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# Global sensitivity analysis and Wasserstein spaces

Jean-Claude Fort<sup>1</sup>, Thierry Klein<sup>2</sup>, and Agnès Lagnoux<sup>3</sup>

<sup>1</sup>MAP5 Université Paris Descartes, SPC, 45 rue des Saints Pères, 75006 Paris, France.

<sup>2</sup>Institut de Mathématiques de Toulouse; UMR5219. Université de Toulouse; ENAC - Ecole Nationale de l'Aviation Civile, Université de Toulouse, France

<sup>3</sup>Institut de Mathématiques de Toulouse; UMR5219. Université de Toulouse; CNRS. UT2J, F-31058 Toulouse, France.

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## Abstract

Sensitivity indices are commonly used to quantify the relative influence of any specific group of input variables on the output of a computer code. In this paper, we focus both on computer codes for which the output is a cumulative distribution function and on stochastic computer codes. We propose a way to perform a global sensitivity analysis for these kinds of computer codes. In the first setting, we define two indices: the first one is based on Wasserstein Fréchet means while the second one is based on the Hoeffding decomposition of the indicators of Wasserstein balls. Further, when dealing with the stochastic computer codes, we define an “ideal version” of the stochastic computer code that fits into the frame of the first setting. Finally, we deduce a procedure to realize a second-level global sensitivity analysis, namely when one is interested in the sensitivity related to the input distributions rather than in the sensitivity related to the inputs themselves. Several numerical studies are proposed as illustrations in the different settings.

**Keywords:** Global sensitivity indices, functional computer codes, stochastic computer codes, second-level uncertainty, Fréchet means, Wasserstein spaces.

**AMS subject classification** 62G05, 62G20, 62G30, 65C60, 62E17.

## 1 Introduction

The use of complex computer models for the analysis of applications from sciences, engineering and other fields is by now routine. For instance, in the area of marine submersion, complex computer codes have been developed to simulate submersion events (see, e.g., [4, 34] for more details). In the context of aircraft design, sensitivity analysis and metamodeling are intensively used to optimize the design of an airplane (see, e.g., [51]). Several other concrete examples of stochastic computer codes can be found in [42].

Often, the models are expensive to run in terms of computational time. Thus it is crucial to understand the global influence of one or several inputs on the output of the system under study with a moderate number of runs afforded [54]. When these inputs are regarded as random elements, this problem is generally called (global) sensitivity analysis. We refer to [17, 52, 58] for an overview of the practical aspects of global sensitivity analysis.

A classical tool to perform global sensitivity analysis consists in computing the Sobol indices. These indices were first introduced in [50] and then considered by [57]. They are well tailored when the output space is  $\mathbb{R}$ . The Sobol indices compare, using the Hoeffding decomposition [33], the conditional variance of the output knowing some of the input variables to the total variance of the output. Many different estimation procedures of the Sobol indices have been proposed and studied in the literature. Some are based on Monte-Carlo or quasi Monte-Carlo design of experiments (see [38, 47] and references therein for more details). More recently a method based on nested Monte-Carlo [28] has been developed. In particular, an efficient estimation of the Sobol indices can be performed through the so-called “Pick-Freeze” method. For the description of this method and its theoretical study (consistency, central limit theorem, concentration inequalities and Berry- Esseen bounds), we refer to [36, 25] and references therein. Some

other estimation procedures are based on different designs of experiments using for example polynomial chaos expansions (see [60] and the reference therein for more details).

Since Sobol indices are variance-based, they only quantify the influence of the inputs on the mean behavior of the code. Many authors proposed other criteria to compare the conditional distribution of the output knowing some of the inputs to the distribution of the output. In [47, 49, 48], the authors use higher moments to define new indices while, in [7, 8, 16], the use of divergences or distances between measures allows to define new indices. In [20], the authors use contrast functions to build indices that are goal-oriented. Although these works define nice theoretical indices, the existence of a relevant statistical estimation procedure is still, in most cases, an open question. The case of vectorial-valued computer codes is considered in [26] where a sensitivity index based on the whole distribution using the Cramér-von-Mises distance is defined. Within this framework, the authors show that the Pick-Freeze estimation procedure provides an asymptotically Gaussian estimator of the index.

Nowadays, the computer code output is often no longer a real-valued multidimensional variable but rather a function computed at various locations. In that sense, it can be considered as a functional output. Some other times, the computer code is stochastic in the sense that the same inputs can lead to different outputs. When the output of the computer code is a function (for instance, a cumulative distribution function) or when the computer code is stochastic, Sobol indices are no longer well tailored. It is then crucial to define indices adapted to the functional or random aspect of the output. When the output is vectorial or valued in an Hilbert space, some generalizations of Sobol indices are available [39, 24]. Nevertheless, these indices are still based on the Hoeffding decomposition of the output; so that they only quantify the relative influence of an input through the variance. More recently, indices based on the whole distribution have been developed [16, 9, 7]. In particular, the method relying on Cramér-von-Mises distance [26] compares the conditionnal cumulative distribution function with the unconditional one by considering the Hoeffding decomposition of half-space indicators (rather than the Hoeffding decomposition of the output itself) and by integrating them. This method was then extend to codes taking values in a Riemannian manifold [21] and then in general metric spaces [27].

In this work, we focus on two kinds of computer codes: 1) computer codes for which the output is the cumulative distribution function of a real random variable and 2) real-valued stochastic computer codes. A first step will consist in performing global sensitivity analysis for these kinds of computer codes. Further, we focus on second-level analysis that corresponds to the sensitivity analysis with respect to the input distribution (see Section 6 for more details on second-level analysis). Then we will deduce how to perform second-level sensitivity analysis using the tools developed in the first step. A code with cumulative distribution function as output can be seen as a code taking values in the space of all probability measures on  $\mathbb{R}$ . This space can be endowed with a metric (for example, the Wasserstein metric [62]). This point of view allows to define at least two different indices for this kind of codes, generalizing the framework of [27]. The first one is based on Wasserstein Fréchet means while the second one is based on the Hoeffding decomposition of the indicators of Wasserstein balls. Further, stochastic codes (see Section 5 for a bibliographical study) can be seen as a “discrete approximation” of codes having cumulative distribution functions as values. Then it is possible to define “natural” indices for such stochastic codes. Finally, second-level sensitivity analysis aims at considering uncertainties on the type of the input distributions and/or on the parameters of the input distributions (see Section 6 for a bibliographical study). Actually, this kind of problem can be embedded in the framework of stochastic codes.

The article is organized as follows. In Section 2, we introduce and precisely define a general class of global sensitivity indices. We also present statistical methods to estimate these indices. In Section 3, we recall some basic facts on Wasserstein distances, Wasserstein costs and Fréchet means. In Section 4, we define and study the statistical properties of two new global sensitivity indices for computer codes valued in general Wasserstein spaces. Further, in Section 5, we study the case of stochastic computer codes. The proof of the main result of this section has been postponed to Section A. Then, Section 6 is dedicated to the sensitivity analysis with respect to the distributions of the input variables. In Section 7, practical advices are given for the practitioners. Finally, we present conclusions, limitations and perspectives in Section 8.

## 2 Sensitivity indices for codes valued in general metric spaces

We consider a black-box code  $f$  defined on a product of measurable spaces  $E = E_1 \times E_2 \times \dots \times E_p$  ( $p \in \mathbb{N}^*$ ) taking its values in a metric space  $\mathcal{X}$ . The output denoted by  $Z$  is then given by

$$Z = f(X_1, \dots, X_p). \quad (1)$$

We denote by  $\mathbb{P}$  the distribution of the output code  $Z$ .

The aim of this work is to give answers to the following questions.

**Question 1** How can we perform Global Sensitivity Analysis (GSA) when the output space is the space of probability distribution functions (p.d.f.) on  $\mathbb{R}$  or the space of cumulative distribution functions (c.d.f.)?

**Question 2** How can we perform GSA for stochastic computer codes?

**Question 3** How can we perform GSA with respect to the choice of the distributions of the input variables?

### 2.1 The general metric spaces sensitivity index

In this section, we recall the definition and the properties of the general metric spaces sensitivity index introduced in [27]. We also discuss several ways of estimation: the Pick-Freeze estimation as introduced in [36], the estimation procedure based on U-statistics proposed in [27], and a rank-based procedure initiated in [23].

