some functions defined iteratively; see [29] and [33, p. 157] for more details. In
41 the field of uncertainty quantification the above decomposition is known as the Sobol-
42 Hoeffding decomposition in reference to [11, 29]. The expectations and the covariances
43 of the individual components in the right-hand side of (1.1) are zero and hence we

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44 have the variance decomposition

$$45 \quad \text{Var } f(X) = \text{Var } f_1(X_1) + \cdots + \text{Var } f_p(X_p) + \cdots ,$$

47 which leads to the so-called Sobol indices

$$48 \quad S_j = \frac{\text{Var } f_j(X_j)}{\text{Var } f(X)} = \frac{\text{Var } \mathbb{E}(f(X)|X_j)}{\text{Var } f(X)} = \frac{\mathbb{E} f(X)f(\tilde{X}_{-j}) - (\mathbb{E} f(X))^2}{\mathbb{E} f(X)^2 - (\mathbb{E} f(X))^2},$$

50 $j = 1, \dots, p$; here \tilde{X}_{-j} stands for an independent copy of X where the j th compo-
 51 nent has been replaced by that of X . Thus the Sobol index associated with the j th
 52 argument of f is defined as the proportion of the total variance associated with the
 53 lower-dimensional function that depends on the j th argument only. Sobol indices are
 54 interpreted as sensitivity measures and used to achieve various goals in uncertainty
 55 quantification [27].

56 If the model is nonadditive (it is said that the inputs “interact” with each other)
 57 then the Sobol indices may be inadequate. To account for interactions, the so-called
 58 total sensitivity indices [12] are often computed along with Sobol indices. The total
 59 sensitivity index associated with the j th argument of f is given by

$$60 \quad S_{T_j} = 1 - \frac{\text{Var } \mathbb{E}(f(X)|X_1, \dots, X_{j-1}, X_{j+1}, \dots, X_p)}{\text{Var } f(X)}.$$

62 The total sensitivity index quantifies the sensitivity of the output of f to its j th
 63 argument through the interactions it may have with the other inputs.

64 There are numerous methods to estimate the sensitivity indices. For simplic-
 65 ity, we describe below Sobol’s original method to estimate S_j through Monte Carlo
 66 sampling [29]. For a review of the many other methods, see [23] or the package
 67 `sensitivity` [16] of the R software for an up-to-date list of many methods, with refer-
 68 ences. Thus, draw two independent sets of inputs $\{X^{(i)}, i = 1, \dots, n\}$, $\{\tilde{X}^{(i)} :=$
 69 $(\tilde{X}_1, \dots, \tilde{X}_p), i = 1, \dots, n\}$ and make p more sets by combining the first two: $\{\tilde{X}_{-j}^{(i)},$
 70 $i = 1, \dots, n\}$, $j = 1, \dots, p$, where

$$71 \quad (1.2) \quad \tilde{X}_{-j}^{(i)} := (\tilde{X}_1^{(i)}, \dots, \tilde{X}_{j-1}^{(i)}, X_j^{(i)}, \tilde{X}_{j+1}^{(i)}, \dots, \tilde{X}_p^{(i)}).$$

73 The first and the p last sets are passed on to the function f which produces the
 74 outputs $\{Y^{(i)}, i = 1, \dots, n\}$ (for the first set) and $\{Y_j^{(i)}, i = 1, \dots, n\}$, $j = 1, \dots, p$
 75 (for the p last sets), which in turn make up the so-called pick-freeze estimator

$$76 \quad (1.3) \quad \hat{S}_j = \frac{\frac{1}{n} \sum_{i=1}^n Y^{(i)} Y_j^{(i)} - \left(\frac{1}{n} \sum_{i=1}^n Y^{(i)}\right)^2}{\frac{1}{n} \sum_{i=1}^n Y^{(i)2} - \left(\frac{1}{n} \sum_{i=1}^n Y^{(i)}\right)^2}.$$

78 This gives a simple procedure to estimate all the Sobol indices S_1, \dots, S_p with $(p+1)n$
 79 runs of the model. The pick-freeze estimator is asymptotically normal [7, 17]. The
 80 above formula can be improved in many ways [12, 17, 21]. Many versions of this
 81 estimator exist, the goal being always to get the most efficient estimator with the least
 82 computations. Sobol indices for multivariate, functional outputs [6, 18] or functional
 83 inputs [15] have been proposed as well.

84 The big difference between a deterministic model and a stochastic model is that
 85 the stochastic model is not a function anymore. To a particular value of the input there
 86 does not correspond any particular value for the output. Instead, there corresponds a

87 range of possible values, assumed to come from a probability distribution depending
 88 on the input. Examples can be found in epidemiology [2, 3, 24, 28] or ecology [31], to
 89 name a few.

90 To do the sensitivity analysis of a stochastic model, several approaches have been
 91 investigated. In [19], to the best of my understanding, the authors carry out the
 92 sensitivity analysis of a stochastic model based on a joint metamodel. In [10], a
 93 stochastic model is seen as a functional relation of the form $Y(\vartheta, \omega) = f(X(\vartheta), \omega)$,
 94 where the X is a random vector on some probability space, ω is a point in some
 95 probability space distinct from that on which X is defined, f is some function and
 96 $Y(\vartheta, \omega)$ is a random variable on the induced product probability space. The quan-
 97 tity $f(X(\vartheta), \omega)$ represents the output of the stochastic model run with input $X(\vartheta)$;
 98 the point ω represents the intrinsic randomness. The idea is then to decompose the
 99 function $\vartheta \mapsto f(X(\vartheta), \omega)$ for each ω and estimate the associated sensitivity indices,
 100 which depend on ω . The estimates are then averaged over ω to make the final sen-
 101 sitivity estimates. In [1], to the best of my understanding, the stochastic model is
 102 represented as a deterministic mapping which with an input associates a probability
 103 density function. The Sobol-Hoeffding decomposition is applied to the mapping which
 104 with an input associates the entropy of the output evaluated at that input. Here the
 105 entropy is the Kullback-Leibler divergence of the output density. In [34], the output
 106 of the stochastic model is seen as a semiparametric statistical model—the generalized
 107 lambda distribution—with parameters depending on the inputs. These parameters
 108 have a polynomial chaos expansion which is estimated by maximum likelihood. Once
 109 the law of the output conditionally on the input has been estimated, its inverse cumu-
 110 lative distribution function is used to turn the stochastic model into a deterministic
 111 model to which standard methods are applied. In [5], the stochastic model is seen as
 112 a mapping that goes from the input space to a space of probability measures equipped
 113 with the Wasserstein distance. Following [8, 9], the Wasserstein space is mapped to
 114 the real line \mathbb{R} with some family of test functions, thus allowing for a standard Sobol-
 115 Hoeffding decomposition which is then averaged over all possible test functions. In
 116 more specific contexts, global sensitivity analysis methods also have been proposed.
 117 For instance, there are methods for stochastic differential equations [4] and chemical
 118 reaction networks [22].

119 In practice, although it has not been formally defined in the literature, another
 120 method has been used for some time [2, 24, 28, 31]. The idea is simple: at each
 121 draw of the input $X^{(i)}$, one produces as many outputs $Y^{(i,1)}, \dots, Y^{(i,m)}$ as possible,
 122 makes the average $m^{-1} \sum_{k=1}^m Y^{(i,k)}$ and does *as if* it were the output of some deter-
 123 ministic model. The same is done with the inputs $\tilde{X}_{-j}^{(i)}$ (1.2) to produce the outputs
 124 $m^{-1} \sum_{k=1}^m Y_j^{(i,k)}$. The obtained estimator is then the same as that in (1.3) but with
 125 $Y^{(i)}$ replaced by $m^{-1} \sum_{k=1}^m Y^{(i,k)}$ and $Y_j^{(i)}$ replaced by $m^{-1} \sum_{k=1}^m Y_j^{(i,k)}$, yielding

(1.4)

$$\hat{S}_j = \frac{\frac{1}{n} \sum_{i=1}^n m^{-1} \sum_{k=1}^m Y^{(i,k)} m^{-1} \sum_{k=1}^m Y_j^{(i,k)} - \left(\frac{1}{n} \sum_{i=1}^n m^{-1} \sum_{k=1}^m Y^{(i,k)} \right)^2}{\frac{1}{n} \sum_{i=1}^n \left(m^{-1} \sum_{k=1}^m Y^{(i,k)} \right)^2 - \left(\frac{1}{n} \sum_{i=1}^n m^{-1} \sum_{k=1}^m Y^{(i,k)} \right)^2}.$$

128 The big advantage for practitioners is that they can use the numerous available and
 129 ready-to-use softwares for deterministic models.

130 To build the estimator (1.4), the stochastic model must be run $mn(p+1)$ times.
 131 The number m is called the number of repetitions and the number n is called the
 132 number of explorations. If the stochastic model is computationally intensive—that

133 is, each model run is time-consuming—, then the estimator is built with limited
 134 resources. In this context, an increase of m must go along with a decrease of n , and
 135 conversely. What is then a good balance between m and n ? How to choose m and
 136 n such that the estimator (1.4) will be the most efficient? This question was asked
 137 by [31].

138 We address this problem by finding a pair (m, n) that minimizes a bound on
 139 the so-called missranking error. The missranking error penalizes bad rankings of the
 140 Sobol indices associated with the inputs. The estimated minimizer is used to build
 141 well-balanced estimators, leading to a two-step procedure to estimate the sensitivity
 142 indices. This two-step procedure is shown to have good asymptotic properties. We
 143 show that the estimator (1.4) is asymptotically normal but may be biased if m goes
 144 to infinity too slowly. If $m/\sqrt{n} \rightarrow \infty$ then it is asymptotically unbiased and converges
 145 to the so-called *sensitivity index of the second kind*. Under the minimal assumption
 146 that a stochastic model is a set of probability measures that capture how the outputs
 147 are drawn, we show that the output, the inputs and some random “noise” are linked
 148 through a function, which the Sobol-Hoeffding decomposition can be applied to. This
 149 yields a new sensitivity index, called *the sensitivity index of the first kind*, with the
 150 advantage that asymptotically unbiased estimators can be built even though m re-
 151 mains fixed. The indices of the first and of the second kinds are complementary as
 152 they offer distinct pieces of information. Interestingly, these indices can be estimated
 153 jointly with no additional cost, the joint estimator is asymptotically normal and the
 154 two kinds of sensitivity indices lead to the same solution for the tradeoff problem.

155 This paper is organized as follows. Section 2 gives a definition of stochastic
 156 models in terms of probability measures and shows how one can construct a functional
 157 representation linking the output, the input and some random noise. Section 3 defines
 158 the indices of both kinds and their estimators. The asymptotic properties are deferred
 159 to Section 5. Section 4 introduces the tradeoff problem, gives a procedure to attack it
 160 and gives some theoretical guarantees. Section 6 illustrates the theory on numerical
 161 simulations. A Conclusion closes the paper.

162 **2. Representations of stochastic models.** The concept of stochastic models
 163 is intuitive and shared by many people but there are different mathematical routes
 164 to describe them. One is given in Section 2.1. It makes minimal distributional as-
 165 sumptions to get to a representation in terms of random variables and establishes the
 166 existence of a function to which the Sobol-Hoeffding decomposition can be applied.
 167 Section 2.2 makes connections with the stochastic models of [10].

168 **2.1. Representing stochastic models from minimal distributional as-**
 169 **sumptions.** A stochastic model is some mechanism that produces outputs at ran-
 170 dom given some inputs. Thus, a stochastic model can be seen as family of probability
 171 measures $\{Q_x, x \in \mathcal{X}\}$ indexed by some input space $\mathcal{X} \subset \mathbb{R}^p$. We assume that each
 172 probability measure Q_x is defined on the measurable space $(\mathbb{R}, \mathcal{B})$, where \mathcal{B} is the
 173 Borel σ -field induced by \mathbb{R} . The law Q_x governs how the outputs are produced given
 174 the input $x \in \mathcal{X} \subset \mathbb{R}^p$. Let us endow \mathbb{R}^p with its product Borel σ -field \mathcal{B}^p and let
 175 P^* be a product probability measure on the measurable space $(\mathbb{R}^p, \mathcal{B}^p)$ such that
 176 $P^*(\mathcal{X}) = 1$. (Thus we assume that $\mathcal{X} \in \mathcal{B}^p$.) The probability measure P^* represents
 177 how the inputs are drawn by the practitioner. In particular, since P^* is a product
 178 probability measure, the inputs are drawn independently.

179 The stochastic experiment that consists of drawing inputs at random according
 180 to P^* and observing the corresponding outputs is fully characterized by the family
 181 $\{Q_x\}$ and the probability measure P^* . This leads us to Definition 2.1.

182 DEFINITION 2.1. *If P^* and $\{Q_x\}$ are probability measures as described above then*
 183 *the pair $(P^*, \{Q_x\})$ is called the complete stochastic model.*

184 Now we look for a representation in terms of random variables that will allow us
 185 to use the Sobol-Hoeffding decomposition later on.

186 LEMMA 2.2. *If $(P^*, \{Q_x\})$ is a complete stochastic model then there exist a proba-*
 187 *bility space (Ω, \mathcal{F}, P) , a random vector $(X, Z) : \Omega \rightarrow \mathbb{R}^{p+1}$ and a function $f : \mathbb{R}^{p+1} \rightarrow$*
 188 *\mathbb{R} such that*

- 189 (i) *$f(x, Z)$ is measurable for every $x \in \mathcal{X}$,*
 - 190 (ii) *$P(f(x, Z) \in B) = Q_x(B)$ for every $x \in \mathcal{X}$ and every $B \in \mathcal{B}$,*
 - 191 (iii) *$P(X \in A, Z \in B) = P^*(A)P(Z \in B)$ for every $A \in \mathcal{B}^p$ and $B \in \mathcal{B}$.*
- 192 *Moreover, if $(X, f(X, Z))$ and $(X', f'(X', Z'))$ are two joint vectors that satisfy the*
 193 *conditions (i), (ii) and (iii) then $(X, f(X, Z)) \stackrel{d}{=} (X', f'(X', Z'))$ where $\stackrel{d}{=}$ means*
 194 *equality in distribution.*

195 Note that the conditions in Lemma 2.2 do not determine the law of Z ; see the
 196 example below.

197 EXAMPLE 1 (The law of Z is not determined). *Let $p = 1$. Let P^* be the*
 198 *standard uniform distribution and Q_x be the Gaussian distribution with mean $x \in \mathbb{R}$*
 199 *and variance 1. Let $\Omega = (0, 1)^2$ endowed with its Borel σ -field and set P to be the*
 200 *product Lebesgue measure. Let $X_1(\omega) = \omega_1$ for $\omega = (\omega_1, \omega_2) \in \Omega$. Let Φ denote the*
 201 *distribution function of the standard Gaussian distribution and denote by Φ^{-1} the*
 202 *inverse of Φ . If $Z(\omega) = \omega_2$ and $f(x, z) = \Phi^{-1}(z) + x$, $x \in \mathbb{R}$, $z \in (0, 1)$, then it is*
 203 *easy to see that (X, Z) and f satisfy the conditions of Lemma 2.2 and the law of Z is*
 204 *the standard uniform distribution. But the conditions of Lemma 2.2 are also satisfied*
 205 *with $Z(\omega) = \sqrt{\omega_2}$ and $f(x, z) = \Phi^{-1}(z^2) + x$, in which case, $P(Z \leq t) = t^2$, $t \in (0, 1)$,*
 206 *that is, the law of Z is the beta distribution with parameter $(2, 1)$.*

207 The indeterminacy of the law of Z is symptomatic of the lack of control of the
 208 intrinsic randomness assumed in our definition of stochastic models. But this is not
 209 an issue because our interest lies in the joint vector $(X, f(X, Z))$, the law of which is
 210 fully characterized by the conditions in Lemma 2.2. To each complete stochastic model
 211 there corresponds a unique law that all vectors $(X, f(X, Z))$ must have, regardless of
 212 the chosen representation. Therefore, the pair $(X, f(X, Z))$ can be used to define the
 213 pair (input, output) of a complete stochastic model, as done in Definition 2.3.

214 DEFINITION 2.3. *If (X, Z) and f satisfy the conditions in Lemma 2.2 then the*
 215 *pair $(X, f(X, Z))$ is called an observation of the complete stochastic model $(P^*, \{Q_x\})$;*
 216 *the random variable X is called the input and $f(X, Z)$ is called the output.*

217 In sum, we have established the existence of random variables on a common
 218 probability space and a function f that characterize the statistical experiment that
 219 consists of drawing inputs and observing the outputs of a stochastic model. The set
 220 of assumptions used to represent outputs and inputs of a stochastic model is minimal:
 221 all we need is a family $\{Q_x\}$ and a probability measure P^* . We remark that the above
 222 formalism of stochastic models can be used to represent physical models [32] as well.

223 **2.2. Links with the stochastic models and the sensitivity indices in [10].**
 224 In [10], the authors consider the model $(X'(\omega'), \varphi(X'(\omega'), \omega''))$, $\omega' \in \Omega'$, $\omega'' \in \Omega''$,
 225 where $(\Omega', \mathcal{F}', P')$ and $(\Omega'', \mathcal{F}'', P'')$ are probability spaces, $X' = (X'_1, \dots, X'_p)$ is a

226 random vector on Ω' and φ is some function. They consider the sensitivity indices

$$227 \quad S_j^{\text{HAG}} = \int_{\Omega''} S_j(\omega'') P''(d\omega''),$$

229 where

$$230 \quad S_j(\omega'') = \frac{\text{Var E}(\varphi(X', \omega'') | X'_j)}{\text{Var } \varphi(X', \omega'')};$$

232 above the variances and the expectation are to be understood as integrals on Ω' with
233 respect to P' .

234 One can choose a representation in Lemma 2.2 that corresponds to the models
235 in [10]. In particular, one can recover the sensitivity indices S_j^{HAG} , $j = 1, \dots, p$. Let
236 us illustrate this with an example. Let $(P^*, \{Q_x\})$ be a complete stochastic model
237 and let $X = (X_1, \dots, X_p)$, Z and f be as in Lemma 2.2. Define

$$238 \quad \tilde{S}_j^{\text{HAG}} = \text{E} \left(\frac{\text{Var}(\text{E}[f(X, Z) | X_j, Z] | Z)}{\text{Var}(f(X, Z) | Z)} \right), \quad j = 1, \dots, p.$$

240 Consider the model in Example 1.1 of [10], given by

$$241 \quad (2.1) \quad \varphi(X'(\omega'), \omega'') = X_1(\omega') + X_2(\omega')\omega'',$$

243 where the law of X'_1 is the uniform distribution on $(0, 1)$, the law of X'_2 is the uniform
244 distribution on $(1, L + 1)$, $L > 0$, and P'' is the standard normal distribution on
245 $\Omega'' = \mathbb{R}$. The indices in Example 1.1 of [10] are given by

$$246 \quad S_1^{\text{HAG}} = \int_{\Omega''} \frac{1}{1 + L^2\omega''} P''(d\omega'') = \int_{\mathbb{R}} \frac{1}{1 + L^2w} \exp\left(-\frac{w^2}{2}\right) \frac{1}{\sqrt{2\pi}} dw$$

248 and $S_2^{\text{HAG}} = 1 - S_1^{\text{HAG}}$.