In [27], the authors performed GSA for codes  $f$  taking values in general metric spaces. To do so, they consider a family of test functions parameterized by  $m \in \mathbb{N}^*$  elements of  $\mathcal{X}$  and defined by

$$\begin{aligned} \mathcal{X}^m \times \mathcal{X} &\rightarrow \mathbb{R} \\ (a, x) &\mapsto T_a(x). \end{aligned}$$

Let  $\mathbf{u} \subset \{1, \dots, p\}$  and  $X_{\mathbf{u}} = (X_i, i \in \mathbf{u})$ . Assuming that the test functions  $T_a$  are  $L^2$ -functions with respect to the product measure  $\mathbb{P}^{\otimes m} \otimes \mathbb{P}$  (where  $\mathbb{P}^{\otimes m}$  is the product  $m$ -times of the distribution of the output code  $Z$ ) on  $\mathcal{X}^m \times \mathcal{X}$ , they allow to define the general metric space (GMS) sensitivity index with respect to  $X_{\mathbf{u}}$  by

$$S_{2,\text{GMS}}^{\mathbf{u}} = \frac{\int_{\mathcal{X}^m} \mathbb{E} \left[ (\mathbb{E}[T_a(Z)] - \mathbb{E}[T_a(Z)|X_{\mathbf{u}}])^2 \right] d\mathbb{P}^{\otimes m}(a)}{\int_{\mathcal{X}^m} \text{Var}(T_a(Z)) d\mathbb{P}^{\otimes m}(a)} = \frac{\int_{\mathcal{X}^m} \text{Var}(\mathbb{E}[T_a(Z)|X_{\mathbf{u}}]) d\mathbb{P}^{\otimes m}(a)}{\int_{\mathcal{X}^m} \text{Var}(T_a(Z)) d\mathbb{P}^{\otimes m}(a)}. \quad (2)$$

Roughly speaking, the previous indices divided into two parts. First, for any value of  $a$ , we consider the numerator  $\mathbb{E}[(\mathbb{E}[T_a(Z)] - \mathbb{E}[T_a(Z)|X_{\mathbf{u}}])^2]$  and the denominator  $\text{Var}(T_a(Z))$  of the classical Sobol index of  $T_a(Z)$ . This part is called the Sobol part. Second, we integrate each part with respect to the measure  $\mathbb{P}^{\otimes m}$ ; it is called the integration part.

As explained in [27], by construction, the indices  $S_{2,\text{GMS}}^{\mathbf{u}}$  lie in  $[0, 1]$  and share the same properties as their Sobol counterparts:

- the different contributions sum to 1; (3)

- they are invariant by translation, by any isometry and by any non-degenerated scaling of  $Z$ . (4)

**Estimation** Three different estimation procedures are available in this context. The two first methods are based on the Pick-Freeze scheme. More precisely, the Pick-Freeze scheme, considered in [36], is a well tailored design of experiment. Namely, let  $X^{\mathbf{u}}$  be the random vector such that  $X_i^{\mathbf{u}} = X_i$  if  $i \in \mathbf{u}$  and  $X_i^{\mathbf{u}} = X'_i$  if  $i \notin \mathbf{u}$  where  $X'_i$  is an independent copy of  $X_i$ . We then set

$$Z^{\mathbf{u}} := f(X^{\mathbf{u}}). \quad (5)$$

Further, the procedure consists in rewriting the variance of the conditional expectation in terms of covariances as follows

$$\text{Var}(\mathbb{E}[Z|X_{\mathbf{u}}]) = \text{Cov}(Z, Z^{\mathbf{u}}). \quad (6)$$

Alternatively, the third estimation procedure that can be seen as an ingenious and effective approximation of the Pick-Freeze scheme is based on rank statistics [23]. Until now, it is unfortunately only available to estimate first-order indices in the case of real-valued inputs.

- **First method - Pick-Freeze.** Introduced in [26], this procedure is based on a double Monte-Carlo scheme to estimate the Cramér-von-Mises (CVM) indices  $S_{2,\text{CVM}}^{\mathbf{u}}$ . More precisely, to estimate  $S_{2,\text{GMS}}^{\mathbf{u}}$  in our context, we consider the following design of experiment consisting in

1. a classical Pick-Freeze  $N$ -sample, that is two  $N$ -samples of  $Z$ :  $(Z_j, Z_j^{\mathbf{u}})$ ,  $1 \leq j \leq N$ ;
2.  $m$  other  $N$ -samples of  $Z$  independent of  $(Z_j, Z_j^{\mathbf{u}})_{1 \leq j \leq N}$ :  $W_{l,k}$ ,  $1 \leq l \leq m$ ,  $1 \leq k \leq N$ .

The empirical estimator of the numerator of  $S_{2,\text{GMS}}^{\mathbf{u}}$  is then given by

$$\begin{aligned} \hat{N}_{2,\text{GMS},\text{PF}}^{\mathbf{u}} = & \frac{1}{N^m} \sum_{1 \leq i_1, \dots, i_m \leq N} \left[ \frac{1}{N} \sum_{j=1}^N T_{W_{1,i_1}, \dots, W_{m,i_m}}(Z_j) T_{W_{1,i_1}, \dots, W_{m,i_m}}(Z_j^{\mathbf{u}}) \right] \\ & - \frac{1}{N^m} \sum_{1 \leq i_1, \dots, i_m \leq N} \left[ \frac{1}{2N} \sum_{j=1}^N (T_{W_{1,i_1}, \dots, W_{m,i_m}}(Z_j) + T_{W_{1,i_1}, \dots, W_{m,i_m}}(Z_j^{\mathbf{u}})) \right]^2 \end{aligned}$$

while the one of the denominator is

$$\begin{aligned} \hat{D}_{2,\text{GMS},\text{PF}}^{\mathbf{u}} = & \frac{1}{N^m} \sum_{1 \leq i_1, \dots, i_m \leq N} \left[ \frac{1}{2N} \sum_{j=1}^N (T_{W_{1,i_1}, \dots, W_{m,i_m}}(Z_j)^2 + T_{W_{1,i_1}, \dots, W_{m,i_m}}(Z_j^{\mathbf{u}})^2) \right] \\ & - \frac{1}{N^m} \sum_{1 \leq i_1, \dots, i_m \leq N} \left[ \frac{1}{2N} \sum_{j=1}^N (T_{W_{1,i_1}, \dots, W_{m,i_m}}(Z_j) + T_{W_{1,i_1}, \dots, W_{m,i_m}}(Z_j^{\mathbf{u}})) \right]^2. \end{aligned}$$

For  $\mathcal{X} = \mathbb{R}^k$ ,  $m = 1$ , and  $T_a$  given by  $T_a(x) = \mathbb{1}_{x \leq a}$ , the index  $S_{2,\text{GMS},\text{PF}}^{\mathbf{u}}$  is nothing more than the index  $S_{2,\text{CVM}}^{\mathbf{u}}$  defined in [26] based on the Cramér-von-Mises distance and on the whole distribution of the output. Its estimator  $\hat{S}_{2,\text{CVM}}^{\mathbf{u}}$  defined as the ratio of  $\hat{N}_{2,\text{GMS},\text{PF}}^{\mathbf{u}}$  and  $\hat{D}_{2,\text{GMS},\text{PF}}^{\mathbf{u}}$  with  $T_a(x) = \mathbb{1}_{x \leq a}$  has been proved to be asymptotically Gaussian [26, Theorem 3.8]. The proof relies on Donsker's theorem and the functional delta method [61, Theorem 20.8]. Analogously, in the general case of  $S_{2,\text{GMS}}^{\mathbf{u}}$ , the central limit theorem is still valid as soon as the collection  $(T_a)_{a \in \mathcal{X}^m}$  forms a Donsker's class of functions.