249 We can build a probability space (Ω, \mathcal{F}, P) , a random vector (X, Z) and a function
250 f such that $\tilde{S}_1^{\text{HAG}} = S_1^{\text{HAG}}$, as shown in Example 2 below.

251 **EXAMPLE 2.** *Let us first extract the induced complete stochastic model. Set $P^*((0, t_1] \times$
252 $(1, t_2]) = t_1(t_2 - 1)/L$ for all $0 < t_1 < 1$, $1 < t_2 < L + 1$, $L > 0$ and $Q_x(-\infty, t] =$
253 $\Phi((t - x_1)/x_2)$ for all $t \in \mathbb{R}$, where $\Phi(t) = \int_{-\infty}^t (2\pi)^{-1/2} e^{-s^2/2} ds$ and $x = (x_1, x_2) \in$
254 $\mathbb{R} \times (0, \infty)$. Now it remains to choose a representation that fulfills the conditions in
255 Lemma 2.2 and ensures that $S_1^{\text{HAG}} = \tilde{S}_1^{\text{HAG}}$. Such a representation can easily be
256 found. For instance, take $\Omega = (0, 1)^3$ endowed with the product Lebesgue measure and
257 put $Z(\omega) = \omega_3$, $X_1(\omega) = F_1^{-1}(\omega_1)$ and $X_2(\omega) = F_2(\omega_2)^{-1}$ for $\omega = (\omega_1, \omega_2, \omega_3) \in \Omega$,
258 where $F_1(t_1) = t_1$ for $0 < t_1 < 1$ and $F_2(t_2) = (t_2 - 1)/L$ for $1 < t_2 < L + 1$. Finally
259 take $f(x, z) = \Phi^{-1}(z)x_2 + x_1$ for $x_1 \in \mathbb{R}$, $x_2 > 0$ and $z \in (0, 1)$. Then the conditions
260 of Lemma 2.2 are fulfilled by construction and the detailed calculations in Appendix A
261 show that $S_1^{\text{HAG}} = \tilde{S}_1^{\text{HAG}}$.*

262 In sum, the stochastic models in [10] can be expressed with the framework of
263 Section 2.1. There is however a difference between [10] and Section 2.1. In [10], the
264 function φ is fixed. It is given as being a part of the stochastic model. In our side,
265 the function f is constructed from the probability measures that we are given in the
266 first place. It is not unique. Consequently, it is unclear whether or not the indices
267 \tilde{S}_1^{HAG} are uniquely determined.

268 **3. The sensitivity indices and their estimators.** In view of Section 2, we
 269 can assume that there are a random vector $(X, Z) \in \mathbb{R}^p \times \mathbb{R}$ with mutually independent
 270 $p+1$ components on some probability space (Ω, \mathcal{F}, P) and a real function f such that
 271 the pair $(X, f(X, Z)) \in \mathbb{R}^p \times \mathbb{R}$ represents a random observation (input, output) of
 272 the stochastic model of interest. To ensure the existence of the sensitivity indices and
 273 later to derive theoretical results for the estimators, we need to assume the following:
 274 there exists some function F with $\mathbb{E} F(X)^8 < \infty$ such that

$$275 \quad (3.1) \quad |f(X, Z)| \leq F(X)$$

276 almost surely. This assumption appears to be mild. In particular every stochastic
 277 model with bounded outputs fulfills the condition.

278 **3.1. Definition of the sensitivity indices.** We define two kinds of sensitivity
 279 indices. The sensitivity indices of the first kind exploit the existence of the function f
 280 by applying the Sobol-Hoeffding decomposition to it directly. The sensitivity indices
 281 of the second kind result from an application of the Sobol-Hoeffding decomposition
 282 to the conditional expectation of $f(X, Z)$ given X , which is a function of X alone.
 283 The indices of the second kind are those to which the estimators (1.4) mentioned in
 284 the Introduction converge.

285 **3.1.1. Indices of the first kind.** Applying the Sobol-Hoeffding decomposition
 286 to f yields

$$287 \quad (3.2) \quad f(X, Z) - f_0 = f_1(X_1) + \cdots + f_p(X_p) + f_{p+1}(Z) + \cdots,$$

289 where $f_0 = \mathbb{E} f(X, Z)$, $f_j(X_j) = \mathbb{E}(f(X, Z) - f_0 | X_j)$, $j = 1, \dots, p$, $f_{p+1}(Z) =$
 290 $\mathbb{E}(f(X, Z) - f_0 | Z)$ and $+\cdots$ stands for the interaction terms. Since X and Z are in-
 291 dependent, we have $\text{Var} f(X, Z) = \text{Var} f_1(X_1) + \cdots + \text{Var} f_p(X_p) + \text{Var} f_{p+1}(Z) + \cdots$,
 292 which leads us to the indices in Definition 3.1.

293 **DEFINITION 3.1** (Sobol indices of the first kind). *The Sobol indices of the first*
 294 *kind are defined as*

$$295 \quad S'_j = \frac{\text{Var} \mathbb{E}(f(X, Z) | X_j)}{\text{Var} f(X, Z)}, \quad j = 1, \dots, p.$$

296 It is important to notice that the indices of the first kind depend on the law
 297 of $(X, f(X, Z))$ only and hence are uniquely determined. Note that total sensitivity
 298 indices could be defined as well but it is unclear whether or not they depend on the
 299 chosen representation.

300 **3.1.2. Indices of the second kind.** Let $g(X) := \mathbb{E}(f(X, Z) | X)$ be the condi-
 301 tional expectation of the output of the stochastic model given the input. The object
 302 g is a function and the Sobol-Hoeffding decomposition can be applied to it, yielding

$$303 \quad g(X) - g_0 = g_1(X_1) + \cdots + g_p(X_p) + \cdots,$$

305 where $g_0 = \mathbb{E} g(X)$, $g_j(X_j) = \mathbb{E}(g(X) - g_0 | X_j)$, $j = 1, \dots, p$ and $+\cdots$ stands for the
 306 interaction terms. Since the components of X are independent, we have $\text{Var} g(X) =$
 307 $\text{Var} g_1(X_1) + \cdots + \text{Var} g_p(X_p) + \cdots$, leading to the indices in Definition 3.2.

308 **DEFINITION 3.2** (Sobol indices of the second kind). *The Sobol indices of the*
 309 *second kind are defined as*

$$310 \quad S''_j = \frac{\text{Var} \mathbb{E}(g(X) | X_j)}{\text{Var} g(X)} = \frac{\text{Var} \mathbb{E}[\mathbb{E}(f(X, Z) | X) | X_j]}{\text{Var} \mathbb{E}(f(X, Z) | X)}, \quad j = 1, \dots, p.$$

311 The total sensitivity indices, defined by

$$312 \quad (3.3) \quad S''_{Tj} = 1 - \frac{\text{Var E}(g(X)|X_1, \dots, X_{j-1}, X_{j+1}, \dots, X_p)}{\text{Var } g(X)},$$

313
314 $j = 1, \dots, p$, are uniquely determined.

315 **3.1.3. Comparison of the definitions.** The sensitivity indices of the first kind
316 provide more refined “first-order” information than the indices of the second kind.
317 Example 3 and 4 illustrate this.

318 **EXAMPLE 3.** Let $f(X, Z) = aX_1 + cX_2\phi(Z)$, where X_1, X_2, Z are independent
319 standard normal variables, a, c are real coefficients and ϕ is a function such that
320 $E\phi(Z) = 0$. Then

$$321 \quad S'_1 = \frac{a^2}{a^2 + c^2 E\phi(Z)^2}, S'_2 = 0, S''_1 = 1 \text{ and } S''_2 = 0.$$

323 According to the sensitivity indices of the second kind, X_1 has the same impor-
324 tance regardless of the value of its coefficient a , while the sensitivity indices of the
325 first kind acknowledge that the importance of X_1 should depend on its coefficient.
326 However, the sensitivity indices of the first kind cannot provide insight into the in-
327 teractions between the inputs. For instance, if a is small then the sum $S'_1 + S'_2$ will
328 be small and hence the contribution to the variance of the output must come from
329 elsewhere. Perhaps it comes from the intrinsic stochasticity of the model or from the
330 interactions.

331 Example 4 returns to the model (2.1).

332 **EXAMPLE 4.** Let $f(X, Z) = \Phi^{-1}(Z)X_2 + X_1$ such that the law of X_1 and that
333 of Z are the uniform distribution on $(0, 1)$, the law of X_2 is the uniform distribution
334 on $(1, L + 1)$, $L > 0$, and Φ^{-1} denotes the inverse distribution function of the stan-
335 dard normal distribution. It is easy to see that $S''_1 = 1$ and $S''_2 = 0$. The detailed
336 calculations in Appendix A show that $S'_2 = 0$ and

$$337 \quad S'_1 = \frac{1}{4(L^2 + 3(L + 1)) + 1}.$$

339 As in Example 3, the sensitivity indices of the second kind do not depend on the
340 coefficient L . The sensitivity indices of the first kind do depend on L but note that
341 $S'_1 + S'_2 \leq 1/13$, indicating that most of the contribution to the output comes from
342 the intrinsic randomness or the interactions.

343 In sum, both kinds of sensitivity indices provide useful insights although neither
344 kind is perfect. The sensitivity indices of the second kind are good indices for doing a
345 sensitivity analysis of the model averaged over the intrinsic randomness but by doing
346 so information may be lost. The sensitivity indices of the first kind provide more
347 refined information into the individual contributions of the inputs but the information
348 is only partial because the knowledge of the interactions and the intrinsic randomness
349 are lacking.

350 **3.2. Construction of the estimators.** We construct estimators for the indices
351 in Definition 3.1 and 3.2 by Monte-Carlo simulation. The input space is “explored”
352 n times; at each exploration two independent input vectors are drawn, combined
353 and passed to the stochastic model which is run m times. The integer n is called
354 the number of explorations and the integer m is called the number of repetitions.

355 The couple (n, m) is called the *design* of the Monte-Carlo sampling scheme. The
 356 total number of calls to the stochastic model is $mn(p + 1)$. The details are given in
 357 Algorithm 3.1.

Algorithm 3.1 Generate a Monte-Carlo sample

for $i = 1$ to n **do**
 draw two independent copies $X^{(i)} = (X_1^{(i)}, \dots, X_p^{(i)})$, $\tilde{X}^{(i)} = (\tilde{X}_1^{(i)}, \dots, \tilde{X}_p^{(i)})$
for $j = 0, 1, \dots, p$ **do**
for $k = 1$ to m **do**
 run the stochastic model at $\tilde{X}_{-j}^{(i)} := (\tilde{X}_1^{(i)}, \dots, \tilde{X}_{j-1}^{(i)}, X_j^{(i)}, \tilde{X}_{j+1}^{(i)}, \dots, \tilde{X}_p^{(i)})$ to
 get an output $Y_j^{(i,k)}$
end for
end for
end for

358 In the algorithm above, $\tilde{X}_{-0}^{(i)} = X^{(i)}$ by convention. By assumption, the objects
 359 $\tilde{X}^{(i)}$, $\tilde{X}_{-j}^{(i)}$ and $Y_j^{(i,k)}$, $j = 0, \dots, p$, $k = 1, \dots, m$, $i = 1, \dots, n$, are random vectors
 360 such that the sets $\{\tilde{X}^{(i)}, \tilde{X}_{-j}^{(i)}, Y_j^{(i,k)} : j = 0, \dots, p; k = 1, \dots, m\}$, $i = 1, \dots, n$, are
 361 i.i.d., $X^{(i)}$ and $\tilde{X}^{(i)}$ are independent and $P(\cap_{j=0}^p \cap_{k=1}^m \{Y_j^{(i,k)} \in B_j^{(k)}\} | X^{(i)}, \tilde{X}^{(i)}) =$
 362 $\prod_{j=0}^p \prod_{k=1}^m P(Y_j^{(i,k)} \in B_j^{(k)} | X^{(i)}, \tilde{X}^{(i)})$ for all Borel sets $B_j^{(k)} \in \mathcal{B}$. It is easy to see that
 363 these conditions characterize the joint law of the set $\{\tilde{X}_{-j}^{(i)}, Y_j^{(i,k)} : j = 0, \dots, p; k =$
 364 $1, \dots, m; i = 1, \dots, n\}$, that is, the inputs and the outputs of Algorithm 3.1.

365 In view of Section 2, assume without loss of generality that there is some function
 366 f and some random variables $Z_j^{(i,k)}$, $j = 0, \dots, p$, $k = 1, \dots, m$, $i = 1, \dots, n$, such that
 367 $Y_j^{(i,k)} = f(\tilde{X}_{-j}^{(i)}, Z_j^{(i,k)})$, where all of the random vectors in the sets $\{\tilde{X}^{(i)}, X^{(i)}, Z_j^{(i,k)} :$
 368 $j = 0, \dots, p; k = 1, \dots, m\}$, $i = 1, \dots, n$, are mutually independent and all of these
 369 sets are i.i.d. We shall use both the notations Y and $f(X, Z)$ to denote the outputs.

370 With the above notation, the estimators (1.4) of the indices of the second kind
 371 are rewritten

$$372 \quad (3.4) \quad \hat{S}_{j;n,m}'' = \frac{\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \frac{1}{m} \sum_{k'=1}^m Y_j^{(i,k')} - \left(\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \right)^2}{\frac{1}{n} \sum_{i=1}^n \left(\frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \right)^2 - \left(\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \right)^2},$$

373 $j = 1, \dots, p$, which are indeed the empirical versions of the indices S_j'' , since

$$374 \quad S_j'' = \frac{\mathbb{E} g(X^{(1)}) g(\tilde{X}_{-j}^{(1)}) - (\mathbb{E} g(X^{(1)}))^2}{\mathbb{E} g(X^{(1)})^2 - (\mathbb{E} g(X^{(1)}))^2}$$

$$375 \quad (3.5) \quad = \frac{\mathbb{E} \mathbb{E}[f(X^{(1)}, Z_0^{(1,1)}) | X^{(1)}] \mathbb{E}[f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) | \tilde{X}_{-j}^{(1)}] - (\mathbb{E} \mathbb{E}[f(X^{(1)}, Z_0^{(1,1)}) | X^{(1)}])^2}{\mathbb{E} \mathbb{E}[f(X^{(1)}, Z_0^{(1,1)}) | X^{(1)}]^2 - (\mathbb{E} \mathbb{E}[f(X^{(1)}, Z_0^{(1,1)}) | X^{(1)}])^2}.$$

377 As said in the Introduction, this estimator is used implicitly by practitioners but has
 378 not been formally studied in the literature. A simplified version with $m = n$ appears
 379 in [13, 14].

380 To estimate the sensitivity indices of the first kind, we exploit a formula similar
381 to (3.5). Indeed, we have

$$\begin{aligned}
 382 \quad S'_j &= \frac{\mathbb{E} f(X^{(1)}, Z_0^{(1,1)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) - (\mathbb{E} f(X^{(1)}, Z_0^{(1,1)}))^2}{\mathbb{E} f(X^{(1)}, Z_0^{(1,1)})^2 - (\mathbb{E} f(X^{(1)}, Z_0^{(1,1)}))^2} \\
 (3.6) \quad &= \frac{\mathbb{E} \mathbb{E}[f(X^{(1)}, Z_0^{(1,1)}) | X^{(1)}] \mathbb{E}[f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) | \tilde{X}_{-j}^{(1)}] - \left(\mathbb{E} \mathbb{E}[f(X^{(1)}, Z_0^{(1,1)}) | X^{(1)}] \right)^2}{\mathbb{E} \mathbb{E}[f(X^{(1)}, Z_0^{(1,1)})^2 | X^{(1)}] - \left(\mathbb{E} \mathbb{E}[f(X^{(1)}, Z_0^{(1,1)}) | X^{(1)}] \right)^2}. \\
 383 \quad & \\
 384 \quad &
 \end{aligned}$$

385 Notice that the upper left, upper right and the lower right terms are identical to the
386 upper left, upper right and the lower right terms in (3.5) respectively. The upper
387 left term is the only term that depends on j and, therefore, it is the only term that
388 permits to discriminate between any two indices of the same kind. For this reason, it
389 is called the *discriminator*. It is denoted by D_j . Formula (3.6) yields the estimator

$$\begin{aligned}
 390 \quad (3.7) \quad \hat{S}'_{j;n,m} &= \frac{\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \frac{1}{m} \sum_{k'=1}^m Y_j^{(i,k')} - \left(\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \right)^2}{\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)^2} - \left(\frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \right)^2}. \\
 391 \quad & \\
 392 \quad & \\
 393 \quad & \\
 394 \quad & \\
 395 \quad &
 \end{aligned}$$

391 Since the estimators for the discriminator are identical, both kinds of sensitivity
392 indices lead to the same estimated ranking of the inputs. All of the $2p$ estimators
393 can be computed with $mn(p+1)$ runs of the stochastic model. In (3.7) and (3.4), if
394 $m=1$ and if the function f does in fact not depend on Z , then the estimators reduce
395 to Sobol estimators [29, 30] for deterministic models.

396 **4. Choosing between Monte-Carlo designs.** The estimators in Section 3
397 depend on the design (n, m) of the Monte-Carlo sampling scheme. To estimate the
398 sensitivity indices in Definition 3.1 and Definition 3.2, the stochastic model has to be
399 called $(p+1)mn$ times.

400 It is reasonable to think of a sensitivity analysis as done the following way. The
401 total number of calls is set to a limit, say T . Then n and m are chosen so that
402 $T = (p+1)mn$. For instance, suppose that one cannot afford more than 150 calls to
403 a model with two inputs. Then $T = 150$, $p = 2$ and one can choose either one of the
404 columns in the following table

405	n	50	25	10	5	2	1
	m	1	2	5	10	25	50.