- **Second method - U-statistics.** As done in [27], this method allows the practitioner to get rid of the additional random variables  $(W_{l,k})$  for  $l \in \{1, \dots, m\}$  and  $k \in \{1, \dots, N\}$ . The estimator is now based on U-statistics and deals simultaneously with the Sobol part and the integration part with respect to  $d\mathbb{P}^{\otimes m}(a)$ . It suffices to rewrite  $S_{2,\text{GMS}}^{\mathbf{u}}$  as

$$S_{2,\text{GMS}}^{\mathbf{u}} = \frac{I(\Phi_1) - I(\Phi_2)}{I(\Phi_3) - I(\Phi_4)}, \quad (7)$$

where,

$$\begin{aligned} \Phi_1(\mathbf{z}_1, \dots, \mathbf{z}_{m+1}) &= T_{z_1, \dots, z_m}(z_{m+1}) T_{z_1, \dots, z_m}(z_{m+1}^{\mathbf{u}}), \\ \Phi_2(\mathbf{z}_1, \dots, \mathbf{z}_{m+2}) &= T_{z_1, \dots, z_m}(z_{m+1}) T_{z_1, \dots, z_m}(z_{m+2}^{\mathbf{u}}), \\ \Phi_3(\mathbf{z}_1, \dots, \mathbf{z}_{m+1}) &= T_{z_1, \dots, z_m}(z_{m+1})^2, \\ \Phi_4(\mathbf{z}_1, \dots, \mathbf{z}_{m+2}) &= T_{z_1, \dots, z_m}(z_{m+1}) T_{z_1, \dots, z_m}(z_{m+2}), \end{aligned} \quad (8)$$

denoting by  $\mathbf{z}_i$  the pair  $(z_i, z_i^{\mathbf{u}})$  and, for  $l = 1, \dots, 4$ ,

$$I(\Phi_l) = \int_{\mathcal{X}^{m(l)}} \Phi_l(\mathbf{z}_1, \dots, \mathbf{z}_{m(l)}) d\mathbb{P}_2^{\mathbf{u}, \otimes m(l)}(\mathbf{z}_1 \dots, \mathbf{z}_{m(l)}), \quad (9)$$

with  $m(1) = m(3) = m + 1$  and  $m(2) = m(4) = m + 2$ . Finally, one considers the empirical version of (7) as estimator of  $S_{2,\text{GMS}}^{\mathbf{u}}$

$$\hat{S}_{2,\text{GMS},\text{Ustat}}^{\mathbf{u}} = \frac{U_{1,N} - U_{2,N}}{U_{3,N} - U_{4,N}}, \quad (10)$$

where, for  $l = 1, \dots, 4$ ,

$$U_{l,N} = \binom{N}{m(l)}^{-1} \sum_{1 \leq i_1 < \dots < i_{m(l)} \leq N} \Phi_l^s(\mathbf{Z}_{i_1}, \dots, \mathbf{Z}_{i_{m(l)}}) \quad (11)$$

and the function

$$\Phi_l^s(\mathbf{z}_1, \dots, \mathbf{z}_{m(l)}) = \frac{1}{(m(l))!} \sum_{\tau \in \mathcal{S}_{m(l)}} \Phi_l(\mathbf{z}_{\tau(1)}, \dots, \mathbf{z}_{\tau(m(l))})$$

is the symmetrized version of  $\Phi_l$ . In [27, Theorem 2.4], the estimator  $\widehat{S}_{2,\text{GMS},\text{U-stat}}^{\mathbf{u}}$  has been proved to be consistent and asymptotically Gaussian.

- **Third method - Rank-based.** In [15], Chatterjee proposes an efficient way based on ranks to estimate a new coefficient of correlation. This estimation procedure can be seen as an approximation of the Pick-Freeze scheme and then has been exploited in [23] to perform a more efficient estimation of  $S_{2,\text{GMS}}^{\mathbf{u}}$ . Nevertheless, this method is only well tailored for estimating first-order indices i.e. in the case of  $\mathbf{u} = \{i\}$  for some  $i \in \{1, \dots, p\}$  and when the input  $X_i \in \mathbb{R}$ .

More precisely, an i.i.d. sample of pairs of real-valued random variables  $(X_{i,j}, Y_j)_{1 \leq j \leq N}$  ( $i \in \{1, \dots, p\}$ ) is considered, assuming for simplicity that the laws of  $X_i$  and  $Y$  are both diffuse (ties are excluded). The pairs  $(X_{i,(1)}, Y_{(1)}), \dots, (X_{i,(N)}, Y_{(N)})$  are rearranged in such a way that

$$X_{i,(1)} < \dots < X_{i,(N)}$$

and, for any  $j = 1, \dots, N$ ,  $Y_{(j)}$  is the output computed from  $X_{i,(j)}$ . Let  $r_j$  be the rank of  $Y_{(j)}$ , that is,

$$r_j = \#\{j' \in \{1, \dots, N\}, Y_{(j')} \leq Y_{(j)}\}.$$

The new correlation coefficient is then given by

$$\xi_N(X_i, Y) = 1 - \frac{3 \sum_{j=1}^{N-1} |r_{j+1} - r_j|}{N^2 - 1}. \quad (12)$$

In [15], it is proved that  $\xi_N(X_i, Y)$  converges almost surely to a deterministic limit  $\xi(X_i, Y)$  which is actually equal to  $S_{2,\text{CVM}}^i$  when  $Y = Z = f(X_1, \dots, X_p)$ . Further, the author also proves a central limit theorem when  $X_i$  and  $Y$  are independent, which is clearly not relevant in the context of sensitivity analysis (SA) (where  $X_i$  and  $Y$  are dependent through the computer code).

In our context, recall that  $\mathbf{u} = \{i\}$  and let  $Y = Z$ . Let also  $\pi_i(j)$  be the rank of  $X_{i,j}$  in the sample  $(X_{i,1}, \dots, X_{i,N})$  of  $X_i$  and define

$$N_i(j) = \begin{cases} \pi_i^{-1}(\pi_i(j) + 1) & \text{if } \pi_i(j) + 1 \leq N, \\ \pi_i^{-1}(1) & \text{if } \pi_i(j) = N. \end{cases} \quad (13)$$

Then the empirical estimator  $\widehat{S}_{2,\text{GMS},\text{Rank}}^i$  of  $S_{2,\text{GMS}}^i$  only requires a  $N$ -sample  $(Z_j)_{1 \leq j \leq N}$  of  $Z$  and is given by the ratio between

$$\begin{aligned} \widehat{N}_{2,\text{GMS},\text{Rank}}^i &= \frac{1}{N^m} \sum_{1 \leq i_1, \dots, i_m \leq N} \left[ \frac{1}{N} \sum_{j=1}^N T_{Z_{i_1}, \dots, Z_{i_m}}(Z_j) T_{Z_{i_1}, \dots, Z_{i_m}}(Z_{N_i(j)}) \right] \\ &\quad - \frac{1}{N^m} \sum_{1 \leq i_1, \dots, i_m \leq N} \left[ \frac{1}{N} \sum_{j=1}^N T_{Z_{i_1}, \dots, Z_{i_m}}(Z_j) \right]^2 \end{aligned} \quad (14)$$

and  $\widehat{D}_{2,\text{GMS},\text{Rank}}^i$

$$\frac{1}{N^m} \sum_{1 \leq i_1, \dots, i_m \leq N} \left[ \frac{1}{N} \sum_{j=1}^N T_{Z_{i_1}, \dots, Z_{i_m}}(Z_j)^2 \right] - \frac{1}{N^m} \sum_{1 \leq i_1, \dots, i_m \leq N} \left[ \frac{1}{N} \sum_{j=1}^N T_{Z_{i_1}, \dots, Z_{i_m}}(Z_j) \right]^2. \quad (15)$$

It is worth mentioning that  $Z_{N_i(j)}$  plays the same role as  $Z_j^i$  (the Pick-Freeze version of  $Z_j$  with respect to  $X_i$ ) in the Pick-Freeze estimation procedure.

## Comparison of the estimation procedures

First, the Pick-Freeze estimation procedure allows the estimation of several sensitivity indices: the classical Sobol indices for real-valued outputs, as well as their generalization for vectorial-valued codes, but also the indices based on higher moments [49] and the Cramér-von-Mises indices which take the whole distribution into account [26, 21]. Practically, this methodology is quite general and easy to implement. Moreover, the Pick-Freeze estimators have desirable statistical properties. More precisely, this estimation scheme has been proved to be consistent and asymptotically normal (i.e. the rate of convergence is  $\sqrt{N}$ ) in [36, 25, 27]. The limiting variances can be computed explicitly, allowing the practitioner to build confidence intervals. In addition, for a given sample size  $N$ , exponential inequalities have been established. Last but not least, the sequence of estimators is asymptotically efficient from such a design of experiment (see, [61] for the definition of the asymptotic efficiency and [25] for more details on the result).

However, the Pick-Freeze estimators have two major drawbacks. First, they rely on a particular experimental design that may be unavailable in practice. Second, it can be unfortunately very time consuming in practice: the number of model calls to estimate all first-order Sobol indices grows linearly with the number of input parameters. For example, if we consider  $p = 99$  input parameters and only  $N = 1000$  calls are allowed, then only a sample of size  $N/(p+1) = 10$  is available to estimate each single first-order Sobol index.

Secondly, the estimation procedure based on U-statistics has the same kind of asymptotic guarantees as the Pick-Freeze estimators (namely, consistency and asymptotic normality). Furthermore, the estimation scheme is reduced to  $2N$  evaluations of the code. Last, using the results of Hoeffding [33] on U-statistics, the asymptotic normality is proved straightforwardly.