406 Denote by $\text{div}_p(T)$ the set of all divisors of $T/(p+1)$ between 1 and $T/(p+1)$.
407 In the example above, $\text{div}_2(150) = \{1, 2, 5, 10, 25, 50\}$. There are as many designs as
408 there are elements in the set $\text{div}_p(T)$. Each one of those elements corresponds to a
409 possible combination for n and m which Algorithm 3.1 can be run with. The resulting
410 estimators require the same number of calls but do not perform equally well. The
411 goal of this section is to find the “best” way to estimate the sensitivity indices.

412 **4.1. Introducing the miss-ranking error and its bound.** To compare the
413 estimators, a measure of performance has to be defined. We shall consider the miss-

414 ranking error (MRE), defined by

$$415 \quad \text{MRE} = \mathbb{E} \left(\sum_{j=1}^p |\hat{R}_{j;n,m} - R_j| \right),$$

416 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
 417 $\hat{R}_{j;n,m}$ is an estimator of R_j . Recall that D_1, \dots, D_p are the upper-left terms in (3.6)
 418 and (3.5). They determine the ranks of the sensitivity indices. The MRE is small
 419 when one succeeds in ranking the inputs from the most to the least important, a task
 420 which is called “factors prioritization” in [27, p. 52]. For simplicity, we assume that
 421 the sensitivity indices, and hence the quantities D_1, \dots, D_p , are distincts, so that they
 422 can be ranked unambiguously. This assumption is mild: even if D_j and $D_{j'}$ only differ
 423 by a small amount, it is still satisfied. Recall that the ranks of the sensitivity indices
 424 of the first kind coincide with the ranks of the sensitivity indices of the second kind.
 425 Thus, the MRE permits to find a unique solution for both kinds of sensitivity indices.

426 The MRE has a bound with interesting mathematical properties. Denote by
 427 $\text{MRE}(T, m)$ the MRE based on T calls to the model with m repetitions, so that the
 428 number of explorations is $T/(p+1)/m$. To shorten the notation, let $(X^{(1)}, \tilde{X}^{(1)}) = \mathbf{X}$,
 429 $f(X^{(1)}, Z_0^{(1,1)}) = Y_0$ and $f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) = Y_j$.

430 **PROPOSITION 4.1.** *Let $\hat{D}_{j;n,m}$, $j = 1, \dots, p$, be the upper-left term in (3.7) or (3.4) ■*
 431 *and put $\hat{R}_{j;n,m} = \sum_{i=1}^p \mathbf{1}(\hat{D}_{i;n,m} \leq \hat{D}_{j;n,m})$. If D_1, \dots, D_p are all distincts then*

$$432 \quad \text{MRE}(T, m) \leq \frac{L}{nm} \left(m \sum_{j=1}^p \text{Var}(\mathbb{E}[Y_0 Y_j | \mathbf{X}]) \right. \\
 433 \quad \quad \quad \left. + \sum_{j=1}^p \mathbb{E}[\text{Var}(Y_0 Y_j | \mathbf{X}) - \text{Var}(Y_0 | \mathbf{X}) \text{Var}(Y_j | \mathbf{X})] \right. \\
 434 \quad \quad \quad \left. + \frac{1}{m} \sum_{j=1}^p \mathbb{E}[\text{Var}(Y_0 | \mathbf{X}) \text{Var}(Y_j | \mathbf{X})] \right), \\
 435$$

436 where

$$437 \quad L = \frac{4(p-1)}{\min_{j < j'} (|D_j - D_{j'}|^2)}.$$

438

439 The constant L tells us that the bound is smaller when the indices are well
 440 separated. The bound goes to zero when the number of explorations goes to infinity.
 441 This is true even if the number of repetitions is fixed. Most interestingly, the bound
 442 separates T and m : substituting $T/(p+1)$ for nm in the denominator of the bound,
 443 we get

$$444 \quad (4.1) \quad \text{MRE}(T, m) \leq \frac{1}{T} v(m), \quad m \in \text{div}_p(T), \\
 445$$

446 where
447

$$448 \quad v(m) = L(p+1) \left(m \sum_{j=1}^p \text{Var}(\mathbb{E}[Y_0 Y_j | \mathbf{X}]) + \sum_{j=1}^p \mathbb{E}[\text{Var}(Y_0 Y_j | \mathbf{X}) - \text{Var}(Y_0 | \mathbf{X}) \text{Var}(Y_j | \mathbf{X})] \right. \\ 449 \quad \left. + \frac{1}{m} \sum_{j=1}^p \mathbb{E}[\text{Var}(Y_0 | \mathbf{X}) \text{Var}(Y_j | \mathbf{X})] \right). \\ 450$$

451 Denote by m_T^\dagger the element $m \in \text{div}_p(T)$ that minimizes $v(m)$. Taking $m = m_T^\dagger$
452 in (4.1), we get the bound

$$453 \quad \text{MRE}(T, m_T^\dagger) \leq \frac{v(m_T^\dagger)}{T} \leq \frac{v(m)}{T}, \quad \text{for all } m \in \text{div}_p(T).$$

454 Thus choosing $m = m_T^\dagger$ and $n = T/(p+1)/m_T^\dagger$ in Algorithm 3.1 ensures that the
455 MRE cannot exceed the least possible bound. The least possible bound $v(m_T^\dagger)/T$
456 is also called *the best obtainable guarantee*. However, m_T^\dagger is unknown and must be
457 estimated.

458 *Remark 4.2.* The choice of T , through the specification of $\text{div}_p(T)$, will influence
459 the quality of the bound. It is clear that choosing $T/(p+1)$ a prime number may not
460 be a good idea because $v(m_T^\dagger)$ will be either $v(1)$ or $v(T/(p+1))$. On the opposite,
461 choosing $T/(p+1)$ a factorial number ensures many more choices (in fact, all).

462 **4.2. A two-stage procedure to estimate the sensitivity indices.** The re-
463 sults in Section 4.1 suggest a two-stage procedure to estimate the sensitivity indices.
464 The procedure is given in Algorithm 4.1. The computational budget is split into two
465 parts K and $T - K$. Denote by m_{T-K}^\dagger the element $m \in \text{div}_p(T - K)$ that minimizes
466 the function $v(m)$. The first K calls to the model are used to estimate m_{T-K}^\dagger . The
467 last $T - K$ calls to the model are used to estimate the sensitivity indices.

Algorithm 4.1 Estimate the sensitivity indices by a two-stage procedure

Stage 1. Choose an integer K such that $K/(p+1)$ and $(T - K)/(p+1)$ are integers
also. Choose integers m_0 and n_0 such that $K = m_0 n_0 (p+1)$. Run Algorithm 3.1
with $m = m_0$ and $n = n_0$. Estimate m_{T-K}^\dagger by an estimator $\hat{m}_{T-K}^\dagger \in \text{div}_p(T - K)$.

Stage 2. Run Algorithm 3.1 with $m = \hat{m}_{T-K}^\dagger$ and

$$n = \frac{T - K}{(p+1)\hat{m}_{T-K}^\dagger}.$$

Compute the sensitivity indices estimators (3.7) and (3.4).

468 In Algorithm 4.1 we need \hat{m}_{T-K}^\dagger an estimator of m_{T-K}^\dagger . Let us build one. Let
469 m^* be the minimizer of v seen as a function on the positive reals. Since v is convex,
470 the minimizer is unique. It follows from (4.1) and Proposition 4.1 that

$$471 \quad (4.2) \quad m^* := \sqrt{\frac{\sum_{j=1}^p \mathbb{E}[\text{Var}(Y_0 | \mathbf{X}) \text{Var}(Y_j | \mathbf{X})]}{\sum_{j=1}^p \text{Var}(\mathbb{E}[Y_0 Y_j | \mathbf{X}])}} = \sqrt{\frac{\sum_{j=1}^p \zeta_{3,j}}{\sum_{j=1}^p \zeta_{1,j}}}, \\ 472$$

473 where $\zeta_{3,j} = \mathbb{E}[\text{Var}(Y_0|\mathbf{X}) \text{Var}(Y_j|\mathbf{X})]$ and $\zeta_{1,j} = \text{Var}(\mathbb{E}[Y_0 Y_j|\mathbf{X}])$, $j = 1, \dots, p$.

474 Let $\varphi_T : (0, \infty) \rightarrow \text{div}_p(T)$, be the function defined by $\varphi_T(x) = 1$ if $0 < x < 1$,
475 $\varphi_T(x) = T/(p+1)$ if $x > T/(p+1)$, and

$$476 \quad \varphi_T(x) = \begin{cases} \lfloor x \rfloor_T & \text{if } \sqrt{\lfloor x \rfloor_T \lceil x \rceil_T} > x \geq 1 \\ \lceil x \rceil_T & \text{if } \sqrt{\lfloor x \rfloor_T \lceil x \rceil_T} \leq x \leq \frac{T}{p+1} \end{cases}$$

478 where

$$479 \quad \lfloor x \rfloor_T = \max\{m \in \text{div}_p(T), m \leq x\}, \quad \lceil x \rceil_T = \min\{m \in \text{div}_p(T), m \geq x\}.$$

481 The function φ_T is piecewise constant with discontinuity points at \sqrt{ij} , where i and
482 j are two consecutive elements of $\text{div}_p(T)$.

483 **PROPOSITION 4.3.** *If $m^* > 0$ then $m_{T-K}^\dagger = \varphi_{T-K}(m^*)$. If, moreover,
484 $\lfloor m^* \rfloor_{T-K} \lceil m^* \rceil_{T-K}$ is not equal to m^{*2} then the minimizer of $v(m)$, $m \in \text{div}_p(T-K)$,
485 is unique.*

486 Proposition 4.3 suggests that m_{T-K}^\dagger can be estimated by applying the function
487 φ_{T-K} to an estimate of m^* . Thus, our problem of estimating m_{T-K}^\dagger boils down to
488 the problem of estimating m^* . Let us find an estimator of m^* . Remember that it has
489 to be based on the first $K = m_0 n_0 (p+1)$ calls to the model. In view of (4.2), put

$$490 \quad (4.3) \quad \hat{m}_K^* := \sqrt{\frac{\sum_{j=1}^p \hat{\zeta}_{3,j}}{\sum_{j=1}^p \hat{\zeta}_{1,j}}},$$

491 where

$$492 \quad \hat{\zeta}_{3,j} =$$

$$493 \quad (4.4) \quad \frac{1}{n_0} \sum_{i=1}^n \frac{1}{m_0} \sum_{k_1=1}^{m_0} f(X^{(i)}, Z_0^{(i,k_1)})^2 \frac{1}{m_0} \sum_{k_2=1}^{m_0} f(\tilde{X}_{-j}^{(i)}, Z_j^{(i,k_2)})^2$$

$$494 \quad (4.5) \quad + \frac{1}{n_0} \sum_{i=1}^n \left(\frac{1}{m_0} \sum_{k_1=1}^{m_0} f(X^{(i)}, Z_0^{(i,k_1)}) \right)^2 \left(\frac{1}{m_0} \sum_{k_2=1}^{m_0} f(\tilde{X}_{-j}^{(i)}, Z_j^{(i,k_2)}) \right)^2$$

$$495 \quad (4.6) \quad - \frac{1}{n_0} \sum_{i=1}^n \left(\frac{1}{m_0} \sum_{k_1=1}^{m_0} f(X^{(i)}, Z_0^{(i,k_1)}) \right)^2 \frac{1}{m_0} \sum_{k_2=1}^{m_0} f(\tilde{X}_{-j}^{(i)}, Z_j^{(i,k_2)})^2$$

$$496 \quad (4.7) \quad - \frac{1}{n_0} \sum_{i=1}^n \frac{1}{m_0} \sum_{k_1=1}^{m_0} f(X^{(i)}, Z_0^{(i,k_1)})^2 \left(\frac{1}{m_0} \sum_{k_2=1}^{m_0} f(\tilde{X}_{-j}^{(i)}, Z_j^{(i,k_2)}) \right)^2,$$

498 and

$$499 \quad \hat{\zeta}_{1,j} =$$

$$500 \quad (4.8) \quad \frac{1}{n_0} \sum_{i=1}^n \left(\frac{1}{m_0} \sum_{k=1}^{m_0} f(X^{(i)}, Z_0^{(i,k)}) f(\tilde{X}_{-j}^{(i)}, Z_j^{(i,k)}) \right)^2$$

$$501 \quad (4.9) \quad - \left(\frac{1}{n_0} \sum_{i=1}^n \frac{1}{m_0} \sum_{k=1}^{m_0} f(X^{(i)}, Z_0^{(i,k)}) f(\tilde{X}_{-j}^{(i)}, Z_j^{(i,k)}) \right)^2.$$

502

503 Notice that $\widehat{\zeta}_{1,j} \geq 0$ and $\widehat{\zeta}_{3,j} \geq 0$ so that $\widehat{m}_K^* \geq 0$. If $m_0 = 1$ then $\widehat{\zeta}_{3,j} = 0$ and hence
 504 $\widehat{m}_K^* = 0$.

505 The estimator \widehat{m}_K^* is consistent and asymptotically normal on some conditions
 506 on the rates of n_0 and m_0 .

507 **THEOREM 4.4.** *Assume (3.1) holds. Let $n_0 \rightarrow \infty$. If m_0 is fixed then*

$$508 \quad \sqrt{n_0} \left(\widehat{m}_K^* - \left[m^* + \frac{C}{m_0} + \epsilon_{m_0} \right] \right) \xrightarrow{d} \mathcal{N}(0, \sigma_{m_0}^2),$$

509 where C is some constant, $\epsilon_{m_0} = C_1/m_0^2 + \dots + C_N/m_0^{N+1}$ for some constants
 510 C_1, \dots, C_N and $\sigma_{m_0}^2$ is some variance depending on m_0 . If $m_0 \rightarrow \infty$ then the above
 511 display with $\epsilon_{m_0} = o(1/m_0)$ and σ_{m_0} replaced by $\lim_{m_0 \rightarrow \infty} \sigma_{m_0}$ is true.

512 Theorem 4.4 shows that \widehat{m}_K^* is asymptotically biased. The bias is polynomial in
 513 $1/m_0$. Corollary 4.5 shows that letting $m_0 \rightarrow \infty$ suffices to get the consistency of \widehat{m}_K^*
 514 but to get a central limit theorem centered around m^* , it is furthermore needed that
 515 $\sqrt{n_0}/m_0 \rightarrow 0$.

516 **COROLLARY 4.5.** *Assume (3.1) holds. Let $n_0 \rightarrow \infty$ and $m_0 \rightarrow \infty$. Then $\widehat{m}_K^* \xrightarrow{P}$
 517 m^* . If, moreover, $\sqrt{n_0}/m_0 \rightarrow 0$, then*

$$518 \quad \sqrt{n_0}(\widehat{m}_K^* - m^*) \xrightarrow{d} \mathcal{N}(0, \lim_{m_0 \rightarrow \infty} \sigma_{m_0}^2).$$

519 Now we have everything that is needed to estimate m_{T-K}^\dagger . Put $\widehat{m}_{T-K}^\dagger =$
 520 $\varphi_{T-K}(\widehat{m}_K^*)$. Proposition 4.6 states that $\widehat{m}_{T-K}^\dagger$ and m_{T-K}^\dagger are equal with proba-
 521 bility going to one.

522 **PROPOSITION 4.6.** *Assume (3.1) holds. Let $n_0 \rightarrow \infty$ and $m_0 \rightarrow \infty$. Then*

$$523 \quad P \left(\widehat{m}_{T-K}^\dagger = m_{T-K}^\dagger \right) \rightarrow 1.$$

524 All the details of Algorithm 4.1 have been given.

525 **4.3. Performance.** To get some insight into the performance of Algorithm 4.1,
 526 we look at the estimators produced in Stage 2, which are built with $T - K$ calls
 527 to the model with $\widehat{m}_{T-K}^\dagger$ repetitions and $(T - K)/(p + 1)/\widehat{m}_{T-K}^\dagger$ explorations. Let
 528 $\widehat{D}_{j;\hat{n},\widehat{m}}$, $j = 1, \dots, p$, be the discriminators of those estimators, so that $\hat{n} = (T -$
 529 $K)/(p + 1)/\widehat{m}_{T-K}^\dagger$ and $\widehat{m} = \widehat{m}_{T-K}^\dagger$. Let $\widehat{R}_{j;\hat{n},\widehat{m}}$ be the rank of $\widehat{D}_{j;\hat{n},\widehat{m}}$ among
 530 $\widehat{D}_{1;\hat{n},\widehat{m}}, \dots, \widehat{D}_{p;\hat{n},\widehat{m}}$. The conditional expectation of $\sum_{j=1}^p |\widehat{R}_{j;\hat{n},\widehat{m}} - R_j|$ given the
 531 outputs produced in Stage 1 is equal to $\text{MRE}(T - K, \widehat{m}_{T-K}^\dagger)$, the MRE based on
 532 $T - K$ calls to the model with $\widehat{m}_{T-K}^\dagger$ repetitions and $(T - K)/(p + 1)/\widehat{m}_{T-K}^\dagger$ explo-
 533 rations. Recall that the estimator $\widehat{m}_{T-K}^\dagger$ is computed with K calls to the model and
 534 by construction $\widehat{m}_{T-K}^\dagger \in \text{div}_p(T - K)$. Equation (4.1) yields

$$536 \quad (4.10) \quad \text{MRE}(T - K, \widehat{m}_{T-K}^\dagger) \leq \frac{1}{T - K} v(\widehat{m}_{T-K}^\dagger),$$

537 where the inequality above is to be understood almost surely, since both sides of
 538 equation are random variables.

539 We shall show that, under conditions on T and K , the bound in (4.10) is in
 540 fact close to the best obtainable guarantee $v(m_T^\dagger)/T$. Suppose for simplicity that
 541

542 $\text{div}_p(T - K) \subset \text{div}_p(T)$. Since $\widehat{m}_{T-K}^\dagger \in \text{div}_p(T - K)$ by construction, we have
 543 $\widehat{m}_{T-K}^\dagger \in \text{div}_p(T)$ and therefore $v(m_T^\dagger)/T \leq v(\widehat{m}_{T-K}^\dagger)/(T - K)$ by definition of m_T^\dagger .
 544 The left hand side is the best guarantee we can hope for and corresponds to the case
 545 where $K = 0$ in Algorithm 4.1. It can be interpreted as the guarantee obtained if we
 546 would know the value of m^* in (4.2), for in that case we would not need to spend
 547 budget in Stage 1 of Algorithm 4.1. We proceed in two steps.

548 **THEOREM 4.7.** *Assume that the conditions of Proposition 4.6 are fulfilled. Suppose*
 549 *furthermore that $K \rightarrow \infty$ such that $K/T \rightarrow 0$. Then*

$$550 \frac{1}{T - K} v(\widehat{m}_{T-K}^\dagger) = \frac{1}{T} v(m_{T-K}^\dagger) (1 + o_P(1)).$$

552 Theorem 4.7 holds without the condition $\text{div}_p(T - K) \subset \text{div}_p(T)$. Imposing this
 553 condition, we get Corollary 4.8 below.

554 **COROLLARY 4.8.** *If, in addition to the conditions of Theorem 4.7, $\text{div}_p(T - K) \subset$*
 555 *$\text{div}_p(T)$ then*

$$556 \text{MRE}(T - K, \widehat{m}_{T-K}^\dagger) \leq \frac{v(m_T^\dagger)}{T} (1 + o_P(1)).$$

558 The result of Corollary 4.8 easily follows from (4.10) and Theorem 4.7 because
 559 $m_{T-K}^\dagger = m_T^\dagger$ as soon as $(T - K)/(p + 1) > m_{T-K}^\dagger$, which happens eventually as T
 560 and K go to infinity because the function v is convex.

561 **5. Asymptotic normality of the sensitivity indices estimators.** The sensi-
 562 tivity indices estimators of Section 3.2 depend on both m and n . It is clear that
 563 n should go to infinity to get central limit theorems. It may be less clear, however,
 564 whether or not m should go to infinity as well. The answer depends on the kind of
 565 the sensitivity index we are looking at.

566 Two frameworks are considered:

- 567 • $n \rightarrow \infty$ and m is fixed;
- 568 • $n \rightarrow \infty$ and $m \rightarrow \infty$.

569 In the second framework $m = m_n$ is a sequence indexed by n that goes to infinity as
 570 n goes to infinity. Denote by \mathbf{S}' (resp. \mathbf{S}'') the column vector with coordinates S'_j
 571 (resp. S''_j), $j = 1, \dots, p$, and denote by $\widehat{\mathbf{S}}'_{n,m}$ (resp. $\widehat{\mathbf{S}}''_{n,m}$) the column vector with
 572 coordinates $\widehat{S}'_{j;n,m}$ given in (3.7) (resp. $\widehat{S}''_{j;n,m}$ given in (3.4)). Theorem 5.1 below
 573 predicts that the joint vector $(\widehat{\mathbf{S}}'_{n,m}, \widehat{\mathbf{S}}''_{n,m})^\top$ is asymptotically normal.

574 **THEOREM 5.1.** *Assume (3.1) holds. Let $n \rightarrow \infty$. If m is fixed then*

$$575 \sqrt{n} \left(\widehat{\mathbf{S}}'_{n,m} - \mathbf{S}' \left[1 - \frac{\widehat{\mathbf{S}}'_{n,m} - \mathbf{S}'}{\text{E Var}(f(X, Z)|X) + m \text{Var E}(f(X, Z)|X)} \right] \right) \xrightarrow{d} \mathcal{N}(0, \Xi_m),$$

576 for some nonnegative matrix Ξ_m of size $2p \times 2p$. If $m \rightarrow \infty$ then, elementwise,
 577 $\lim_{m \rightarrow \infty} \Xi_m$ exists and the above display with Ξ_m replaced by $\lim_{m \rightarrow \infty} \Xi_m$ is true.

578 A blockwise reading of Theorem 5.1 shows that the behaviors of $\widehat{\mathbf{S}}'_{n,m}$ and $\widehat{\mathbf{S}}''_{n,m}$
 579 differ. While $\widehat{\mathbf{S}}'_{n,m}$ is asymptotically unbiased even if m is kept fixed, $\widehat{\mathbf{S}}''_{n,m}$ is asymptot-
 580 ically biased in general even if m goes to infinity. The estimator $\widehat{\mathbf{S}}''_{n,m}$ under-estimates
 581 \mathbf{S}'' . The bias, given by

$$582 \mathbf{S}'' \frac{\text{E Var}(f(X, Z)|X)}{\text{E Var}(f(X, Z)|X) + m \text{Var E}(f(X, Z)|X)},$$

583

584 is null whenever f actually does not depend on Z , and large whenever the stochastic
585 model is highly stochastic.

586 Corollary 5.2 below shows that m must go to infinity fast enough to avoid the
587 estimator to be concentrated around the wrong target.

588 COROLLARY 5.2. *Assume (3.1) holds. Let $n \rightarrow \infty$. If $m \rightarrow \infty$ such that $\sqrt{n}/m \rightarrow$
589 0 then*

$$590 \quad \sqrt{n} \left(\widehat{\mathbf{S}}''_{n,m} - \mathbf{S}'' \right) \xrightarrow{d} \mathcal{N}(0, \Xi_{22}),$$

591 where Ξ_{22} is the lower-right block of the matrix $\lim_{m \rightarrow \infty} \Xi_m$ given in Theorem 5.1.

592 The difference between $\widehat{\mathbf{S}}'_{n,m}$ and $\widehat{\mathbf{S}}''_{n,m}$ is due to the difference between the lower-
593 left terms in (3.7) and (3.4). While the lower-left term in (3.7) is unbiased for all n
594 and m , the lower-left term in (3.4) has a bias depending on m which propagates to the
595 estimator of the sensitivity indices. (The calculations are carried out in Appendix D.)
596 From a statistical perspective, it is more difficult to estimate the sensitivity indices of
597 the second kind than to estimate the sensitivity indices of the first kind. To estimate
598 the former, one needs to repeat the model many times. To estimate the later, this is
599 not necessary.

600 **6. Numerical tests.** Section 6.1 illustrates how the MRE responds to a change
601 in the Monte-Carlo design. In Section 6.1 the total budget T is kept fixed. Section 6.2
602 illustrates how the sensitivity indices estimators behave asymptotically. In Section 6.2
603 the total budget T increases.

604 **6.1. Comparison of Monte-Carlo designs.** The effect of the number of rep-
605 etitions on the sensitivity indices estimators and the effect of the calibration in the
606 two-stage procedure are examined in two kinds of experiments: the “direct” experi-
607 ments and the “calibration” experiments.

608 In the direct experiments, the sensitivity indices are estimated directly with the
609 given number of repetitions. Increasing numbers of repetitions m are tested. (Since
610 the budget is fixed, this goes with decreasing numbers of explorations.) For each m ,
611 the mean squared errors (MSEs), given by $\mathbb{E} \sum_{j=1}^p (\widehat{S}'_{j;n,m} - S'_j)^2$ and $\mathbb{E} \sum_{j=1}^p (\widehat{S}''_{j;n,m} -$
612 $S''_j)^2$, are estimated with replications. They are also split into the sum of the squared
613 biases and the sum of the variances to get further insight about the behavior of the
614 estimators. The MREs are estimated as well. A normalized version is considered:
615 it is the MRE divided by the number of variables. For models with two inputs, the
616 normalized MRE is interpreted directly as the probability that the two inputs are
617 ranked incorrectly.

618 In the calibration experiments, the sensitivity indices are estimated with the two-
619 stage procedure, the results of which depend on the calibration parameters K and
620 m_0 . Various calibration parameters are tested to see their effect on the MRE. The
621 budgets for the direct experiments and the calibration experiments are the same so
622 that the numbers can be compared. In particular, the direct experiments correspond
623 to the case $K = 0$ in the calibration experiments.

624 A linear model of the form $Y = X_1 + \beta X_2 + \sigma Z$, where X_1, X_2, Z , are standard
625 normal random variables and β, σ are real coefficients, has been considered because
626 the sensitivity indices are explicit and hence the performance of the estimators can
627 be evaluated easily. The quantity m^* is explicit: the formula is given in Appendix E.

628 **6.1.1. High noise context.** The coefficients are $\beta = 1.2$ and $\sigma = 4$. The
629 sensitivity indices are $S'_1 = 0.05$, $S'_2 = 0.08$, $S''_1 = 0.41$ and $S''_2 = 0.59$. The real

$K/3$	m_0				n_0			
	2	5	10	20	20	10	5	2
400	0.43	0.42	0.42	-	-	0.42	0.39	0.40
200	0.38	0.39	0.37	-	-	0.35	0.35	0.34
100	0.36	0.37	-	-	-	-	0.32	0.30
50	0.39	0.33	-	-	-	-	0.33	0.31

Table 1: Normalized MRE in the linear model with high noise for various calibrations: $K/(p+1) = 50, 100, 200, 400$ and $m_0 = 2, 5, 10, 20, \dots$. For instance, for $K/(p+1) = 200 = m_0 n_0$, the normalized MRE is available for $m_0 = 2, 5, 10, 20, 40, 100$.

630 m^* is about 5.8. The total budget is $T = 3 \times 500 = 1500$ and hence $\text{div}_2(1500) =$
631 $\{1, 2, 4, 5, 10, 20, 25, 50, 100, 125, 250, 500\}$. The integer m_{1500}^\dagger is equal to $\varphi_{1500}(m^*) =$
632 5. Since the budget is kept fixed, the numbers of explorations are, respectively,
633 500, 250, 125, 100, 50, 25, 20, 10, 5, 4, 2, 1. The number of replications is 1500.

634 The results of the direct experiment are given in Figure 1 for $m = 1, 2, 4, 5, 10,$
635 20, 25. The MSE of first kind does not vary with the number of repetitions and is
636 much lower than the MSE of second kind, see (c). The estimators of the second kind
637 are highly biased for small numbers of repetitions (a) and they have a higher variance
638 for larger numbers of repetitions (b). The fact that the bias is high for small numbers
639 of repetitions agrees with the theory, according to which the bias should vanish as m
640 goes to infinity. Overall, the sensitivity indices of the second kind seem to be much
641 harder to estimate than the indices of the first kind, the estimators of which have a
642 negligible bias and a very small variance whatever the number of repetitions.

643 According to Figure 1(c), the normalized MRE curve has a banana shape with a
644 minimum of about slightly less than 30% reached around $m \in \{5, 10\}$ and endpoints
645 with a value of about 35%. A value of 30% means that the probability of ranking
646 the inputs correctly is about 70%. The region of observed optimal performance $m \in$
647 $\{5, 10\}$ coincides with $m_{1500}^\dagger = 5$, the point at which the bound is minimal.

648 The results of the calibration experiment is given in Table 1 for the normalized
649 MRE. The lowest MREs are reached at the bottom right of the table, with values
650 corresponding to $2 \leq m \leq 10$ in Figure 1 (c). Optimal performance is reached with
651 very few explorations in the first stage of the two-stage procedure. In this case, the
652 estimator \widehat{m}_K^* has a small bias but a high variance. It seems to be better than an
653 estimator with a small variance but a large bias. This might be explained by the low
654 curvature of the MRE curve.

655 **6.1.2. Low noise context.** The coefficients are $\beta = 1.2$ and $\sigma = 0.9$. The
656 sensitivity indices are $S'_1 = 0.31$, $S'_2 = 0.44$, $S''_1 = 0.41$ and $S''_2 = 0.59$. The real
657 m^* is about 0.30 and hence the integer m_{1500}^\dagger is equal to 1. As expected, these
658 numbers are smaller than the ones found in the high noise context. The total budget
659 is $T = 3 \times 500 = 1500$. The number of replications is 500.

660 The results for the direct experiment are given in Figure 2. The MSE of first
661 kind increases with the number of repetitions, see (c): this is due to the increase
662 of the variance (b), while the bias is negligible (a). As in the high noise context,
663 the estimators of the second kind have a decreasing bias and an increasing variance,
664 although the decrease of the bias is of much less magnitude. This agrees with the
665 theory, where we have seen that, for the sensitivity indices of the second kind, the
666 biases of the estimators are small when the noise of the model is low.

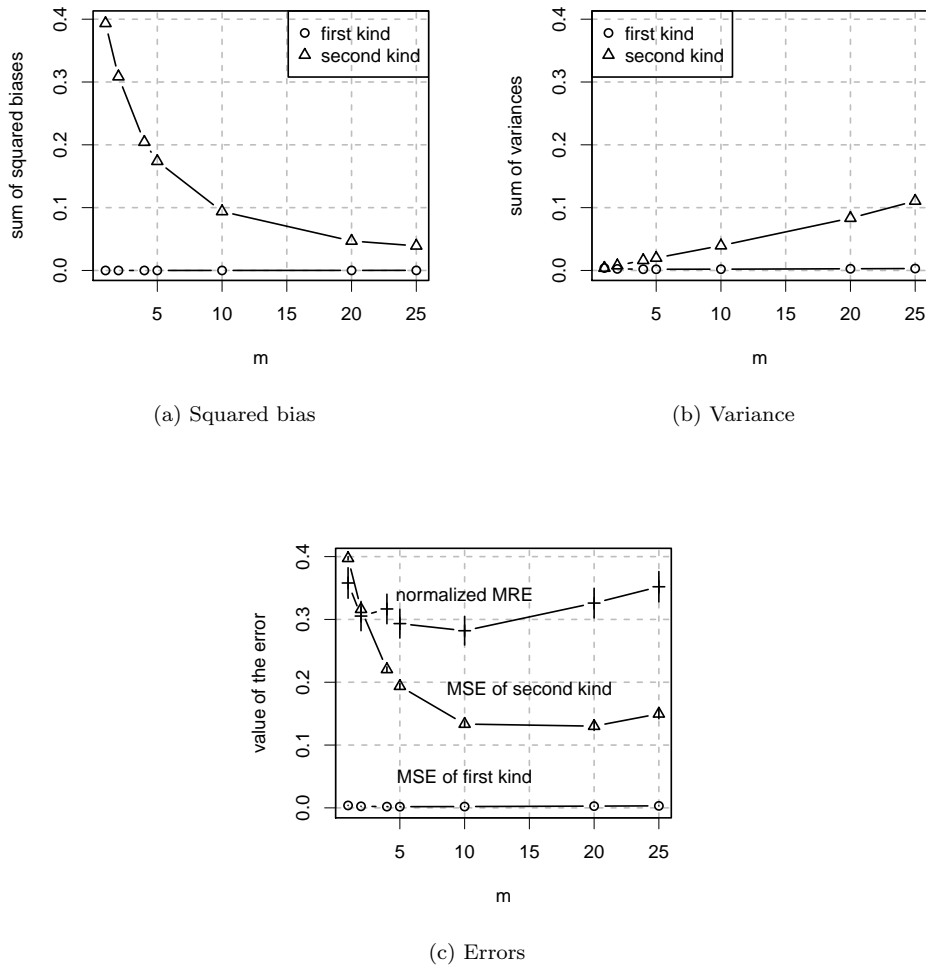


Fig. 1: Sum of squared biases (a), sum of variances (b) and errors (c) of the sensitivity indices estimators for the linear model in the high noise setting. Confidence intervals of level 95% are added in (c).

667 In Figure 2 (c), the normalized MRE varies a lot. It increases from about 2% at
 668 $m = 1$ to 30% at $m = 25$. Thus, unlike in the high noise setting, choosing a good
 669 number of repetitions is important. The best performance is achieved at $m = 1$, which
 670 coincides with the minimizer $m_{1500}^{\dagger} = 1$ of the bound.

671 The results of the calibration experiment for the normalized MRE is given in
 672 Table 2. The best performance is reached at the bottom left of the table with numbers
 673 that correspond to the optimal performance in Figure 2 (c). Moreover, notice that a
 674 large spectrum of calibration parameters (K, m_0) yield low errors.

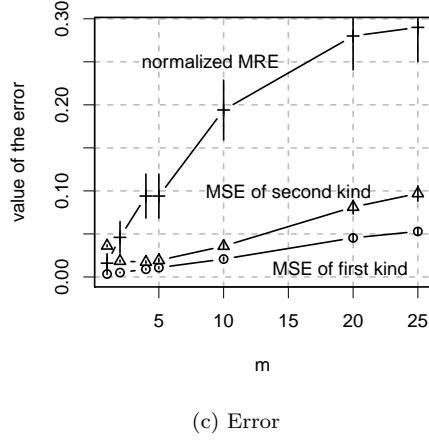
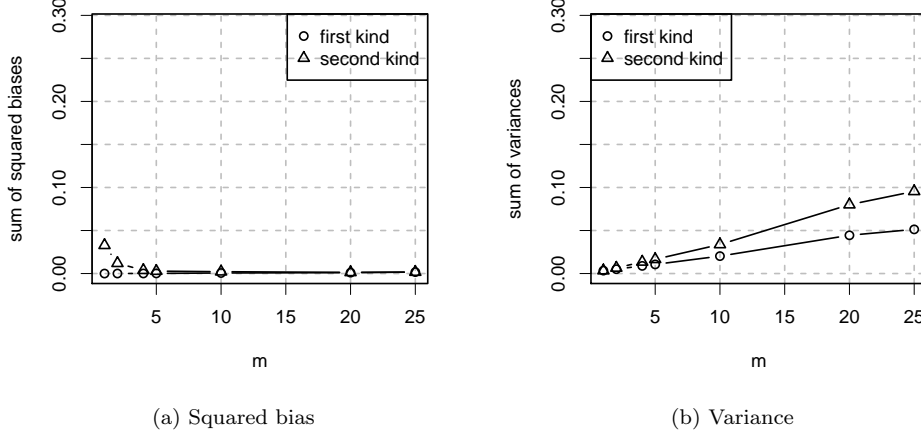


Fig. 2: Sum of squared biases (a), sum of variances (b) and errors (c) of the sensitivity indices estimators for the linear model in the low noise context. Confidence intervals of level 95% are added in (c).

$K/3$	m_0				n_0			
	2	5	10	20	20	10	5	2
400	0.18	0.15	0.17	-	-	0.16	0.18	0.20
200	0.05	0.04	0.04	-	-	0.06	0.05	0.07
100	0.02	0.04	-	-	-	-	0.04	0.04
50	0.03	0.02	-	-	-	-	0.02	0.04

Table 2: Normalized MRE in the linear model with low noise for various calibrations: $K/(p + 1) = 50, 100, 200, 400$ and $m_0 = 2, 5, 10, 20, \dots$. For instance, for $K/(p + 1) = 200 = m_0 n_0$, the normalized MRE is available for $m_0 = 2, 5, 10, 20, 40, 100$.