Finally, embedding Chatterjee’s method in the GSA framework (called rank-based method in this framework) thereby eliminates the two drawbacks of the classical Pick-Freeze estimation. Indeed, the strength of the rank-based estimation procedure lies in the fact that only one  $N$ -sample of  $Z$  is required while  $(m+2)$  samples of size  $N$  are necessary in the Pick-Freeze estimation of a single index (worse,  $(m+1+p)$  samples of size  $N$  are required when one wants to estimate  $p$  indices). Using a single sample of size  $N$ , it is now possible to estimate at the same time all the first-order Sobol indices, first-order Cramér-von-Mises indices, and other useful first-order sensitivity indices as soon as all inputs are real valued. More generally, the rank-based method allows for the estimation of a large class of GSA indices which includes the Sobol indices and the higher-order moment indices proposed by Owen [47, 49, 48]. In addition, the rank-based estimator has nice theoretical properties. For instance, the estimator of the Sobol index  $S^i$  has been proved to be consistent and asymptotically Gaussian (see, e.g., Theorem 3.3 in [23]).

## 2.2 The universal sensitivity index

In this section, the aim is to generalize the already-known general metric space index  $S_{2,\text{GMS}}^{\mathbf{u}}$  presented in the previous section. Here, we then define a new index that we call the “universal sensitivity index” and we denote by  $S_{2,\text{Univ}}^{\mathbf{u}}$ .

To do so, observe that Formula (2) can be generalized in the following ways.

1. The point  $a$  in the definition of the test functions can be allowed to belong to another measurable space than  $\mathcal{X}^m$ .
2. The probability measure  $\mathbb{P}^{\otimes m}$  in (2) can be replaced by any “admissible” probability measure.

Such generalizations lead to the definition of a universal sensitivity index and its procedures of estimation.

**Definition 2.1.** Let  $a$  belongs to some measurable space  $\Omega$  endowed with some probability measure  $\mathbb{Q}$ . For any  $\mathbf{u} \subset \{1, \dots, p\}$ , we define the *universal sensitivity index* with respect to  $X_{\mathbf{u}}$  by

$$S_{2,\text{Univ}}^{\mathbf{u}}(T_a, \mathbb{Q}) = \frac{\int_{\Omega} \mathbb{E} \left[ (\mathbb{E}[T_a(Z)] - \mathbb{E}[T_a(Z)|X_{\mathbf{u}}])^2 \right] d\mathbb{Q}(a)}{\int_{\Omega} \text{Var}(T_a(Z)) d\mathbb{Q}(a)} = \frac{\int_{\Omega} \text{Var}(\mathbb{E}[T_a(Z)|X_{\mathbf{u}}]) d\mathbb{Q}(a)}{\int_{\Omega} \text{Var}(T_a(Z)) d\mathbb{Q}(a)}. \quad (16)$$

Notice that the index  $S_{2,\text{Univ}}^{\mathbf{u}}(T_a, \mathbb{Q})$  is obtained by the integration over  $a$  with respect to  $\mathbb{Q}$  of the Hoeffding decomposition of  $T_a(Z)$ . Hence, by construction, this index lies in  $[0, 1]$  and shares the same properties as its Sobol counterparts, namely the two previously cited properties in (3) and (4).

The universality is twofold. First, it allows to consider more general relevant indices. Secondly, this definition encompasses, as particular cases, the classical sensitivity indices. Indeed,

- the so-called Sobol index  $S^{\mathbf{u}}$  with respect to  $X_{\mathbf{u}}$  is  $S_{2,\text{Univ}}^{\mathbf{u}}(\text{Id}, \mathbb{P})$ , with  $\text{Id}$  the identity test function;
- the Cramér-von-Mises index  $S_{2,\text{CVM}}^{\mathbf{u}}$  with respect to  $X_{\mathbf{u}}$  is  $S_{2,\text{Univ}}^{\mathbf{u}}(\mathbb{1}_{\leq a}, \mathbb{P}^{\otimes d})$  where  $\mathcal{X} = \mathbb{R}^d$  and  $\Omega = \mathcal{X}$ ;
- the general metric space sensitivity index  $S_{2,\text{GMS}}^{\mathbf{u}}$  with respect to  $X_{\mathbf{u}}$  is  $S_{2,\text{Univ}}^{\mathbf{u}}(\mathbb{1}_{\leq a}, \mathbb{P}^{\otimes m})$  where  $\Omega = \mathcal{X}^m$ .

An example where  $\mathbb{Q}$  is different from  $\mathbb{P}$  will be considered in Section 4.

**Estimation** Here, we assume that  $\mathbb{Q}$  is different from  $\mathbb{P}^{\otimes m}$  and we follow the same tracks as for the estimation of  $S_{2,\text{GMS}}^{\mathbf{u}}$  in Section 2.1.

- First method - Pick-Freeze. We use the same design of experiment as in the first method of Section 2.1 but instead of considering that the  $m$  additional  $N$ -samples  $(W_{l,k})$  for  $l \in \{1, \dots, m\}$  and  $k \in \{1, \dots, N\}$  are drawn with respect to the distribution  $\mathbb{P}$  of the output, they are now drawn with respect to  $\mathbb{Q}$ . More precisely, we consider the following design of experiment consisting in
  1. a classical Pick-Freeze sample, that is two  $N$ -samples of  $Z$ :  $(Z_j, Z_j^{\mathbf{u}})$ ,  $1 \leq j \leq N$ ;
  2.  $m$   $\mathbb{Q}$ -distributed  $N$ -samples  $W_{l,k}$ ,  $l \in \{1, \dots, m\}$  and  $k \in \{1, \dots, N\}$  that are independent of  $(Z_j, Z_j^{\mathbf{u}})$  for  $1 \leq j \leq N$ .

The empirical estimator of the numerator of  $S_{2,\text{Univ}}^{\mathbf{u}}$  is then given by

$$\begin{aligned} \hat{N}_{2,\text{Univ},\text{PF}}^{\mathbf{u}} = & \frac{1}{N^m} \sum_{1 \leq i_1, \dots, i_m \leq N} \left[ \frac{1}{N} \sum_{j=1}^N T_{W_{1,i_1}, \dots, W_{m,i_m}}(Z_j) T_{W_{1,i_1}, \dots, W_{m,i_m}}(Z_j^{\mathbf{u}}) \right] \\ & - \frac{1}{N^m} \sum_{1 \leq i_1, \dots, i_m \leq N} \left[ \frac{1}{2N} \sum_{j=1}^N (T_{W_{1,i_1}, \dots, W_{m,i_m}}(Z_j) + T_{W_{1,i_1}, \dots, W_{m,i_m}}(Z_j^{\mathbf{u}})) \right]^2 \end{aligned}$$

while the one of the denominator is

$$\begin{aligned} \hat{D}_{2,\text{Univ},\text{PF}}^{\mathbf{u}} = & \frac{1}{N^m} \sum_{1 \leq i_1, \dots, i_m \leq N} \left[ \frac{1}{2N} \sum_{j=1}^N (T_{W_{1,i_1}, \dots, W_{m,i_m}}(Z_j)^2 + T_{W_{1,i_1}, \dots, W_{m,i_m}}(Z_j^{\mathbf{u}})^2) \right] \\ & - \frac{1}{N^m} \sum_{1 \leq i_1, \dots, i_m \leq N} \left[ \frac{1}{2N} \sum_{j=1}^N (T_{W_{1,i_1}, \dots, W_{m,i_m}}(Z_j) + T_{W_{1,i_1}, \dots, W_{m,i_m}}(Z_j^{\mathbf{u}})) \right]^2. \end{aligned}$$

As previously, it is straightforward (as soon as the collection  $(T_a)_{a \in \mathcal{X}^m}$  forms a Donsker's class of functions) to adapt the proof of Theorem [26, Theorem 3.8] to prove the asymptotic normality of the estimator.

- Second method - U-statistics. This method is not relevant in this case since  $\mathbb{Q} \neq \mathbb{P}^{\otimes d}$ .
- Third method - Rank-based. Here, the design of experiment reduces to
  1. a  $N$ -sample of  $Z$ :  $Z_j$ ,  $1 \leq j \leq N$ ;
  2. a  $N$ -sample of  $W$  that is  $\mathbb{Q}$ -distributed:  $W_k$ ,  $1 \leq k \leq N$ , independent of  $Z_j$ ,  $1 \leq j \leq N$ .

Assume as previously  $\mathbf{u} = \{i\}$  and  $N_i(\cdot)$  be defined in (13). The empirical estimator  $\hat{S}_{2,\text{Univ},\text{Rank}}^i$  of  $S_{2,\text{Univ}}^i$  is then given by the ratio between

$$\begin{aligned} \hat{N}_{2,\text{Univ},\text{Rank}}^i = & \frac{1}{N^m} \sum_{1 \leq i_1, \dots, i_m \leq N} \left[ \frac{1}{N} \sum_{j=1}^N T_{W_{i_1}, \dots, W_{i_m}}(Z_j) T_{W_{i_1}, \dots, W_{i_m}}(Z_{N_i(j)}) \right] \\ & - \frac{1}{N^m} \sum_{1 \leq i_1, \dots, i_m \leq N} \left[ \frac{1}{N} \sum_{j=1}^N T_{W_{i_1}, \dots, W_{i_m}}(Z_j) \right]^2 \end{aligned} \quad (17)$$



and  $\widehat{D}_{2,\text{Univ,Rank}}^i$

$$\frac{1}{N^m} \sum_{1 \leq i_1, \dots, i_m \leq N} \left[ \frac{1}{N} \sum_{j=1}^N T_{W_{i_1}, \dots, W_{i_m}}(Z_j)^2 \right] - \frac{1}{N^m} \sum_{1 \leq i_1, \dots, i_m \leq N} \left[ \frac{1}{N} \sum_{j=1}^N T_{W_{i_1}, \dots, W_{i_m}}(Z_j) \right]^2. \quad (18)$$

We recall that this last method only applies for first-order sensitivity indices and real-valued input variables.

### 2.3 A sketch of answer to Questions 1 to 3

In the sequel, we discuss how pertinent choices of the metric, of the class of test functions  $T_a$  and of the probability measure  $\mathbb{Q}$  can provide answers to Questions 1 to 3 raised at the beginning of Section 2. For instance, in order to answer to Question 1, we can consider that  $\mathcal{X} = \mathcal{M}_q(\mathbb{R})$  is the space of probability measures  $\mu$  on  $\mathbb{R}$  having finite  $q$ -moments that we endow with the Wasserstein metric  $W_q$  (see Section 3.1 for some recalls on Wasserstein metrics). We propose two possible approaches to define interesting sensitivity indices in this framework.

- In Section 4.1, we use (2) with  $m = 2$ ,  $a = (\mu_1, \mu_2)$  and  $T_a(Z) = \mathbb{1}_{Z \in B(\mu_1, \mu_2)}$  where  $B(\mu_1, \mu_2)$  is the open ball defined by  $\{\mu \in \mathcal{M}_q(\mathbb{R}), W_q(\mu, \mu_1) < W_q(\mu_1, \mu_2)\}$ .
- In Section 4.2, we use the notion of Fréchet means on Wasserstein spaces (see Section 3.2) and the index defined in (16) with appropriate choices of  $a$ ,  $T_a$ , and  $\mathbb{Q}$ .

The case of stochastic computer codes raised in Question 2 will be addressed as follows. A computer code (to be defined) valued in  $\mathcal{M}_q(\mathbb{R})$  will be seen as an ideal case of stochastic computer codes. Finally, it will be possible to treat Question 3 using the framework of Question 2.

## 3 Wasserstein spaces and random distributions

### 3.1 Definition

For any  $q \geq 1$ , we define the  $q$ -Wasserstein distance between two probability distributions that are  $L^q$ -integrable and characterized by their c.d.f.'s  $F$  and  $G$  on  $\mathbb{R}^p$  by

$$W_q(F, G) = \min_{X \sim F, Y \sim G} \left( \mathbb{E}[\|X - Y\|^q]^{1/q} \right),$$

where  $X \sim F$  and  $Y \sim G$  mean that  $X$  and  $Y$  are random variables with respective c.d.f.'s  $F$  and  $G$ . We define the Wasserstein space  $\mathcal{W}_q(\mathbb{R}^p)$  as the space of all measures defined on  $\mathbb{R}^p$  endowed with the  $q$ -Wasserstein distance  $W_q$  with finite  $q$ -moments. In the sequel, any measure is identified to its c.d.f. or in some cases to its p.d.f. In the unidimensional case ( $p = 1$ ), it is a well known fact that  $W_q(F, G)$  has an explicitly expression given by

$$W_q(F, G) = \left( \int_0^1 |F^-(v) - G^-(v)|^q dv \right)^{1/q} = \mathbb{E}[|F^-(U) - G^-(U)|^q]^{1/q}, \quad (19)$$

where  $F^-$  and  $G^-$  are the generalized inverses of the increasing functions  $F$  and  $G$  and  $U$  is a random variable uniformly distributed on  $[0, 1]$ . Of course,  $F^-(U)$  and  $G^-(U)$  have c.d.f.'s  $F$  and  $G$ . The representation (19) of the  $q$ -Wasserstein distance when  $p = 1$  can be generalized to a wider class of "contrast functions". For more details on Wasserstein spaces, one can refer to [62] and [6] and the references therein.

**Definition 3.1.** We call *contrast function* any application  $c$  from  $\mathbb{R}^2$  to  $\mathbb{R}$  satisfying the "measure property"  $\mathcal{P}$  defined by

$$\mathcal{P} : \forall x \leq x' \text{ and } \forall y \leq y', c(x', y') - c(x', y) - c(x, y') + c(x, y) \leq 0,$$

meaning that  $c$  defines a negative measure on  $\mathbb{R}^2$ .

For instance,  $c(x, y) = -xy$  satisfies  $\mathcal{P}$ . If  $c$  satisfies  $\mathcal{P}$ , any function of the form  $a(x) + b(y) + c(x, y)$  also satisfies  $\mathcal{P}$ . If  $C$  is a convex real function,  $c(x, y) = C(x - y)$  satisfies  $\mathcal{P}$ . In particular,  $c(x, y) = (x - y)^2 = x^2 + y^2 - 2xy$  satisfies  $\mathcal{P}$  and actually so does  $c(x, y) = |x - y|^q$  as soon as  $q \geq 1$ .

**Definition 3.2.** We define the *Skorokhod space*  $\mathcal{D} := \mathcal{D}([0, 1])$  of all distribution functions as the space of all non-decreasing functions from  $\mathbb{R}$  to  $[0, 1]$  that are right-continuous with left-hand limits with limit 0 (resp. 1) in  $-\infty$  (resp.  $+\infty$ ) equipped with the supremum norm.

**Definition 3.3.** For any  $F \in \mathcal{D}$ , any  $G \in \mathcal{D}$ , and any positive contrast function  $c$ , we define the *c-Wasserstein cost* by

$$W_c(F, G) = \min_{X \sim F, Y \sim G} \mathbb{E}[c(X, Y)] < +\infty.$$

Obviously,  $W_q^q = W_c$  with  $c(x, y) = |x - y|^q$ . The following theorem has been established by Cambanis, Simon, and Stout in [12].

**Theorem 3.4.** *Let  $c$  be a contrast function. Then*

$$W_c(F, G) = \int_0^1 c(F^-(v), G^-(v)) dv = \mathbb{E}[c(F^-(U), G^-(U))],$$

where  $U$  is a random variable uniformly distributed on  $[0, 1]$ .

### 3.2 Extension of the Fréchet mean to contrast functions

In this section, we recall the classical definition of the notion of the Fréchet mean which is a natural extension of the classical mean for general metric spaces and then we extend this definition to the notion of a Fréchet feature.

**Definition 3.5.** We call a *loss function* any positive and measurable function  $l$ . Then, we define a *Fréchet feature*  $\mathcal{E}_l[X]$  of a random variable  $X$  taking values in a measurable space  $\mathcal{M}$  (whenever it exists) as

$$\mathcal{E}_l[X] \in \underset{\theta \in \mathcal{M}}{\operatorname{Argmin}} \mathbb{E}[l(X, \theta)]. \quad (20)$$

When  $\mathcal{M}$  is a metric space endowed with a distance  $d$ , the Fréchet feature with  $l = d^2$  corresponds to the classical Fréchet mean (see [22]). In particular,  $\mathcal{E}_{d^2}[X]$  minimizes  $\mathbb{E}[d^2(X, \theta)]$  which is an extension of the definition of the classical mean in  $\mathbb{R}^p$  which minimizes  $\mathbb{E}[\|X - \theta\|^2]$ .

Now we consider  $\mathcal{M} = \mathcal{D}$  and  $l = W_c$ . Further, (20) becomes

$$\mathcal{E}_{W_c}[\mathbb{F}] \in \underset{G \in \mathcal{D}}{\operatorname{Argmin}} \mathbb{E}[W_c(\mathbb{F}, G)].$$

where  $\mathbb{F}$  is a measurable function from a measurable space  $\Omega$  to  $\mathcal{D}$ .