675 **6.2. Asymptotic behavior of the sensitivity indices estimators.** To illus-
 676 trate the asymptotic behavior of the sensitivity indices estimators, Sobol's g-function,
 677 a benchmark in sensitivity analysis [25, 20], is considered. Sobol's g-function is given
 678 by

$$679 \quad g(U_1, \dots, U_{p+1}) = \prod_{j=1}^{p+1} \frac{|4U_j - 2| + a_j}{1 + a_j},$$

681 where the a_j are nonnegative and the U_j are independent standard uniform random
 682 variables. The less a_j the more U_j is important. Elementary calculations show that
 683 the first-order Sobol index associated with U_j is given by

$$684 \quad S_j^{(a_1, \dots, a_{p+1})} = \frac{1}{3(1 + a_j)^2} \left(-1 + \prod_{j=1}^{p+1} \frac{(4/3 + a_j^2 + 2a_j)}{(1 + a_j)^2} \right)^{-1}.$$

686 To build a stochastic model out of Sobol's g-function, we let one of the U_j play
 687 the role of Z . For instance if U_i , $1 \leq i \leq p + 1$, were to play this role, then the
 688 stochastic model would be

$$689 \quad (6.1) \quad Y = f(X_1, \dots, X_p, Z) = g(X_1, \dots, X_{i-1}, Z, X_i, \dots, X_p).$$

691 Of course Y and f above depend on i . In the rest of this section we choose arbitrarily
 692 $i = 2$ and $p = 4$.

693 The Sobol indices of the first and of the second kind (in the sense of Definition 3.1
 694 and 3.2) are then easily seen to be

$$695 \quad S'_j = \begin{cases} S_j^{(a_1, \dots, a_{p+1})} & \text{if } 1 \leq j \leq i - 1 \\ S_{j+1}^{(a_1, \dots, a_{p+1})} & \text{if } i \leq j \leq p \end{cases}$$

697 and $S''_j = S_j^{(b_{i1}, \dots, b_{ip})}$, where

$$698 \quad b_{ij} = \begin{cases} a_j & \text{if } 1 \leq j \leq i - 1, \\ a_{j+1} & \text{if } i \leq j \leq p. \end{cases}$$

700 For each kind of Sobol index, we produced 500 estimates of the p Sobol indices
 701 and computed the values of the mean squared error (MSE) by averaging over the
 702 500 replications and summing over the p indices. We tested $n = 100, 500, 2500$ and
 703 $m = 1, 10, 100$.

704 The MSEs are shown in Figure 3. Let us look at 3a. As n increases, the decrease
 705 is linear for each m . This indicates that the MSEs go to zero at a polynomial rate,
 706 even if m is fixed (look at the line $m = 1$). This agrees with the theoretical results
 707 of Section 5. The picture is different for the estimator of Sobol indices of the second
 708 kind. In 3b, the curve for $m = 1$ is not a straight line, indicating that the MSE may
 709 not go to zero. Indeed, the MSE for m fixed is not expected to go to zero because
 710 of the bias depending on m . To make the MSE go to zero, one has to force m go to
 711 infinity.

712 Figure 4, which shows the distribution of the estimates for the index associated
 713 to X_1 , better explains this phenomenon. Here the bias is apparent for $m = 1$ and
 714 vanishes as m goes to infinity. The bias for the indices associated with the other
 715 inputs is not as large (not shown here).

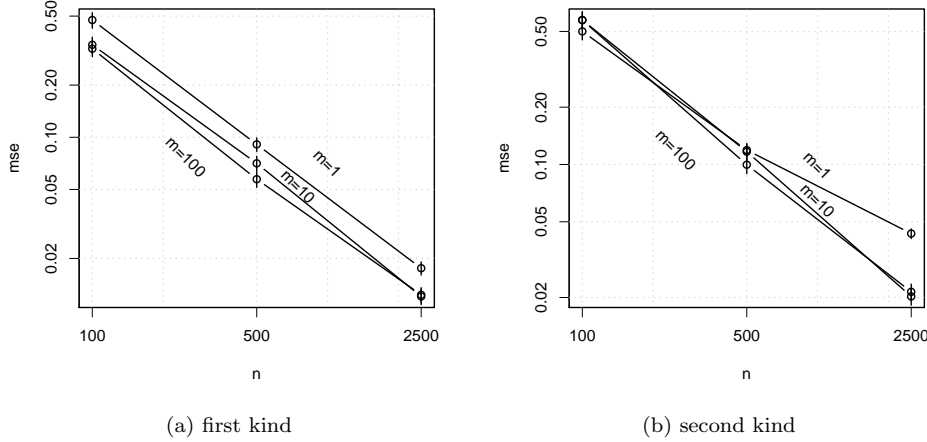


Fig. 3: MSEs for the Sobol index estimators of the first and second kind (logarithmic scale).

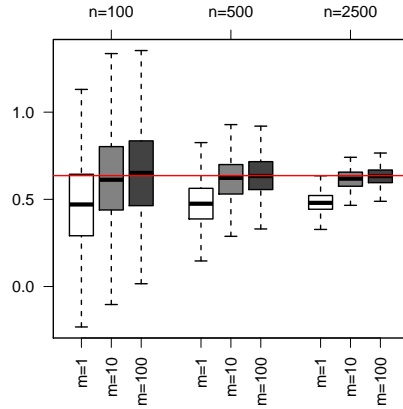


Fig. 4: Boxplots of the estimates for the Sobol index of the second kind associated with X_1 . The red horizontal line is the truth.

716 **7. Conclusion.** The practical method that consists of repeating the stochastic
 717 model at each exploration of the input space was analysed in the context of global
 718 sensitivity analysis. To find a tradeoff between the number of explorations n and the
 719 number of repetitions m , a bound on the missranking error (MRE) was found and
 720 minimized, leading to a solution in closed form. A two-step procedure was imple-
 721 mented to estimate the sensitivity indices. It was shown to have good asymptotic
 722 properties. Two sensitivity indices were considered. The sensitivity index of the first
 723 kind results from the existence of a function that links the output, the inputs and

724 some random noise in stochastic models defined through probability measures. The
 725 sensitivity index of the second kind is the population version of the estimator (1.4). An
 726 asymptotic analysis of the estimators was conducted. It was found that the estimators
 727 for the indices of the second kind may be asymptotically biased if m goes to infinity
 728 too slowly, while the estimators for the indices of the first kind are asymptotically
 729 unbiased even if m remains fixed. To test the theory, simulation experiments were
 730 conducted and the bias of the sensitivity estimator of the second kind was confirmed.
 731 Optimal compromises between repetitions and explorations have been identified and
 732 compared with the output of the two-stage procedure.

733 This work opens many research directions. First, the sensitivity estimators of the
 734 two stages could be aggregated to build estimators with a lower variance. Second,
 735 other methods might be developed to optimize the Monte-Carlo sampling scheme. For
 736 instance the MSE might be approximated or asymptotic variance-covariance matrices
 737 might be minimized. Third, multilevel Monte-Carlo sampling schemes might be con-
 738 sidered to alleviate the bias issue. Fourth, a finite-sample analysis could be conducted
 739 to get insight into the tradeoff K is subjected to. Fifth, since the bias is known, it
 740 could be estimated to build bias-corrected sensitivity indices estimators. Sixth, the
 741 problem of choosing a number of calls with many divisors must be addressed. It may
 742 be worth to call the model a bit less if this permits to have a better set $\text{div}_p(T)$. Sev-
 743 enth, the connection between our representation of stochastic models and that of [10]
 744 could be investigated further.

745 Appendix A. Calculations of some sensitivity indices.

746 **A.1. Calculations for \tilde{S}_1^{HAG} in Example 2.** We have

$$747 \quad \tilde{S}_1^{\text{HAG}} = \mathbb{E} \left(\frac{\text{Var}(\mathbb{E}[f(X, Z)|X_j, Z]|Z)}{\text{Var}(f(X, Z)|Z)} \right) = \int_{\Omega} \frac{\text{Var}(\mathbb{E}[f(X, Z)|X_j, Z]|Z)}{\text{Var}(f(X, Z)|Z)} dP.$$

748
749

750 Since the term inside the integral is a function of Z and the law of Z is the standard
 751 uniform distribution, a change of measures yields

$$752 \quad \tilde{S}_1^{\text{HAG}} = \int_{(0,1)} \frac{\text{Var}(\mathbb{E}[f(X, z)|X_j, Z = z]|Z = z)}{\text{Var}(f(X, z)|Z = z)} dz = \int_{(0,1)} \frac{\text{Var}(\mathbb{E}[f(X, z)|X_1])}{\text{Var}(f(X, z))} dz.$$

754 It remains to know what the ratio inside the integral is. We have

$$755 \quad \begin{aligned} \text{Var}(f(X, z)) &= \text{Var}(\Phi^{-1}(z)X_2 + X_1) = \Phi^{-1}(z)^2 \text{Var}(X_2) + \text{Var}(X_1) \\ &= \Phi^{-1}(z)^2 \frac{L^2}{12} + \frac{1}{12}, \end{aligned}$$

756
757
758 and

$$759 \quad \begin{aligned} \text{Var}(\mathbb{E}[f(X, z)|X_1]) &= \text{Var}(\mathbb{E}[\Phi^{-1}(z)X_2 + X_1|X_1]) \\ 760 &= \text{Var}(\Phi^{-1}(z) \mathbb{E}[X_2|X_1] + \mathbb{E}[X_1|X_1]) \\ 761 &= \text{Var}(\Phi^{-1}(z) \mathbb{E}[X_2] + X_1) \\ 762 &= \text{Var}(X_1) \\ 763 &= \frac{1}{12} \\ 764 \end{aligned}$$

765 and hence

$$766 \quad \widetilde{S}_1^{\text{HAG}} = \int_{(0,1)} \frac{1}{\Phi^{-1}(z)^2 L^2 + 1} dz = \int_{-\infty}^{\infty} \frac{1}{z^2 L + 1} \frac{1}{\sqrt{2\pi}} e^{-z^2/2} dz.$$

768 **A.2. Calculations for S'_1 in Example 4.** The sensitivity index of the first
769 kind associated with the first input is given by

$$770 \quad S'_1 = \frac{\text{Var}[\text{E}(X_1 + X_2\Phi^{-1}(Z)|X_1)]}{\text{Var}[X_1 + X_2\Phi^{-1}(Z)]}.$$

772 The numerator is given by $\text{Var}[\text{E}(X_1 + X_2\Phi^{-1}(Z)|X_1)] = \text{Var}[X_1 + \text{E}(X_1\Phi^{-1}(Z))] =$
773 $\text{Var}[X_1] = 1/12$. The denominator is given by $\text{Var}[X_1 + X_2\Phi^{-1}(Z)] = \text{Var}[X_1] +$
774 $\text{Var}[X_2\Phi^{-1}(Z)] = 1/12 + \text{Var}[X_2\Phi^{-1}(Z)]$, where

$$775 \quad \begin{aligned} \text{Var}[X_2\Phi^{-1}(Z)] &= \text{Var}[\text{E}(X_2\Phi^{-1}(Z)|Z)] + \text{E}(\text{Var}[X_2\Phi^{-1}(Z)|Z]) \\ 776 \quad &= \text{Var}\left[\Phi^{-1}(Z)\left(\frac{L}{2} + 1\right)\right] + \int_0^1 \Phi^{-1}(z)^2 \text{Var}[X_2] dz \\ 777 \quad &= \left(\frac{L}{2} + 1\right)^2 + \frac{L^2}{12}, \end{aligned}$$

779 so that

$$780 \quad S'_1 = \frac{1/12}{1/12 + (L/2 + 1)^2 + L^2/12} = \frac{1}{4(L^2 + 3(L + 1)) + 1}.$$

782 Appendix B. Proofs.

783 **B.1. Proof of Lemma 2.2.** Since P^* is a product probability measure, we
784 can write $P^* = \otimes_{j=1}^p P_j^*$. Let $\Omega = (0, 1)^{p+1}$ endowed with its Borel σ -field and let
785 P be the product Lebesgue measure $\lambda^{\otimes_{j=1}^{p+1}}$. If F_j denotes the distribution function
786 corresponding to P_j^* then, for $\omega = (\omega_1, \dots, \omega_{p+1}) \in \Omega$, put $X_j(\omega) = F_j^{\leftarrow}(\omega_j) :=$
787 $\inf\{x_j \in \mathbb{R} : F_j(x_j) \geq \omega_j\}$ for all $j = 1, \dots, p$ and $Z(\omega) = \omega_{p+1}$. Take $f(x, z) =$
788 $F_x^{\leftarrow}(z) := \inf\{t \in \mathbb{R} : F_x(t) \geq z\}$, $z \in (0, 1)$, where F_x is the cumulative distribution
789 function associated with Q_x . Standard probability techniques show that $f(x, Z)$ is
790 measurable for every x . Moreover, for every $t \in \mathbb{R}$,

$$791 \quad \begin{aligned} P(f(x, Z) \leq t) \\ 792 \quad &= P(Z \leq F_x(t)) = \lambda^{\otimes_{j=1}^{p+1}}\{\omega \in \Omega : \omega_{p+1} \leq F_x(t)\} = \lambda(0, F_x(t)) = F_x(t). \end{aligned}$$

794 Finally, by the same token,

$$795 \quad \begin{aligned} P(X_1 \leq t_1, \dots, X_p \leq t_p, Z \leq t_{p+1}) \\ 796 \quad &= P\{\omega : \omega_1 \leq F_1(t_1), \dots, \omega_p \leq F_p(t_p), \omega_{p+1} \leq t_{p+1}\} = t_{p+1} \prod_{j=1}^p F_j(t_j). \end{aligned}$$

798 The proof is complete.

799 **Proof of Proposition 4.1.** Assume without loss of generality that $D_1 < \dots <$
800 D_p . We first prove the following Lemma. For convenience, the subscripts n and m
801 are left out.

802 LEMMA B.1. *Let $i < j$. Then*

$$803 \quad P(\widehat{D}_i - \widehat{D}_j \geq 0) \leq \frac{\text{Var } \widehat{D}_i + \text{Var } \widehat{D}_j}{\frac{1}{2}|D_i - D_j|^2}.$$

805 *Proof. We have*

$$806 \quad P(\widehat{D}_i - \widehat{D}_j \geq 0) \leq P(|\widehat{D}_i - D_i| + |\widehat{D}_j - D_j| \geq D_j - D_i)$$

$$807 \quad \leq P(|\widehat{D}_i - D_i|^2 + |\widehat{D}_j - D_j|^2 \geq \frac{1}{2}|D_j - D_i|^2)$$

808

810 *and the claim follows from Markov's inequality.*

811 We now prove Proposition 4.1. Recall that $D_1 < \dots < D_p$. We have

$$812 \quad \sum_{i=1}^p \mathbb{E} |\widehat{R}_i - R_i| \leq \sum_{i=1}^p \sum_{j=1}^p \mathbb{E} |\mathbf{1}(\widehat{D}_j \leq \widehat{D}_i) - \mathbf{1}(D_j \leq D_i)|$$

$$813 \quad \leq \sum_{i=1}^p \sum_{j \neq i} \frac{\text{Var } \widehat{D}_i + \text{Var } \widehat{D}_j}{\frac{1}{2}|D_i - D_j|^2}$$

$$814 \quad \leq \frac{4(p-1)}{\min_{j < j'} |D_j - D_{j'}|^2} \sum_{i=1}^p \text{Var } \widehat{D}_i,$$

816 where the second inequality holds by Lemma B.1 and because

$$817 \quad \mathbb{E} |\mathbf{1}(\widehat{D}_j \leq \widehat{D}_i) - \mathbf{1}(D_j \leq D_i)| = \begin{cases} \mathbb{E} |\mathbf{1}(\widehat{D}_j > \widehat{D}_i)| & \text{if } j < i, \\ 0 & \text{if } j = i, \\ \mathbb{E} |\mathbf{1}(\widehat{D}_j \leq \widehat{D}_i)| & \text{if } j > i. \end{cases}$$

819 It remains to calculate the variances. But this is done in Lemma D.3 in Appendix D,
820 where it is found that

$$821 \quad \text{Var } \widehat{D}_j = \frac{1}{n} \{ \text{Var } \mathbb{E}[Y_0 Y_j | \mathbf{X}] + \frac{1}{m} (\mathbb{E} \text{Var}[Y_0 Y_j | \mathbf{X}] - \text{Var}[Y_0 | \mathbf{X}] \text{Var}[Y_j | \mathbf{X}])$$

$$822 \quad + \frac{1}{m^2} \mathbb{E} \text{Var}[Y_0 | \mathbf{X}] \text{Var}[Y_j | \mathbf{X}] \}.$$

824 **Proof of Proposition 4.3.** We distinguish between three cases: $0 < m^* < 1$,
825 $m^* > (T-K)/(p+1)$ and $1 \leq m^* \leq (T-K)/(p+1)$. Recall that m_{T-K}^\dagger is the
826 minimizer of $v(m)$, m in $\text{div}_p(T-K)$.

827 If $0 < m^* < 1$ then by definition $\varphi_{T-K}(m^*) = 1$ and by convexity $v(m^*) \leq$
828 $v(1) \leq v(m)$ for all m in $\text{div}_p(T-K)$. Therefore $m_{T-K}^\dagger = 1$.

829 If $m^* > (T-K)/(p+1)$ then by definition $\varphi_{T-K}(m^*) = (T-K)/(p+1)$ and by
830 convexity $v(m^*) \leq v((T-K)/(p+1)) \leq v(m)$ for all m in $\text{div}_p(T-K)$. Therefore
831 $m_{T-K}^\dagger = (T-K)/(p+1)$.

832 If $1 \leq m^* \leq (T-K)/(p+1)$ then by definition

$$833 \quad \varphi_{T-K}(m^*) = \begin{cases} \lrcorner m^* \lrcorner_{T-K} & \text{if } \sqrt{\lrcorner m^* \lrcorner_{T-K} \lrcorner m^* \lrcorner_{T-K}} > m^* \\ \lrcorner m^* \lrcorner_{T-K} & \text{if } \sqrt{\lrcorner m^* \lrcorner_{T-K} \lrcorner m^* \lrcorner_{T-K}} \leq m^*. \end{cases}$$

834

835 By convexity m_{T-K}^\dagger must be $\llcorner m^* \lrcorner_{T-K}$ or $\lrcorner m^* \lrcorner_{T-K}$. If $\llcorner m^* \lrcorner_{T-K} = \lrcorner m^* \lrcorner_{T-K}$ then
 836 $m_{T-K}^\dagger = \lrcorner m^* \lrcorner_{T-K} = \varphi_{T-K}(m^*)$. Otherwise, since $v(x) = \zeta_1 x + \zeta_2 + \zeta_3/x$, $x > 0$,
 837 for some constants ζ_1, ζ_2 and ζ_3 such that $\zeta_3/\zeta_1 = m^*$, we have

$$838 \quad v(\llcorner m^* \lrcorner_{T-K}) < v(\lrcorner m^* \lrcorner_{T-K}) \text{ iff } \sqrt{\llcorner m^* \lrcorner_{T-K} \lrcorner m^* \lrcorner_{T-K}} > \frac{\zeta_3}{\zeta_1} = m^*.$$

840 Therefore $\varphi_{T-K}(m^*) = m_{T-K}^\dagger$.

841 Let us prove that the minimizer of $v(m)$, $m \in \text{div}_p(T-K)$, is unique if $m^* \neq$
 842 $\sqrt{\llcorner m^* \lrcorner_{T-K} \lrcorner m^* \lrcorner_{T-K}}$. If it were not, then we would have $v(\llcorner m^* \lrcorner_{T-K})$
 843 $= v(\lrcorner m^* \lrcorner_{T-K})$. But this implies $m^* = \sqrt{\llcorner m^* \lrcorner_{T-K} \lrcorner m^* \lrcorner_{T-K}}$, which is a contra-
 844 diction.

845 **Proof of Theorem 4.4.** In this proof m_0 and n_0 are denoted by m and n ,
 846 respectively. In view of (4.3) and (4.4)–(4.9), we have

$$847 \quad \widehat{m}_K^* = \sqrt{\frac{\sum_{j=1}^p \widehat{\zeta}_{3,j}}{\sum_{j=1}^p \widehat{\zeta}_{1,j}}} = \sqrt{\frac{\sum_{j=1}^p \frac{1}{n} \sum_{i=1}^n \xi_{j;m,i}^{(4.4)} + \xi_{j;m,i}^{(4.5)} - \xi_{j;m,i}^{(4.6)} - \xi_{j;m,i}^{(4.7)}}{\sum_{j=1}^p \frac{1}{n} \sum_{i=1}^n \xi_{j;m,i}^{(4.8)} - \left(\frac{1}{n} \sum_{i=1}^n \xi_{j;m,i}^{(4.9)}\right)^2}},$$

849 where the $\xi_{j;m,i}^{(e)}$, $i = 1, \dots, n$, $j = 1, \dots, p$, $e = 4.4, \dots, 4.9$, are implicitly defined
 850 through (4.4)–(4.9). Let

$$851 \quad \bar{\xi} = \frac{1}{n} \sum_{i=1}^n \xi_{m,i},$$

$$852 \quad \xi_{m,i} = (\xi_{1;m,i}^\top, \dots, \xi_{p;m,i}^\top)^\top, \quad i = 1, \dots, n,$$

$$853 \quad \xi_{j;m,i} = (\xi_{j;m,i}^{(4.4)}, \dots, \xi_{j;m,i}^{(4.9)})^\top, \quad j = 1, \dots, p, \quad i = 1, \dots, n.$$

855 Let s be the function defined by

$$856 \quad s(\mathbf{x}) = \sqrt{\frac{\sum_{j=1}^p x_j^{(4.4)} + x_j^{(4.5)} - x_j^{(4.6)} - x_j^{(4.7)}}{\sum_{j=1}^p x_j^{(4.8)} - x_j^{(4.9)2}},$$

858 where $\mathbf{x} = (\mathbf{x}_1^\top, \dots, \mathbf{x}_p^\top)^\top$, $\mathbf{x}_j = (x_j^{(4.4)}, \dots, x_j^{(4.9)})^\top$, $j = 1, \dots, p$. With the above
 859 notation we have $\widehat{m}_K^* = s(\bar{\xi})$. Moreover, elementary calculations show that

$$860 \quad (\text{B.1}) \quad \mathbb{E} \xi_{m,1} = \boldsymbol{\theta} + \sum_{\nu=1}^4 \frac{\mathbf{C}_\nu}{m^\nu},$$

862 where the \mathbf{C}_ν are vectors of constants, $\boldsymbol{\theta} = (\boldsymbol{\theta}_1^\top, \dots, \boldsymbol{\theta}_p^\top)^\top$ and

$$863 \quad \boldsymbol{\theta}_j = \mathbb{E} \begin{pmatrix} Y_0^{(1,1)2} Y_j^{(1,1)2} \\ Y_0^{(1,1)} Y_0^{(1,2)} Y_j^{(1,1)} Y_j^{(1,2)} \\ Y_0^{(1,1)} Y_0^{(1,2)} Y_j^{(1,1)2} \\ Y_j^{(1,1)} Y_j^{(1,2)} Y_0^{(1,1)2} \\ Y_0^{(1,1)} Y_0^{(1,2)} Y_j^{(1,1)} Y_j^{(1,2)} \\ Y_j^{(1,1)} Y_0^{(1,1)} \end{pmatrix}.$$

864

865 Check that $m^* = s(\boldsymbol{\theta})$. A concatenation of two Taylor expansions yield

$$\begin{aligned}
866 \quad & \sqrt{n}(\bar{\boldsymbol{\xi}} - \mathbb{E} \boldsymbol{\xi}_{m,1})^\top \dot{s}(\mathbb{E} \boldsymbol{\xi}_{m,1}) + \frac{1}{2}(\bar{\boldsymbol{\xi}} - \mathbb{E} \boldsymbol{\xi}_{m,1})^\top \ddot{s}_{n,m}(\bar{\boldsymbol{\xi}} - \mathbb{E} \boldsymbol{\xi}_{m,1}) \\
867 \quad (\text{B.2}) \quad & = \sqrt{n}(s(\bar{\boldsymbol{\xi}}) - s(\mathbb{E} \boldsymbol{\xi}_{m,1})) \\
868 \quad & = \sqrt{n}(s(\bar{\boldsymbol{\xi}}) - s(\boldsymbol{\theta}) - (\mathbb{E} \boldsymbol{\xi}_{m,1} - \boldsymbol{\theta})^\top \dot{s}(\boldsymbol{\theta}) - \frac{1}{2}(\mathbb{E} \boldsymbol{\xi}_{m,1} - \boldsymbol{\theta})^\top \ddot{s}_m(\mathbb{E} \boldsymbol{\xi}_{m,1} - \boldsymbol{\theta})), \\
869
\end{aligned}$$

870 where \dot{s} is the gradient of s , $\ddot{s}_{n,m}$ is the Hessian matrix of s at a point between $\bar{\boldsymbol{\xi}}$
871 and $\boldsymbol{\theta}_m$, and, \ddot{s}_m is the Hessian matrix of s at a point between $\mathbb{E} \boldsymbol{\xi}_{m,1}$ and $\boldsymbol{\theta}$. It
872 follows from (B.1) that $(\mathbb{E} \boldsymbol{\xi}_{m,1} - \boldsymbol{\theta})^\top \dot{s}(\boldsymbol{\theta})$ is clearly of the form $\sum_{\nu=1}^4 C_\nu/m^\nu$ for some
873 constants C_ν . Putting

$$\begin{aligned}
874 \quad \epsilon_m &= \frac{1}{2}(\mathbb{E} \boldsymbol{\xi}_{m,1} - \boldsymbol{\theta})^\top \ddot{s}_m(\mathbb{E} \boldsymbol{\xi}_{m,1} - \boldsymbol{\theta}) + \sum_{\nu=2}^4 \frac{C_\nu}{m^\nu}, \\
875
\end{aligned}$$

876 it follows from (B.2) that

$$\begin{aligned}
878 \quad (\text{B.3}) \quad & \sqrt{n}(\bar{\boldsymbol{\xi}} - \mathbb{E} \boldsymbol{\xi}_{m,1})^\top \dot{s}(\mathbb{E} \boldsymbol{\xi}_{m,1}) + \frac{1}{2}(\bar{\boldsymbol{\xi}} - \mathbb{E} \boldsymbol{\xi}_{m,1})^\top \ddot{s}_{n,m}(\bar{\boldsymbol{\xi}} - \mathbb{E} \boldsymbol{\xi}_{m,1}) \\
879 \quad & = \sqrt{n}(\widehat{m}_K^* - m^* - \frac{C_1}{m} - \epsilon_m). \\
880
\end{aligned}$$

881 If m is fixed then Lemma C.2 in Appendix C yields

$$\begin{aligned}
882 \quad & \sqrt{n}(\bar{\boldsymbol{\xi}} - \mathbb{E} \boldsymbol{\xi}_{m,1}) \rightarrow \mathcal{N}(0, \Sigma_m),
\end{aligned}$$

884 for some variance-covariance matrix Σ_m of size $6p \times 6p$. Moreover, the second term in
885 the left-hand side of (B.3) is $o_P(1)$ by Cauchy-Schwartz's inequality and the continuity
886 of the second derivatives of s . The first term goes to $\mathcal{N}(0, \dot{s}(\mathbb{E} \boldsymbol{\xi}_{m,1})^\top \Sigma_m \dot{s}(\mathbb{E} \boldsymbol{\xi}_{m,1}))$
887 and hence the claim follows with $\sigma_m^2 = \dot{s}(\mathbb{E} \boldsymbol{\xi}_{m,1})^\top \Sigma_m \dot{s}(\mathbb{E} \boldsymbol{\xi}_{m,1})$ and $C = C_1$.

888 If $m \rightarrow \infty$ then again Lemma C.2 in Appendix C applies: we have

$$\begin{aligned}
889 \quad & \sqrt{n}(\bar{\boldsymbol{\xi}} - \mathbb{E} \boldsymbol{\xi}_{m,1}) \rightarrow \mathcal{N}(0, \lim_{m \rightarrow \infty} \Sigma_m). \\
890
\end{aligned}$$

891 Since $\epsilon_m - \sum_{\nu=2}^4 C_\nu/m^\nu = o(m^{-1})$, \dot{s} is continuous and $\mathbb{E} \boldsymbol{\xi}_{m,1} \rightarrow \boldsymbol{\theta}$, the claim follows.
892 The proof is complete.

893 **Proof of Proposition 4.6.** By definition, $\widehat{m}_{T-K}^\dagger = \varphi_{T-K}(\widehat{m}_K^*)$ and $m_{T-K}^\dagger =$
894 $\varphi_{T-K}(m^*)$. The function φ_{T-K} is piecewise constant and has $|\text{div}_p(T-K)| - 1$ points
895 of discontinuity of the form $\sqrt{i\bar{j}}$, where i and j are two consecutive members of

$$\begin{aligned}
896 \quad & \text{div}_p(T-K) \setminus \left\{ 1, \frac{T-K}{p+1} \right\}. \\
897
\end{aligned}$$

898 Denote the set of discontinuity points by \mathcal{D}_{T-K} . Clearly,

$$\begin{aligned}
899 \quad & \mathcal{D}_{T-K} \subset \{\sqrt{i\bar{j}} : i \text{ and } j \text{ are two consecutive integers}\} = \mathcal{E}.
\end{aligned}$$

901 There exists an open interval that contains m^* but does not contain any points of
902 \mathcal{E} and hence does not contain any points of \mathcal{D}_{T-K} , whatever T and K . If \widehat{m}_K^* is in
903 this interval then there are no discontinuity points between m^* and \widehat{m}_K^* and hence
904 $\widehat{m}_{T-K}^\dagger = \varphi_{T-K}(\widehat{m}_K^*) = \varphi_{T-K}(m^*) = m_{T-K}^\dagger$. By Corollary 4.5, the probability of
905 that event goes to one as m_0 and n_0 go to infinity.

906 **Proof of Theorem 4.7.** Let $\varepsilon > 0$. An obvious algebraic manipulation and
 907 Taylor's expansion yield

$$908 \quad P \left(\left| \frac{\frac{1}{T-K} v(\widehat{m}_{T-K}^\dagger) - \frac{1}{T} v(m_{T-K}^\dagger)}{\frac{1}{T} v(m_{T-K}^\dagger)} > \varepsilon \right| \right)$$

$$909 \quad \leq P \left(\left| \frac{T}{T-K} (\widehat{m}_{T-K}^\dagger - m_{T-K}^\dagger) v'(\widetilde{m}) + \frac{K}{T-K} v(m_{T-K}^\dagger) \right| > v(m_{T-K}^\dagger) \varepsilon \right),$$

911 where \widetilde{m} denotes a real between $\widehat{m}_{T-K}^\dagger$ and m_{T-K}^\dagger . A decomposition of the probability
 912 above according to whether $\widehat{m}_{T-K}^\dagger - m_{T-K}^\dagger \neq 0$ or $\widehat{m}_{T-K}^\dagger - m_{T-K}^\dagger = 0$ yields the
 913 bound

$$914 \quad P \left(\widehat{m}_{T-K}^\dagger - m_{T-K}^\dagger \neq 0 \right) + P \left(\frac{K}{T-K} > \varepsilon \right).$$

916 The first term goes to zero by Proposition 4.6. The second term goes to zero because
 917 $K/T \rightarrow 0$.

918 **Proof of Theorem 5.1.** The proof is based on the results in Appendix C. The
 919 Sobol estimators in (3.7) and (3.4) are of the form

$$920 \quad \widehat{S}'_{j;n,m} = \frac{\frac{1}{n} \sum_{i=1}^n \xi_{j;m,i}^{\text{UL}} - \left(\frac{1}{n} \sum_{i=1}^n \xi_{m,i}^{\text{UR}} \right)^2}{\frac{1}{n} \sum_{i=1}^n \xi_{m,i}^{\text{LL}} - \left(\frac{1}{n} \sum_{i=1}^n \xi_{m,i}^{\text{UR}} \right)^2}, \quad j = 1, \dots, p,$$

922 and

$$923 \quad \widehat{S}''_{j;n,m} = \frac{\frac{1}{n} \sum_{i=1}^n \xi_{j;m,i}^{\text{UL}} - \left(\frac{1}{n} \sum_{i=1}^n \xi_{m,i}^{\text{UR}} \right)^2}{\frac{1}{n} \sum_{i=1}^n \xi_{m,i}^{\text{LL}} - \left(\frac{1}{n} \sum_{i=1}^n \xi_{m,i}^{\text{UR}} \right)^2}, \quad j = 1, \dots, p,$$

925 where the notation is obvious. Denote $\boldsymbol{\xi}_{m,i} := (\xi_{1;m,i}^{\text{UL}}, \dots, \xi_{p;m,i}^{\text{UL}}, \xi_{m,i}^{\text{UR}}, \xi_{m,i}^{\text{LL}}, \xi_{m,i}^{\text{LL}})^\top$.
 926 Elementary but burdensome calculations show that

$$927 \quad \mathbb{E} \boldsymbol{\xi}_{m,1} = \begin{pmatrix} \mathbb{E} \mathbb{E}[f(X, Z)|X] \mathbb{E}[f(\widetilde{X}_{-1}, Z)|\widetilde{X}_{-1}] \\ \vdots \\ \mathbb{E} \mathbb{E}[f(X, Z)|X] \mathbb{E}[f(\widetilde{X}_{-p}, Z)|\widetilde{X}_{-p}] \\ \mathbb{E} f(X, Z) \\ \mathbb{E} f(X, Z)^2 \\ \mathbb{E} \mathbb{E}[f(X, Z)|X]^2 + \frac{\mathbb{E} \text{Var}[f(X, Z)|X]}{m} \end{pmatrix}.$$

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

$$929 \quad s(x_1, \dots, x_p, x_{p+1}, x_{p+2}, x_{p+3})$$

$$930 \quad = \left(\frac{x_1 - x_{p+1}^2}{x_{p+2} - x_{p+1}^2}, \dots, \frac{x_p - x_{p+1}^2}{x_{p+2} - x_{p+1}^2}, \frac{x_1 - x_{p+1}^2}{x_{p+3} - x_{p+1}^2}, \dots, \frac{x_p - x_{p+1}^2}{x_{p+3} - x_{p+1}^2} \right).$$

933 Clearly, we have

$$934 \quad s \left(\frac{1}{n} \sum_{i=1}^n \boldsymbol{\xi}_{m,i} \right) = \begin{pmatrix} \widehat{S}'_{n,m} \\ \widehat{S}''_{n,m} \end{pmatrix}$$

935 and

$$936 \quad s(\mathbf{E} \boldsymbol{\xi}_{m,1}) = \left(\mathbf{S}'' \left[1 - \frac{\mathbf{S}'}{\mathbf{E} \operatorname{Var}[f(X,Z)|X] + m \operatorname{Var} \mathbf{E}[f(X,Z)|X]} \right] \right).$$

937 If m is fixed then Lemma C.2 in Appendix C yields

$$938 \quad \sqrt{n} \left(\frac{1}{n} \sum_{i=1}^n \boldsymbol{\xi}_{m,i} - \mathbf{E} \boldsymbol{\xi}_{m,1} \right) \xrightarrow{d} \mathcal{N}(0, \Sigma_m),$$

939 for some nonnegative matrix Σ_m of size $(p+3) \times (p+3)$ and the result follows by the
940 delta-method.

941 If $m \rightarrow \infty$, Lemma C.2 still holds with the variance-covariance matrix replaced
942 by its limit. Taylor's expansion yields

$$\begin{aligned} 943 \quad & \sqrt{n} \left(s \left(\frac{1}{n} \sum_{i=1}^n \boldsymbol{\xi}_{m,i} \right) - s(\mathbf{E} \boldsymbol{\xi}_{m,1}) \right) \\ 944 \quad & = \sqrt{n} \left(\left(\frac{1}{n} \sum_{i=1}^n \boldsymbol{\xi}_{m,i} - \mathbf{E} \boldsymbol{\xi}_{m,1} \right) \dot{s}_m \right. \\ 945 \quad & \quad \left. + \frac{1}{2} \left(\frac{1}{n} \sum_{i=1}^n \boldsymbol{\xi}_{m,i} - \mathbf{E} \boldsymbol{\xi}_{m,1} \right)^\top \ddot{s}_{n,m} \left(\frac{1}{n} \sum_{i=1}^n \boldsymbol{\xi}_{m,i} - \mathbf{E} \boldsymbol{\xi}_{m,1} \right) \right), \end{aligned}$$

947 where \dot{s}_m is the gradient of s at $\mathbf{E} \boldsymbol{\xi}_{m,1}$ and $\ddot{s}_{n,m}$ is the Hessian matrix of s at a
948 point between $n^{-1} \sum_i \boldsymbol{\xi}_{m,i}$ and $\mathbf{E} \boldsymbol{\xi}_{m,1}$. Since that point goes to a constant and s has
949 continuous second derivatives, it holds that $\ddot{s}_{n,m}$ goes to a constant as well. So does
950 \dot{s}_m and the claim follows by Slutsky's lemma.