In the next theorem, we propose a very general non-parametric framework for which we have existence and uniqueness of the Fréchet means.

**Theorem 3.6.** *Let  $c$  be a positive contrast function. Assume that the application defined by  $(\omega, v) \in \Omega \times (0, 1) \mapsto \mathbb{F}^-(\omega, v) \in \mathbb{R}$  is measurable. In addition, assume that  $\mathcal{E}_c[\mathbb{F}]$  exists and is unique. Then there exists a unique Fréchet mean of  $\mathbb{E}[c(\mathbb{F}^-(v), s)]$  denoted by  $\mathcal{E}_c[\mathbb{F}^-](v)$  and we have*

$$(\mathcal{E}_c[\mathbb{F}])^-(v) = \mathcal{E}_c[\mathbb{F}^-](v) = \underset{s \in \mathbb{R}}{\operatorname{Argmin}} \mathbb{E}[c(\mathbb{F}^-(v), s)].$$

*Proof of Theorem 3.6.* Since  $c$  satisfies  $\mathcal{P}$ , we have

$$\mathbb{E}[W_c(\mathbb{F}, G)] = \mathbb{E} \left[ \int_0^1 c(\mathbb{F}^-(v), G^-(v)) dv \right] = \int_0^1 \mathbb{E}[c(\mathbb{F}^-(v), G^-(v))] dv,$$

by Fubini's theorem. Now, for all  $v \in (0, 1)$ , the quantity  $\mathbb{E}[c(\mathbb{F}^-(v), G^-(v))]$  is minimum for  $G^-(v) = \mathcal{E}_c[\mathbb{F}^-](v)$ .

$$\int_0^1 \mathbb{E}[c(\mathbb{F}^-(v), \mathcal{E}_c[\mathbb{F}^-](v))] dv \leq \int_0^1 \mathbb{E}[c(\mathbb{F}^-(v), G^-(v))] dv$$

and, in particular, for  $G^- = \mathcal{E}_c[\mathbb{F}]^-$ , one gets

$$\int_0^1 \mathbb{E}[c(\mathbb{F}^-(v), \mathcal{E}_c[\mathbb{F}^-](v))]dv \leq \int_0^1 \mathbb{E}[c(\mathbb{F}^-(v), \mathcal{E}_c[\mathbb{F}]^-(v))]dv.$$

Conversely, by the definition of  $\mathcal{E}_c[\mathbb{F}]^-$ , we have for all  $G$ ,

$$\int_0^1 \mathbb{E}[c(\mathbb{F}^-(v), \mathcal{E}_c[\mathbb{F}]^-(v))]dv \leq \int_0^1 \mathbb{E}[c(\mathbb{F}^-(v), G^-(v))]dv$$

and, in particular, for  $G^- = \mathcal{E}_c[\mathbb{F}^-]$ , one gets

$$\int_0^1 \mathbb{E}[c(\mathbb{F}^-(v), \mathcal{E}_c[\mathbb{F}]^-(v))]dv \leq \int_0^1 \mathbb{E}[c(\mathbb{F}^-(v), \mathcal{E}_c[\mathbb{F}^-](v))]dv.$$

278 The theorem then follows by the uniqueness of the minimizer.  $\square$

279 In the previous theorem, we propose a very general non-parametric framework for the random element  
 280  $\mathbb{F}$  together with some assumptions on existence and uniqueness of the Fréchet feature and measurability  
 281 of the map  $(\omega, v) \mapsto \mathbb{F}^-(\omega, v)$ . Nevertheless, it is possible to construct explicit parametric models for  $\mathbb{F}$   
 282 for which these assumptions are satisfied. For instance, the authors of [5] ensure measurability for some  
 283 parametric models on  $\mathbb{F}$  using results of [19]. Notice that, in [20], a new sensitivity index is defined for  
 284 each feature associated to a contrast function. In Section 4.2, we will restrict our analysis to Fréchet  
 285 means and hence to Sobol indices.

### 286 3.3 Examples

287 The Fréchet mean in the  $\mathcal{W}_2(\mathbb{R})$ -space is the inverse function  $v \mapsto \mathbb{E}[\mathbb{F}^-(v)]$ . Another example is the  
 288 Fréchet median. Since the median in  $\mathbb{R}$  is related to the  $L^1$ -cost, the Fréchet  $\mathcal{W}_1(\mathbb{R})$ -median of a random  
 289 c.d.f. is

$$\text{Med}(\mathbb{F})^-(v) \in \text{Med}(\mathbb{F}^-(v)).$$

290 More generally, we recall that, for  $\alpha \in (0, 1)$ , the  $\alpha$ -quantile in  $\mathbb{R}$  is the Fréchet feature associated to  
 291 the contrast function  $c_\alpha(x, y) = (1 - \alpha)(y - x)\mathbb{1}_{x-y < 0} + \alpha(x - y)\mathbb{1}_{x-y \geq 0}$ , also called the *pinball function*.  
 292 Then we can define an  $\alpha$ -quantile  $q_\alpha(\mathbb{F})$  of a random c.d.f. as

$$q_\alpha(\mathbb{F})^-(v) \in q_\alpha(\mathbb{F}^-(v)),$$

293 where  $q_\alpha(X)$  is the set of the  $\alpha$ -quantiles of a random variable  $X$  taking values in  $\mathbb{R}$ . Naturally, taking  
 294  $\alpha = 1/2$  leads to the median.

295 Let us illustrate the previous definitions on an example. Let  $X$  be a random variable with c.d.f.  $F_0$   
 296 which is assumed to be increasing and continuous (hence  $\mathbb{F}^- = \mathbb{F}^{-1}$ ). Let also  $m$  and  $\sigma$  be two real  
 297 random variables such that  $\sigma > 0$ . Then we consider the random c.d.f.  $\mathbb{F}$  of  $\sigma X + m$

$$\mathbb{F}(x) = F_0\left(\frac{x - m}{\sigma}\right) \quad \text{and} \quad \mathbb{F}^{-1}(v) = \sigma F_0^{-1}(v) + m.$$

298 Naturally, the Fréchet mean of  $\mathbb{F}$  is  $\mathcal{E}[\mathbb{F}](x) = F_0((x - \mathbb{E}[m])/\mathbb{E}[\sigma])$  and its  $\alpha$ -quantile is given by

$$q_\alpha(\mathbb{F})^{-1}(v) = q_\alpha(\sigma F_0^{-1}(v) + m).$$

## 299 4 Sensitivity analysis in general Wasserstein spaces

300 In this section, we particularize the indices defined in Section 2.2 in the specific context of general  
 301 Wasserstein spaces. Moreover, we exploit the framework of Section 3 to define a new index based on  
 302 Fréchet means in such general Wasserstein spaces.

303 More precisely, we consider here that our computer code is  $\mathcal{W}_q(\mathbb{R})$ -valued; namely, the output of an  
 304 experiment is the c.d.f. or the p.d.f. of a measure  $\mu \in \mathcal{W}_q(\mathbb{R})$ . For instance, in [10], [40] and [46], the

authors deal with p.d.f.-valued computer codes (and stochastic computer codes). In other words, they define the following application

$$\begin{aligned} f : E &\rightarrow \mathcal{F} \\ x &\mapsto f_x \end{aligned} \quad (21)$$

where  $\mathcal{F}$  is the set of p.d.f.'s

$$\mathcal{F} = \left\{ g \in L^1(\mathbb{R}); g \geq 0, \int_{\mathbb{R}} g(t)dt = 1 \right\}.$$

Here, we choose to identify any element of  $\mathcal{W}_q(\mathbb{R})$  with its c.d.f. In this framework, the output of the computer code is then a c.d.f. denoted by

$$\mathbb{F} = f(X_1, \dots, X_p). \quad (22)$$

Moreover,  $\mathbb{P}$  denotes the law of the c.d.f.  $\mathbb{F}$  and we set  $q = 2$ . The case of a general value of  $q$  can be handled analogously.