951 **Appendix C. A unified treatment of the asymptotics.** All estimators in
952 this paper have a common form, given by

$$953 \quad (\text{C.1}) \quad \frac{1}{n} \sum_{i=1}^n \boldsymbol{\xi}_{m,i},$$

954 with

$$955 \quad (\text{C.2}) \quad \boldsymbol{\xi}_{m,i} = \prod_{l=1}^L \frac{1}{m} \sum_{k=1}^m \prod_{j=0}^p Y_j^{(i,k) b_{j;l}},$$

957 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
958 $b_{j;l}$, $j = 0, \dots, p$, $l = 1, \dots, L$, are nonnegative coefficients. The coefficients are
959 arranged in a matrix $(b_{j;l})$ with L rows and $p+1$ columns, where $b_{j;l}$ is the element in
960 the l th row and $(j+1)$ th column. This way, all estimators of the form (C.1) and (C.2),
961 or, equivalently, all summands (C.2), can be represented by a matrix. We sometimes
962 write $\boldsymbol{\xi}_{m,i} \simeq (b_{j;l})$, where $(b_{j;l})$ is the matrix of size $L \times (p+1)$ with coefficients $b_{j;l}$,
963 $j = 0, \dots, p$, $l = 1, \dots, L$.

964 **C.1. Examples.** The estimator

$$965 \quad \frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \frac{1}{m} \sum_{k'=1}^m Y_j^{(i,k')}$$

966

967 is of the form (C.1) and (C.2) with $L = 2$ and coefficients

$$968 \quad \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 969 & 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \end{pmatrix},$$

970 where the non-null columns are the first and the $(j + 1)$ th ones. The estimators

$$971 \quad \frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)}, \quad \frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)2},$$

$$972 \quad \frac{1}{n} \sum_{i=1}^n \left(\frac{1}{m} \sum_{k=1}^m Y_0^{(i,k)} \right)^2$$

974 are of the form (C.1) and (C.2) with $L = 2$ and coefficients

$$975 \quad \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 976 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}, \quad \begin{pmatrix} 2 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 977 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \end{pmatrix},$$

$$976 \quad \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 977 & 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \end{pmatrix},$$

978 respectively.

979 **The estimators of Section 4.** In view of (4.4)–(4.9), the estimators $\widehat{\zeta}_{3,j}$ and
980 $\widehat{\zeta}_{1,j}$ can be expressed in terms of estimators of the form (C.1) and (C.2): we have

$$981 \quad \widehat{\zeta}_{3,j} = \frac{1}{n} \sum_{i=1}^n \xi_{j;m,i}^{(4.4)} + \xi_{j;m,i}^{(4.5)} - \xi_{j;m,i}^{(4.6)} - \xi_{j;m,i}^{(4.7)} \quad \text{and,}$$

$$982 \quad \widehat{\zeta}_{1,j} = \frac{1}{n} \sum_{i=1}^n \xi_{j;m,i}^{(4.8)} - \left(\frac{1}{n} \sum_{i=1}^n \xi_{j;m,i}^{(4.9)} \right)^2,$$

984 where

$$985 \quad \xi_{j;m,i}^{(4.4)}, \quad \xi_{j;m,i}^{(4.5)}$$

$$986 \quad \xi_{j;m,i}^{(4.6)}, \quad \xi_{j;m,i}^{(4.7)}$$

$$987 \quad \xi_{j;m,i}^{(4.8)}, \quad \xi_{j;m,i}^{(4.9)}$$

989 are all of the form (C.2) with $L = 4$ and coefficients

$$990 \quad \begin{pmatrix} 2 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 991 & 0 & 0 & \cdots & 0 & 2 & 0 & \cdots & 0 \\ 992 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 993 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 994 & 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 995 & 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 996 & 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \end{pmatrix},$$

$$991 \quad \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 992 & 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 993 & 0 & 0 & \cdots & 0 & 2 & 0 & \cdots & 0 \\ 994 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}, \quad \begin{pmatrix} 2 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 995 & 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 996 & 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 997 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \end{pmatrix},$$

$$992 \quad \begin{pmatrix} 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 993 & 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 994 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 995 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 996 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 997 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 998 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \end{pmatrix},$$

994 respectively. In the matrices above, the first and $j + 1$ th columns are nonnull.

995 **The estimators of Section 5.** The Sobol estimators in (3.7) and (3.4) are of
 996 the form (C.1) and (C.2) with $L = 2$ and coefficients

$$997 \quad \xi_{1;m,i}^{\text{UL}} \simeq \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \end{pmatrix}, \dots, \xi_{p;m,i}^{\text{UL}} \simeq \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 1 \end{pmatrix}$$

998 for the upper left (UL) terms,

$$999 \quad \xi_{m,i}^{\text{UR}} \simeq \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \end{pmatrix}$$

1000 for the upper right (UR) term,

$$1001 \quad \xi_{m,i}^{\text{LL}} \simeq \begin{pmatrix} 2 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \end{pmatrix}$$

1002 for the lower left (LL) term of $\widehat{S}'_{j;n,m}$ and

$$1003 \quad \xi_{m,i}^{\text{LL}} \simeq \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 1 & 0 & \cdots & 0 \end{pmatrix}$$

1004 for the lower left (LL) term of $\widehat{S}''_{j;n,m}$.

1005 **C.2. A central limit theorem.** For each n , the random variables $\xi_{m,1}, \dots, \xi_{m,n}$
 1006 are independent and identically distributed. Denote by $\mathcal{E}_{m,i}(L)$ the set of all sum-
 1007 mands (C.2). In other words, $\mathcal{E}_{m,i}(L)$ is the set of all nonnegative matrices of size
 1008 $L \times (p+1)$. This set has useful properties, gathered in Proposition C.1 for subsequent
 1009 use.

1010 **PROPOSITION C.1.** *Let ξ be an element of $\mathcal{E}_{m,i}(L)$ with coefficients $(b_{j;l})$. The*
 1011 *following statements are true.*

1012 (i) *If ξ' is an element of $\mathcal{E}_{m,i}(L)$ with coefficients $(b'_{j;l})$ then $\xi\xi'$ is an element of*
 1013 *$\mathcal{E}_{m,i}(2L)$ with coefficients*

$$1014 \quad \begin{pmatrix} b_{0;1} & \cdots & b_{p;1} \\ \vdots & & \vdots \\ b_{0;L} & \cdots & b_{p;L} \\ b'_{0;1} & \cdots & b'_{p;1} \\ \vdots & & \vdots \\ b'_{0;L} & \cdots & b'_{p;L} \end{pmatrix}.$$

1016 (ii) *The limit of $\mathbb{E}\xi$ exists as $m \rightarrow \infty$.*

1017 (iii) *If there exists some function F such that $|f(x, z)| \leq F(x)$ for all x and z in the*
 1018 *domain of definition of f then*

$$1019 \quad |\xi| \leq \left(\bigvee_{j=0}^p F_j(\mathbf{X}^{(i)}) \right)^{\sum_{j=0}^p \sum_{l=1}^L b_{j;l}},$$

1020 *where $F_j(\mathbf{X}^{(i)})$ is $F(X^{(i)})$ if $j = 0$ and $F(\widetilde{X}_{-j}^{(i)})$ if $j \geq 1$.*

1021 *Proof.* The proof of (i) is trivial. Let us prove (ii). We have

$$\begin{aligned}
1022 \quad \mathbb{E} \xi &= \frac{1}{m^L} \sum_{(k_1, \dots, k_L) \in \{1, \dots, m\}^L} \mathbb{E} \prod_{l=1}^L \prod_{j=0}^p Y_j^{(1, k_l) b_{j;l}} \\
1023 \quad &= \frac{1}{m^L} \sum_{(k_1, \dots, k_L) \in \{1, \dots, m\}^L} \mathbb{E} \mathbb{E} \left(\prod_{l=1}^L \prod_{j=0}^p Y_j^{(1, k_l) b_{j;l}} \middle| \mathbf{X}^{(1)} \right) \\
1024 \quad (\text{C.3}) \quad &= \frac{1}{m^L} \sum_{(k_1, \dots, k_L) \in \{1, \dots, m\}^L} \mathbb{E} \prod_{j=0}^p \mathbb{E} \left(\prod_{l=1}^L Y_j^{(1, k_l) b_{j;l}} \middle| \mathbf{X}^{(1)} \right). \\
1025
\end{aligned}$$

1026 Since (i) $\mathbf{X}^{(1)}$ and $\{\mathbf{Z}^{(1, k)}, k = 1, \dots, m\}$ are independent and (ii) the law of

$$1027 \quad (\mathbf{Z}^{(1, k_1)}, \dots, \mathbf{Z}^{(1, k_L)})$$

1028 is invariant through any permutation of distinct k_1, \dots, k_L , all the inner expectations
1029 in (C.3) are equal to some others. For if k_1, \dots, k_L are distinct then

$$1030 \quad \mathbb{E} \left(\prod_{l=1}^L Y_j^{(1, k_l) b_{j;l}} \middle| \mathbf{X}^{(1)} \right) = \mathbb{E} \left(\prod_{l=1}^L Y_j^{(1, l) b_{j;l}} \middle| \mathbf{X}^{(1)} \right)$$

1031
1032 for all $j = 0, \dots, p$. The number of inner expectations equal to the one above is
1033 $m(m-1) \cdots (m-L+1)$, a polynomial in m with degree L . If some components of
1034 the tuple (k_1, \dots, k_L) are equal, then we can always write

$$1035 \quad \mathbb{E} \left(\prod_{l=1}^L Y_j^{(1, k_l) b_{j;l}} \middle| \mathbf{X}^{(1)} \right) = \mathbb{E} \left(\prod_{l=1}^{L'} Y_j^{(1, l) \beta_{j;l}} \middle| \mathbf{X}^{(1)} \right)$$

1036
1037 for some $L' \leq L$ and coefficients $\beta_{j;l}$. It is easy to see that the number of inner expecta-
1038 tions equal to the one above is a polynomial in m with degree at most L . (Looking
1039 at examples helps to see this; see e.g. the proof of Lemma D.2 in Appendix D.)
1040 Therefore, the sum in (C.3) is also a polynomial in m with degree at most L and the
1041 claim follows ($\mathbb{E} \xi$ can be zero). To prove (iii), simply remember that, by assumption,
1042 $|Y^{(1, k)}| \leq F(X^{(1)})$ and $|Y_j^{(1, k)}| \leq F(\tilde{X}_{-j}^{(1)})$ for all k and all j . \square

1043 Two frameworks are considered:

- 1044 • $n \rightarrow \infty$ and m is fixed;
- 1045 • $n \rightarrow \infty$ and $m \rightarrow \infty$.

1046 In the second framework m_n is a sequence indexed by n that goes to infinity as n goes
1047 to infinity.

1048 LEMMA C.2. Let $\xi_{m,i}^{(I)}$, $I = 1, \dots, N$, be elements of $\mathcal{E}_{m,i}(L)$ with coefficients
1049 $(b_{j;l}^{(I)})$. Assume

$$1050 \quad \mathbb{E} F(X^{(1)})^2 \sum_{j=0}^p \sum_{l=1}^L b_{j;l}^{(I)} < \infty$$

1051 for all $I = 1, \dots, N$. Let $n \rightarrow \infty$. If m is fixed then

$$1052 \quad \sqrt{n} \left[\frac{1}{n} \sum_{i=1}^n \xi_{m,i}^{(1)} - \mathbb{E} \xi_{m,1}^{(1)}, \dots, \frac{1}{n} \sum_{i=1}^n \xi_{m,i}^{(N)} - \mathbb{E} \xi_{m,1}^{(N)} \right]^\top \xrightarrow{d} \mathcal{N}(0, \Sigma_m),$$

1053

1054 where Σ_m is the variance-covariance matrix of $\boldsymbol{\xi}_{m,i} = (\xi_{m,i}^{(1)}, \dots, \xi_{m,i}^{(N)})^\top$. If $m \rightarrow$
 1055 ∞ then $\lim_{m \rightarrow \infty} \Sigma_m$ exists elementwise and the above display with Σ_m replaced by
 1056 $\lim_{m \rightarrow \infty} \Sigma_m$ is true.

1057 *Proof.* Let m be fixed. By Proposition C.1 (i), $\xi_{m,i}^{(I)2}$, $I = 1, \dots, N$, belongs to
 1058 $\mathcal{E}_{m,i}(2L)$ and has coefficients

$$1059 \quad \xi_{m,i}^{(I)2} \simeq \begin{pmatrix} b_{0;1}^{(I)} & \cdots & b_{p;1}^{(I)} \\ \vdots & & \vdots \\ b_{0;L}^{(I)} & \cdots & b_{p;L}^{(I)} \\ b_{0;1}^{(I)} & \cdots & b_{p;1}^{(I)} \\ \vdots & & \vdots \\ b_{0;L}^{(I)} & \cdots & b_{p;L}^{(I)} \end{pmatrix}.$$

1061 Thus, denoting $\sum_{j=0}^p \sum_{l=1}^L b_{j;l}^{(I)}$ by β , Proposition C.1 (iii) yields

$$1062 \quad (C.4) \quad \xi_{m,i}^{(I)2} \leq \bigvee_{j=0}^p F_j(\mathbf{X}^{(i)})^{2\beta}$$

1064 and hence

$$1065 \quad \mathbb{E} \xi_{m,i}^{(I)2} \leq \mathbb{E} \bigvee_{j=0}^p F_j(\mathbf{X}^{(1)})^{2\beta} \leq (p+1) \mathbb{E} \left(F(X^{(1)}) \right)^{2\beta} < \infty.$$

1067 Therefore we can apply the central limit theorem to finish the proof for m fixed.

1068 Let $m \rightarrow \infty$. According to Lindeberg-Feller's central limit theorem (see e.g. [33]),
 1069 it suffices to show

1070 (i) for all $\epsilon > 0$,

$$1071 \quad \sum_{i=1}^n \mathbb{E} \left\| \frac{1}{\sqrt{n}} \boldsymbol{\xi}_{m,i} \right\|^2 \mathbf{1} \left\{ \left\| \frac{1}{\sqrt{n}} \boldsymbol{\xi}_{m,i} \right\| > \epsilon \right\} \rightarrow 0,$$

1073 and

1074 (ii) the limit $\sum_{i=1}^n \text{Cov}(\boldsymbol{\xi}_{m,i}/\sqrt{n})$ exists and is finite.

1075 Let us show (i). Denoting $\mathbf{X} = (X^{(1)}, \tilde{X}^{(1)})$, we have

$$1076 \quad \sum_{i=1}^n \mathbb{E} \left\| \frac{\boldsymbol{\xi}_{m,i}}{\sqrt{n}} \right\|^2 \mathbf{1} \{ \|\boldsymbol{\xi}_{m,i}\| > \sqrt{n}\epsilon \} = \mathbb{E} \|\boldsymbol{\xi}_{m,1}\|^2 \mathbf{1} \{ \|\boldsymbol{\xi}_{m,1}\| > \sqrt{n}\epsilon \}$$

$$1077 \quad = \mathbb{E} \sum_{I=1}^N \xi_{m,1}^{(I)2} \mathbf{1} \{ \|\boldsymbol{\xi}_{m,1}\| > \sqrt{n}\epsilon \}$$

$$1078 \quad = \sum_{I=1}^N \mathbb{E} \left[\mathbb{E} \left(\xi_{m,1}^{(I)2} \mathbf{1} \{ \|\boldsymbol{\xi}_{m,1}\| > \sqrt{n}\epsilon \} \mid \mathbf{X} \right) \right].$$

1079

1080 By (C.4), we have

$$\begin{aligned}
1081 \quad \mathbb{E} \left(\xi_{m,1}^{(I)2} \mathbf{1} \{ \|\xi_{m,1}\| > \sqrt{n}\epsilon \} | \mathbf{X} \right) &\leq \bigvee_{j=0}^p F_j(\mathbf{X}^{(1)})^{2\beta} P(\|\xi_{m,1}\| > \sqrt{n}\epsilon | \mathbf{X}) \\
1082 \quad &\leq \bigvee_{j=0}^p F_j(\mathbf{X}^{(1)})^{2\beta} \frac{\sum_{I=1}^N \mathbb{E} \left(\xi_{m,1}^{(I)2} | \mathbf{X} \right)}{n\epsilon^2} \\
1083 \quad &\leq \frac{N \bigvee_{j=0}^p F_j(\mathbf{X}^{(1)})^{4\beta}}{n\epsilon^2}, \\
1084
\end{aligned}$$

1085 where the last inequality holds by using (C.4) once more. The upper bound goes to
1086 zero and is dominated by an integrable function. Thus, we can apply the dominated
1087 convergence theorem to complete the proof.

1088 Let us show that (ii) holds. We have $\sum_{i=1}^n \text{Cov}(\xi_{m,i}/\sqrt{n}) = \text{Cov}(\xi_{m,1})$. The
1089 element (I, J) in this matrix is given by $\mathbb{E} \xi_{m,1}^{(I)} \xi_{m,1}^{(J)} - \mathbb{E} \xi_{m,1}^{(I)} \mathbb{E} \xi_{m,1}^{(J)}$. Remember that
1090 $\mathbb{E} \xi_{m,1}^{(I)2} < \infty$, $I = 1, \dots, N$, and hence $\mathbb{E} \xi_{m,1}^{(I)} \xi_{m,1}^{(J)} \leq \mathbb{E} \xi_{m,1}^{(I)2}/2 + \mathbb{E} \xi_{m,1}^{(J)2}/2 < \infty$. Therefore
1091 the limit of $\text{Cov} \xi_{m,1}$ exists and is finite. The proof is complete. \square

1092 **Appendix D. Explicit moment calculations.** Explicit moment calculations
1093 are given for the summands in the proof of Theorem 5.1. In this section, $\mathbb{E} f(X, Z)$
1094 and $\mathbb{E} \mathbb{E}[f(X, Z) | X]^2$ are denoted by μ and D , respectively. Recall that the upper-left
1095 term in (3.6) and (3.5) is denoted by D_j . The moments are given in Lemma D.1
1096 and Lemma D.2. The variances and covariances are given in Lemma D.3. Let $\mathbf{X} =$
1097 $(X^{(1)}, \tilde{X}^{(1)})$. Whenever there is a superscript \mathbf{X} added to the expectation symbol \mathbb{E}
1098 or the variance symbol Var , this means that these operators are to be understood
1099 conditionally on \mathbf{X} . An integral with respect to $\mathbf{P}^*(d\mathbf{x})$ means that we integrate with
1100 respect to the law of \mathbf{X} .