#### 4.1 Sensitivity analysis using Equation (2) and Wasserstein balls

Consider  $F$ ,  $F_1$ , and  $F_2$  three elements of  $\mathcal{W}_2(\mathbb{R})$  and, for  $a = (F_1, F_2)$ , the family of test functions

$$T_a(F) = T_{(F_1, F_2)}(F) = \mathbb{1}_{W_2(F_1, F) \leq W_2(F_1, F_2)}. \quad (23)$$

Then, for all  $\mathbf{u} \subset \{1, \dots, p\}$ , the already known index  $S_{2, \text{GMS}}^{\mathbf{u}}$  of (2) becomes

$$\begin{aligned} S_{2, W_2}^{\mathbf{u}} &= S_{2, \text{Univ}}^{\mathbf{u}}((F_1, F_2, F) \mapsto T_{F_1, F_2}(F), \mathbb{P}^{\otimes 2}) \\ &= \frac{\int_{\mathcal{W}_2(\mathbb{R}) \times \mathcal{W}_2(\mathbb{R})} \mathbb{E} \left[ \left( \mathbb{E}[\mathbb{1}_{W_2(F_1, \mathbb{F}) \leq W_2(F_1, F_2)}] - \mathbb{E}[\mathbb{1}_{W_2(F_1, \mathbb{F}) \leq W_2(F_1, F_2)} | X_{\mathbf{u}}] \right)^2 \right] d\mathbb{P}^{\otimes 2}(F_1, F_2)}{\int_{\mathcal{W}_2(\mathbb{R}) \times \mathcal{W}_2(\mathbb{R})} \text{Var}(\mathbb{1}_{W_2(F_1, \mathbb{F}) \leq W_2(F_1, F_2)}) d\mathbb{P}^{\otimes 2}(F_1, F_2)} \\ &= \frac{\int_{\mathcal{W}_2(\mathbb{R}) \times \mathcal{W}_2(\mathbb{R})} \text{Var}(\mathbb{E}[\mathbb{1}_{W_2(F_1, \mathbb{F}) \leq W_2(F_1, F_2)} | X_{\mathbf{u}}]) d\mathbb{P}^{\otimes 2}(F_1, F_2)}{\int_{\mathcal{W}_2(\mathbb{R}) \times \mathcal{W}_2(\mathbb{R})} \text{Var}(\mathbb{1}_{W_2(F_1, \mathbb{F}) \leq W_2(F_1, F_2)}) d\mathbb{P}^{\otimes 2}(F_1, F_2)}. \end{aligned} \quad (24)$$

As explained in Section 2.1,  $S_{2, W_2}^{\mathbf{u}}$  is obtained by integration over  $a$  with respect to  $\mathbb{P}$  of the Hoeffding decomposition of  $T_a(\mathbb{F})$ . Hence, by construction, this index lies in  $[0, 1]$  and shares the two properties previously cited in (3) and (4).

#### 4.2 Sensitivity analysis using Equation (16) and Fréchet means

In the classical framework where the output  $Z$  is real, we recall that the Sobol index with respect to  $X_{\mathbf{u}}$  is defined by

$$S^{\mathbf{u}} = \frac{\text{Var}(\mathbb{E}[Z | X_{\mathbf{u}}])}{\text{Var}(Z)} = \frac{\text{Var}(Z) - \mathbb{E}[\text{Var}(Z | X_{\mathbf{u}})]}{\text{Var}(Z)}, \quad (25)$$

by the property of the conditional expectation. On the one hand, we extend this formula to the framework of this section where the output of interest is the c.d.f.  $\mathbb{F}$  and we define a new index  $S^{\mathbf{u}}(\mathbb{F})$  given by

$$S^{\mathbf{u}}(\mathbb{F}) = \frac{\text{Var}(\mathbb{F}) - \mathbb{E}[\text{Var}(\mathbb{F} | X_{\mathbf{u}})]}{\text{Var}(\mathbb{F})},$$

where  $\text{Var}(\mathbb{F}) = \mathbb{E}[W_2^2(\mathbb{F}, \mathcal{E}_{W_2}(\mathbb{F}))]$  with  $\mathcal{E}_{W_2}(\mathbb{F})$  the Fréchet mean of  $\mathbb{F}$ . From Theorem 3.6, we get

$$\text{Var}(\mathbb{F}) = \mathbb{E} \left[ \int_0^1 |\mathbb{F}^-(v) - \mathcal{E}(\mathbb{F})^-(v)|^2 dv \right] = \mathbb{E} \left[ \int_0^1 |\mathbb{F}^-(v) - \mathbb{E}[\mathbb{F}^-(v)]|^2 dv \right] = \int_0^1 \text{Var}(\mathbb{F}^-(v)) dv$$

leading to

$$S^{\mathbf{u}}(\mathbb{F}) = \frac{\int_0^1 \text{Var}(\mathbb{F}^-(v)) dv - \int_0^1 \mathbb{E}[\text{Var}(\mathbb{F}^-(v) | X_{\mathbf{u}})] dv}{\int_0^1 \text{Var}(\mathbb{F}^-(v)) dv} = \frac{\int_0^1 \text{Var}(\mathbb{E}[\mathbb{F}^-(v) | X_{\mathbf{u}}]) dv}{\int_0^1 \text{Var}(\mathbb{F}^-(v)) dv}. \quad (26)$$

Another point of view is to consider (16), with  $m = 1$ ,

$$T_v(\mathbb{F}) = \mathbb{F}^-(v), \quad (27)$$

and with  $\mathbb{Q}$  the uniform probability measure on  $[0, 1]$ . In that case,

$$\text{Var}(\mathbb{F}) = \mathbb{E} \left[ \int_0^1 |\mathbb{F}^-(v) - \mathcal{E}_{W_2}(\mathbb{F})^-(v)|^2 dv \right] = \int_0^1 \text{Var}(\mathbb{F}^-(v)) dv = \mathbb{E}[W_2^2(\mathbb{F}, \mathcal{E}_{W_2}(\mathbb{F}))].$$

Then

$$S_{2, \text{Univ}}^{\mathbf{u}}(T_v, \mathcal{U}([0, 1])) = \frac{\int_0^1 \mathbb{E} \left[ (\mathcal{E}_{W_2}(\mathbb{F})^-(v) - \mathcal{E}_{W_2}(\mathbb{F}|X_{\mathbf{u}})^-(v))^2 \right] dv}{\int_0^1 \text{Var}(\mathbb{F}^-(v)) dv} = \frac{\mathbb{E} [W_2^2(\mathcal{E}_{W_2}(\mathbb{F}|X_{\mathbf{u}}), \mathcal{E}_{W_2}(\mathbb{F}))]}{\mathbb{E} [W_2^2(\mathbb{F}, \mathcal{E}_{W_2}(\mathbb{F}))]}.$$

is exactly the same as  $S^{\mathbf{u}}(\mathbb{F})$  in (26). Thus, as explained in Section 2.2,  $S^{\mathbf{u}}(\mathbb{F})$  lies in  $[0, 1]$  and has the two properties previously cited in (3) and (4).

Notice that the index defined by (26) is a non-trivial example of the Universal sensitivity index defined in (16).

### 4.3 Estimation procedure

As noticed in the previous section, both

$$S_{2, W_2}^{\mathbf{u}} = S_{2, \text{Univ}}^{\mathbf{u}}(T_a, \mathbb{P}^{\otimes 2})$$

with  $T_a$  defined in (23) and

$$S^{\mathbf{u}}(\mathbb{F}) = S_{2, \text{Univ}}^{\mathbf{u}}(T_v, \mathcal{U}([0, 1]))$$

with  $T_v$  defined in (27), are particular cases of indices of the form (16).

When  $a$  belongs to the same space as the output and when  $\mathbb{Q}$  is equal to  $\mathbb{P}^{\otimes m}$ , we first use the Pick-Freeze estimations of the indices given in (24) and (26). To do so, it is convenient once again to use (6) leading to

$$S_{2, W_2}^{\mathbf{u}} = \frac{\int_{\mathcal{W}_2(\mathbb{R}) \times \mathcal{W}_2(\mathbb{R})} \text{Cov}(\mathbb{1}_{W_2(F_1, \mathbb{F}) \leq W_2(F_1, F_2)}, \mathbb{1}_{W_2(F_1, \mathbb{F}^{\mathbf{u}}) \leq W_2(F_1, F_2)}) d\mathbb{P}^{\otimes 2}(F_1, F_2)}{\int_{\mathcal{W}_2(\mathbb{R}) \times \mathcal{W}_2(\mathbb{R})} \text{Var}(\mathbb{1}_{W_2(F_1, \mathbb{F}) \leq W_2(F_1, F_2)}) d\mathbb{P}^{\otimes 2}(F_1, F_2)} \quad (28)$$

and

$$S^{\mathbf{u}}(\mathbb{F}) = \frac{\int_0^1 \text{Cov}(\mathbb{F}^-(v), \mathbb{F}^{-, \mathbf{u}}(v)) dv}{\int_0^1 \text{Var}(\mathbb{F}^-(v)) dv} \quad (29)$$

where  $\mathbb{F}^{\mathbf{u}}$  and  $\mathbb{F}^{-, \mathbf{u}}$  are respectively the Pick-Freeze versions of  $\mathbb{F}$  and  $\mathbb{F}^-$ . Secondly, one may resort to the estimations based on U-statistics together on the Pick-Freeze design of experiment. Thirdly, it is also possible and easy to obtain rank-based estimations in the vein of (12).