1101 LEMMA D.1 (Moments of order 1). *The moments of order 1 are given by*

$$\begin{aligned}
1102 \quad \mathbb{E} \xi_{j;m1}^{UL} &= D_j, \\
1103 \quad \mathbb{E} \xi_{m1}^{UR} &= \mu, \\
1104 \quad \mathbb{E} \xi_{m1}^{ULL} &= \frac{1}{m} \mathbb{E} \text{Var}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) + D. \\
1105
\end{aligned}$$

1106

1107 *Proof.* One has

$$\begin{aligned}
1108 \quad \mathbb{E} \xi_{j;m1}^{UL} &= \frac{1}{m^2} \sum_{k,k'} \mathbb{E} f(X^{(1)}, Z^{(1,k)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,k')}) \\
1109 \quad &= \frac{1}{m^2} \sum_{k,k'} \int \mathbb{E} f(x, Z^{(1,k)}) f(\tilde{x}_{-j}, Z_j^{(1,k')}) \mathbf{P}^*(d\mathbf{x}) \\
1110 \quad &= \mathbb{E} f(X^{(1)}, Z^{(1,1)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \\
1111 \quad &= D_j,
\end{aligned}$$

1113 where the integral is taken with respect to the law of $\mathbf{x} = (x, \tilde{x})$, and,

$$\begin{aligned}
1114 \quad \mathbb{E} \xi_{m1}^{\prime\prime LL} &= \frac{1}{m^2} \sum_{k, k'} \mathbb{E} f(X^{(1)}, Z^{(1,k)}) f(X^{(1)}, Z^{(1,k')}) \\
1115 &= \frac{1}{m} \mathbb{E} \text{Var}^X f(X, Z) + \mathbb{E} (\mathbb{E}^X f(X, Z))^2 \\
1116 &= \frac{1}{m} \mathbb{E} \text{Var}^X f(X, Z) + D. \\
1117
\end{aligned}$$

1118 The proof for ξ_{m1}^{UR} is similar. □

1119 LEMMA D.2 (Moments of order 2). *The moments of order 2 are given by*

$$\begin{aligned}
1120 \quad \mathbb{E} \xi_{j;m1}^{(UL)2} &= \text{Var} \mathbb{E}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) + D_j^2 \\
1121 &+ \frac{1}{m} [\mathbb{E} \text{Var}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \\
1122 &- \text{Var}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) \text{Var}^{\mathbf{X}} f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)})] \\
1123 &+ \frac{1}{m^2} \mathbb{E} \text{Var}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) \text{Var}^{\mathbf{X}} f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}), \\
1124 \quad \mathbb{E} \xi_{m1}^{(UR)2} &= \frac{1}{m} \mathbb{E} \text{Var}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) + \mathbb{E} (\mathbb{E}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}))^2, \\
1125 \quad \mathbb{E} \xi_{m1}^{\prime\prime (LL)2} &= \frac{m(m-1)(m-2)(m-3)}{m^4} \\
1126 &\mathbb{E} f(X^{(1)}, Z^{(1,1)}) f(X^{(1)}, Z^{(1,2)}) f(X^{(1)}, Z^{(1,3)}) f(X^{(1)}, Z^{(1,4)}) \\
1127 &+ \frac{\binom{4}{2} m(m-1)(m-2)}{m^4} \mathbb{E} f(X^{(1)}, Z^{(1,1)})^2 f(X^{(1)}, Z^{(1,2)}) f(X^{(1)}, Z^{(1,3)}) \\
1128 &+ \frac{\binom{4}{3} m(m-1)}{m^4} \mathbb{E} f(X^{(1)}, Z^{(1,1)})^3 f(X^{(1)}, Z^{(1,2)}) \\
1129 &+ \frac{m}{m^4} \mathbb{E} f(X^{(1)}, Z^{(1,1)})^4 \\
1130 &+ \frac{\binom{4}{2} m(m-1)/2}{m^4} \mathbb{E} f(X^{(1)}, Z^{(1,1)})^2 f(X^{(1)}, Z^{(1,2)})^2 \\
1131 \\
1132
\end{aligned}$$

1133 *Proof.* Let us first deal with $\xi_{j;m1}^{\text{UL}}$. We have

$$\begin{aligned}
1135 \quad \mathbb{E} \xi_{j;m1}^{\text{UL}2} &= \frac{1}{m^4} \sum_{k_1, k_2, k_3, k_4} \mathbb{E} f(X^{(1)}, Z^{(1, k_1)}) f(X^{(1)}, Z^{(1, k_2)}) \\
1136 &f(\tilde{X}_{-j}^{(1)}, Z_j^{(1, k_3)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1, k_4)})
\end{aligned}$$

1138 where, in the sum, the indices run over $1, \dots, m$. We split the sum into four parts.
1139 The first contains the $m^2(m-1)^2$ terms that satisfy $k_1 \neq k_2$ and $k_3 \neq k_4$. In this
1140 part, all the terms are equal to

$$1141 \quad (\text{term 1}) \quad \mathbb{E} \left(\mathbb{E}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \right)^2.$$

1143 The second part contains the $m^2(m-1)$ terms that satisfy $k_1 \neq k_2$ and $k_3 = k_4$ and
1144 that are equal to

$$1145 \quad (\text{term 2}) \quad \mathbb{E} f(X^{(1)}, Z^{(1,1)}) f(X^{(1)}, Z^{(1,2)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)})^2.$$

1147 The third part contains the $m^2(m-1)$ terms that satisfy $k_1 = k_2$ and $k_3 \neq k_4$ and
1148 that are equal to

$$1149 \quad (\text{term 3}) \quad \mathbb{E} f(X^{(1)}, Z^{(1,1)})^2 f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,2)}).$$

1151 Finally, the fourth part contains the m^2 terms that satisfy $k_1 = k_2$ and $k_3 = k_4$ and
1152 are equal to

$$1153 \quad (\text{term 4}) \quad \mathbb{E} f(X^{(1)}, Z^{(1,1)})^2 f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)})^2.$$

1155 (One can see that the number of terms is m^4 .) Thus,

$$1156 \quad \mathbb{E} \xi_{m1}^{(\text{UL})2} = (\text{term 1}) \\ 1157 \quad + \frac{1}{m} [(\text{term 2}) + (\text{term 3}) - 2(\text{term 1})] \\ 1158 \quad + \frac{1}{m^2} [(\text{term 1}) - (\text{term 2}) - (\text{term 3}) + (\text{term 4})].$$

1160 Furthermore, $[(\text{term 1}) - (\text{term 2}) - (\text{term 3}) + (\text{term 4})]$ is equal to

$$1161 \quad \int \left(\mathbb{E}^{\mathbf{X}} f(x, Z) f(\tilde{x}_{-j}, Z_j) \right)^2 \\ 1162 \quad - \mathbb{E}^{\mathbf{X}} f(x, Z^{(1,1)}) f(x, Z^{(1,2)}) f(\tilde{x}_{-j}, Z_j^{(1,1)})^2 \\ 1163 \quad - \mathbb{E}^{\mathbf{X}} f(x, Z^{(1,1)})^2 f(\tilde{x}_{-j}, Z_j^{(1,1)}) f(\tilde{x}_{-j}, Z_j^{(1,2)}) \\ 1164 \quad + \mathbb{E}^{\mathbf{X}} f(x, Z^{(1,1)})^2 f(\tilde{x}_{-j}, Z_j^{(1,1)})^2 d\mathbf{P}^*(\mathbf{x}) \\ 1165 \quad = \int \left(\mathbb{E}^{\mathbf{X}} f(x, Z) \right)^2 \left(\mathbb{E}^{\mathbf{X}} f(\tilde{x}_{-j}, Z_j) \right)^2 \\ 1166 \quad - \left(\mathbb{E}^{\mathbf{X}} f(x, Z) \right)^2 \mathbb{E}^{\mathbf{X}} f(\tilde{x}_{-j}, Z_j)^2 \\ 1167 \quad - \mathbb{E}^{\mathbf{X}} f(x, Z)^2 \left(\mathbb{E}^{\mathbf{X}} f(\tilde{x}_{-j}, Z_j) \right)^2 \\ 1168 \quad + \mathbb{E}^{\mathbf{X}} f(x, Z)^2 \mathbb{E}^{\mathbf{X}} f(\tilde{x}_{-j}, Z_j)^2 d\mathbf{P}^*(\mathbf{x}) \\ 1169 \quad = \int \text{Var}^{\mathbf{X}} f(X, Z) \text{Var}^{\mathbf{X}} f(\tilde{X}_{-j}, Z_j) d\mathbf{P}^*(\mathbf{x}).$$

1171 Likewise, we find that $[(\text{term 2}) + (\text{term 3}) - 2(\text{term 1})]$ is equal to

$$1173 \quad \mathbb{E} \text{Var}^{\mathbf{X}} f(X, Z) f(\tilde{X}_{-j}, Z_j) - \text{Var}^{\mathbf{X}} f(X, Z) \text{Var}^{\mathbf{X}} f(\tilde{X}_{-j}, Z_j),$$

1174 and term 1 is $\text{Var} \mathbb{E}^{\mathbf{X}} f(X, Z) f(\tilde{X}_{-j}, \tilde{Z}) + D_j^2$.

1175 We now deal with ξ_{m1}^{LL} . We have

$$1177 \quad \mathbb{E} \xi_{m1}^{\text{LL}2} = \frac{1}{m^4} \sum_{k_1, k_2, k_3, k_4} \mathbb{E} f(X^{(1)}, Z^{(1, k_1)}) f(X^{(1)}, Z^{(1, k_2)}) \\ 1178 \quad f(X^{(1)}, Z^{(1, k_3)}) f(X^{(1)}, Z^{(1, k_4)}).$$

1180 The sum is split into five parts. The first part consists of the $m(m-1)(m-2)(m-3)$
1181 terms with different indices; those terms are equal to

$$1182 \quad \mathbb{E} f(X^{(1)}, Z^{(1,1)}) f(X^{(1)}, Z^{(1,2)}) f(X^{(1)}, Z^{(1,3)}) f(X^{(1)}, Z^{(1,4)}).$$

1183 The second part consists of the $\binom{4}{2}m(m-1)(m-2)$ terms with exactly two equal
 1184 indices; those terms are equal to

$$1185 \quad \mathbb{E} f(X^{(1)}, Z^{(1,1)})^2 f(X^{(1)}, Z^{(1,2)}) f(X^{(1)}, Z^{(1,3)}).$$

1186 The third part consists of the $\binom{4}{3}m(m-1)$ terms with exactly three equal indices;
 1187 those terms are equal to

$$1188 \quad \mathbb{E} f(X^{(1)}, Z^{(1,1)})^3 f(X^{(1)}, Z^{(1,2)}).$$

1189 The fourth part consists of the m terms with exactly four equal indices; those terms
 1190 are equal to

$$1191 \quad \mathbb{E} f(X^{(1)}, Z^{(1,1)})^4.$$

1192 The fifth and last part consists of the $\binom{4}{2}m(m-1)/2$ terms with exactly two pairs of
 1193 equal indices; those terms are equal to

$$1194 \quad \mathbb{E} f(X^{(1)}, Z^{(1,1)})^2 f(X^{(1)}, Z^{(1,2)})^2.$$

1195 (One can check that the total number of terms is m^4 .)

□

1196 LEMMA D.3 (Variances and covariances).

$$\begin{aligned}
1197 \quad (i) \quad & \text{Var } \xi_{m1}^{UL} = \text{Var } \mathbf{E}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \\
1198 \quad & + \frac{1}{m} [\mathbf{E} \text{Var}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \\
1199 \quad & - \text{Var}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) \text{Var}^{\mathbf{X}} f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)})] \\
1200 \quad & + \frac{1}{m^2} \mathbf{E} \text{Var}^{\mathbf{X}} f(X^{(1)}, Z^{(1,1)}) \text{Var}^{\mathbf{X}} f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}), \\
1201 \quad (ii) \quad & \text{Cov}(\xi_{m1}^{UL}, \xi_{m1}^{UR}) = \frac{m-1}{m} \mathbf{E} f(X^{(1)}, Z^{(1,1)}) f(X^{(1)}, Z^{(1,2)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \\
1202 \quad & + \frac{1}{m} \mathbf{E} f(X^{(1)}, Z^{(1,1)})^2 f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) - D_j \mu \\
1203 \quad (iii) \quad & \text{Cov}(\xi_{m1}^{UL}, f(X, Z)^2) = \frac{1}{m} \mathbf{E} f(X^{(1)}, Z^{(1,1)})^3 f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \\
1204 \quad (iii) \quad & + \frac{m-1}{m} \mathbf{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 \\
1205 \quad (iv) \quad & \text{Var } \xi_{m1}^{UR} = \frac{1}{m} \text{Var } f(X, Z) \\
1206 \quad (v) \quad & \text{Cov}(\xi_{m1}^{UR}, f(X, Z)^2) = \frac{1}{m} f(X, Z)^3 \\
1207 \quad & + \frac{m-1}{m} \mathbf{E} f(X^{(1)}, Z^{(1,1)})^2 f(X^{(1)}, Z^{(1,2)}) - \mu \kappa \\
1208 \quad (vi) \quad & \text{Cov}(\xi_{m_{n1}}^{UL}, \xi_{m_{n1}}^{ULL}) = \frac{m}{m^3} \mathbf{E} f(X^{(1)}, Z^{(1,1)})^3 f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \\
1209 \quad & + \frac{3m(m-1)}{m^3} \mathbf{E} f(X^{(1)}, Z^{(1,1)})^2 f(X^{(1)}, Z^{(1,2)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \\
1210 \quad & + \frac{m(m-1)(m-2)}{m^3} \mathbf{E} f(X^{(1)}, Z^{(1,1)}) f(X^{(1)}, Z^{(1,2)}) \\
1211 \quad & f(X^{(1)}, Z^{(1,3)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \\
1212 \quad & - \mathbf{E} f(X^{(1)}, Z^{(1,1)}) f(\tilde{X}_{-j}^{(1)}, Z_j^{(1,1)}) \\
1213 \quad & \left\{ \frac{1}{m} \mathbf{E} f(X^{(1)}, Z^{(1,1)})^2 + \frac{m-1}{m} \mathbf{E} f(X^{(1)}, Z^{(1,1)}) f(X^{(1)}, Z^{(1,2)}) \right\} \\
1214 \quad & \\
1215 \quad &
\end{aligned}$$

1216 *Proof.* The proof follows from direct calculations. \square

1217 Appendix E. Calculations for the linear model.

1218 LEMMA E.1. Suppose that $f(X, Z) = \beta_0 + \beta_{p+1}Z + \sum_{j=1}^p \beta_j X_j$ where $X =$
1219 (X_1, \dots, X_p) , Z_k, \tilde{Z}_{ik} are independent, $\mathbf{E} X_j = \mathbf{E} Z = 0$, $\mathbf{E} X_j^2 = \mathbf{E} Z^2 = 1$, $\mathbf{E} X_j^3 = 0$,
1220 $\mathbf{E} X_j^4 = 3$. Then the squared optimal number of repetitions is given by

$$1221 \quad (m_i^*)^2 = \frac{\beta_{p+1}^4}{(\beta_0 + \beta_i)^2 - 2\beta_0^4 + (\sum_{j=0}^p \beta_j^2)^2}$$

1222 and the discriminator (the upper-left term in (3.6) and (3.5)) is

$$1223 \quad \beta_0^2 + \beta_i^2.$$

1224

1225 *Proof.* We have

$$1226 \quad m_i^* = \frac{A_i + B_i + C_i + D_i}{E_i},$$

1227 with

$$\begin{aligned} 1228 \quad A_i &= \mathbb{E} f(X, Z_1)^2 f(\tilde{X}_{-i}, \tilde{Z}_{i1})^2 \\ 1229 \quad B_i &= \mathbb{E} f(X, Z_1) f(\tilde{X}_{-i}, \tilde{Z}_{i1}) f(X, Z_2) f(\tilde{X}_{-i}, \tilde{Z}_{i2}) \\ 1230 \quad C_i &= -\mathbb{E} f(X, Z_1)^2 f(\tilde{X}_{-i}, \tilde{Z}_{i1}) f(\tilde{X}_{-i}, \tilde{Z}_{i2}) \\ 1231 \quad D_i &= -\mathbb{E} f(\tilde{X}_{-i}, \tilde{Z}_{i1})^2 f(X, Z_1) f(X, Z_2) \\ 1232 \quad E_i &= B - [\mathbb{E} f(X, Z_1) f(\tilde{X}_{-i}, \tilde{Z}_{i1})]^2 \end{aligned}$$

1234 where $X = (X_1, \dots, X_p)$, Z_k, \tilde{Z}_{ik} are independent, $\mathbb{E} X_j = \mathbb{E} Z = 0$, $\mathbb{E} X_j^2 = \mathbb{E} Z^2 = 1$,
1235 $\mathbb{E} X_j^3 = 0$, $\mathbb{E} X_j^4 = 3$. We deal with the case

$$1236 \quad f(X, Z) = \beta_0 + \beta_{p+1} Z + \sum_{j=1}^p \beta_j X_j.$$

1237 We calculate the terms one by one as follows. We have

$$\begin{aligned} 1238 \quad A_j &= \mathbb{E} \left(\beta_0 + \sum_{j=1}^p \beta_j X_j \right)^2 \left(\beta_0 + \beta_i X_i + \sum_{j:1 \leq j \neq i} \beta_j \tilde{X}_j \right)^2 \\ 1239 \quad &+ \left(\beta_0 + \sum_{j=1}^p \beta_j X_j \right)^2 \beta_{p+1}^2 \tilde{Z}_{i1}^2 + \beta_{p+1}^4 Z_1^2 \tilde{Z}_{i1}^2 \\ 1240 \quad &+ \beta_{p+1}^2 Z_1^2 \left(\beta_0 + \beta_i X_i + \sum_{j:1 \leq j \neq i} \beta_j \tilde{X}_j \right)^2 \\ 1241 \quad &= A_{j1} + A_{j2} + A_{j3}, \end{aligned}$$

1243 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 some-
1244 what tedious calculations yield

$$1245 \quad \mathbb{E}(A1) = \beta_0^4 + 3\beta_i^4 + 6\beta_0^2 \beta_i^2 + 2(\beta_0^2 + \beta_i^2) \sum_{j:1 \leq j \neq i} \beta_j^2 + \left(\sum_{j:1 \leq j \neq i} \beta_j^2 \right)^2.$$

1247 Similar calculations show that $B_j = A_{j1}$, $C_j = -A_{j1} - A_{j3}$, $D_j = -A_{j1} - A_{j3}$,
1248 $E_j = A_{j1} - (\beta_0^2 + \beta_i^2)^2$. Thus,

$$1249 \quad (m_i^*)^2 = \frac{\beta_{p+1}^4}{(\beta_0 + \beta_i)^2 - 2\beta_0^4 + (\sum_{j=0}^p \beta_j^2)^2}. \quad \square$$

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1254

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