### 4.4 Numerical comparison of both indices

**Example 4.1** (Toy model). Let  $X_1, X_2, X_3$  be three independent and positive random variables. We consider the c.d.f.-valued code  $f$  for which the output is given by

$$\mathbb{F}(t) = \frac{t}{1 + X_1 + X_2 + X_1 X_3} \mathbb{1}_{0 \leq t \leq 1 + X_1 + X_2 + X_1 X_3} + \mathbb{1}_{1 + X_1 + X_2 + X_1 X_3 < t}, \quad (30)$$

so that

$$\mathbb{F}^{-1}(v) = v(1 + X_1 + X_2 + X_1 X_3). \quad (31)$$

In addition, one gets

$$\begin{aligned} \text{Var}(\mathbb{F}^{-1}(v)) &= v^2 (\text{Var}(X_1(1 + X_3)) + \text{Var}(X_2)) \\ &= v^2 (\text{Var}(X_1)\text{Var}(X_3) + \text{Var}(X_1)(1 + \mathbb{E}[X_3])^2 + \text{Var}(X_3)\mathbb{E}[X_1]^2 + \text{Var}(X_2)) \end{aligned}$$

and

$$\begin{aligned}\mathbb{E}[\mathbb{F}^{-1}(v)|X_1] &= v\left(1 + X_1(1 + \mathbb{E}[X_3]) + \mathbb{E}[X_2]\right), \\ \mathbb{E}[\mathbb{F}^{-1}(v)|X_2] &= v\left(1 + \mathbb{E}[X_1](1 + \mathbb{E}[X_3]) + X_2\right), \\ \mathbb{E}[\mathbb{F}^{-1}(v)|X_3] &= v\left(1 + \mathbb{E}[X_1](1 + X_3) + \mathbb{E}[X_2]\right), \\ \mathbb{E}[\mathbb{F}^{-1}(v)|X_1, X_3] &= v\left(1 + X_1(1 + X_3) + \mathbb{E}[X_2]\right),\end{aligned}$$

and finally

$$\begin{aligned}\text{Var}(\mathbb{E}[\mathbb{F}^{-1}(v)|X_1]) &= v^2(1 + \mathbb{E}[X_3])^2 \text{Var}(X_1), \\ \text{Var}(\mathbb{E}[\mathbb{F}^{-1}(v)|X_2]) &= v^2 \text{Var}(X_2), \\ \text{Var}(\mathbb{E}[\mathbb{F}^{-1}(v)|X_3]) &= v^2 \mathbb{E}[X_1]^2 \text{Var}(X_3), \\ \text{Var}(\mathbb{E}[\mathbb{F}^{-1}(v)|X_1, X_3]) &= v^2 (\text{Var}(X_1)\text{Var}(X_3) + \text{Var}(X_1)(1 + \mathbb{E}[X_3])^2 + \text{Var}(X_3)\mathbb{E}[X_1]^2).\end{aligned}$$

338 For  $\mathbf{u} = \{i\} \in \{1, 2, 3\}$  or  $\mathbf{u} = \{1, 3\}$ , it remains to plug the previous formulas in (26) to get the explicit  
339 expressions of the indices  $S^{\mathbf{u}}(\mathbb{F})$ .

340 Now, in order to get a closed formula for the indices defined in (24), we assume  $X_i$  is Bernoulli  
341 distributed with parameter  $0 < p_i < 1$  for  $i = 1, 2$ , and  $3$ . In (24), the distributions  $F_1$  and  $F_2$  can  
342 be either  $\mathcal{U}([0, 1])$ ,  $\mathcal{U}([0, 2])$ ,  $\mathcal{U}([0, 3])$ , or  $\mathcal{U}([0, 4])$  with respective probabilities  $q_1 = (1 - p_1)(1 - p_2)$ ,  
343  $q_2 = (1 - p_1)p_2 + p_1(1 - p_2)(1 - p_3)$ ,  $q_3 = p_1((1 - p_2)p_3 + p_2(1 - p_3))$ , and  $q_4 = p_1p_2p_3$ . In the sequel, we  
344 give, for all sixteen possibilities for the distribution of  $(F_1, F_2)$ , the corresponding contributions for the  
345 numerator and for the denominator of (24).

With probability  $p_{1,1} = (1 - p_1)^2(1 - p_2)^2$ ,  $F_1$  and  $F_2 \sim \mathcal{U}([0, 1])$ . Then  $W_2^2(F_1, F_2) = 0$ ,  $W_2^2(F_1, \mathbb{F}) = \frac{1}{3}(X_1 + X_2 + X_1X_3)^2$ , and  $W_2^2(F_1, \mathbb{F}) \leq W_2^2(F_1, F_2)$  if and only if  $X_1 + X_2 + X_1X_3 = 0$ . Since  $\mathbb{P}(X_1 + X_2 + X_1X_3 = 0) = (1 - p_1)(1 - p_2)$ , the contribution  $d_{1,1}$  to the denominator is thus

$$d_{1,1} = q_{1,1}(1 - q_{1,1}) \quad \text{with } q_{1,1} = (1 - p_1)(1 - p_2).$$

Moreover,

$$\mathbb{E}[\mathbb{1}_{X_1+X_2+X_1X_3=0}|X_1] = \mathbb{P}(X_1 + X_2 + X_1X_3 = 0|X_1) = \mathbb{1}_{X_1=0}\mathbb{P}(X_2 = 0) = (1 - p_2)\mathbb{1}_{X_1=0}.$$

so that, the contribution to the numerator is given by

$$n_{1,1}^1 = \text{Var}(\mathbb{E}[\mathbb{1}_{X_1+X_2+X_1X_3=0}|X_1]) = p_1(1 - p_1)(1 - p_2)^2.$$

346 Similarly, one gets

$$n_{1,1}^2 = \text{Var}(\mathbb{E}[\mathbb{1}_{X_1+X_2+X_1X_3=0}|X_2]) = p_2(1 - p_2)(1 - p_1)^2 \quad \text{and} \quad n_{1,1}^3 = 0.$$

347 Moreover, regarding the indices with respect to  $X_1$  and  $X_3$ ,

$$\mathbb{E}[\mathbb{1}_{X_1+X_2+X_1X_3=0}|X_1, X_3] = \mathbb{P}(X_1 + X_2 + X_1X_3 = 0|X_1, X_3) = \mathbb{1}_{X_1=0}\mathbb{P}(X_2 = 0) = (1 - p_2)\mathbb{1}_{X_1=0}$$

348 and the contribution to the numerator is given by

$$n_{1,1}^{1,3} = \text{Var}(\mathbb{E}[\mathbb{1}_{X_1+X_2+X_1X_3=0}|X_1, X_3]) = p_1(1 - p_1)(1 - p_2)^2.$$

The remaining fifteen cases can be treated similarly and are gathered (with the first case developed above) in the following table. Finally, one may compute the explicit expression of  $S_{2,W_2}^{\mathbf{u}}$

$$S_{2,W_2}^{\mathbf{u}} = \frac{\int_{\mathcal{W}_2(\mathbb{R}) \times \mathcal{W}_2(\mathbb{R})} \text{Cov}(\mathbb{1}_{W_2(F_1, \mathbb{F}) \leq W_2(F_1, F_2)}, \mathbb{1}_{W_2(F_1, \mathbb{F}^{\mathbf{u}}) \leq W_2(F_1, F_2)}) d\mathbb{P}^{\otimes 2}(F_1, F_2)}{\int_{\mathcal{W}_2(\mathbb{R}) \times \mathcal{W}_2(\mathbb{R})} \text{Var}(\mathbb{1}_{W_2(F_1, \mathbb{F}) \leq W_2(F_1, F_2)}) d\mathbb{P}^{\otimes 2}(F_1, F_2)} = \frac{\sum_{k,l} p_{k,l} n_{k,l}^{\mathbf{u}}}{\sum_{k,l} p_{k,l} d_{k,l}}.$$

Some numerical values have not been explicated in the table but given below

$$\text{Case 2} \quad \text{Var}(\mathbb{1}_{X_1=1}(1 - (1 - p_2)\mathbb{1}_{X_3=0})) = p_1(1 - p_1)(1 - (1 - p_2)(1 - p_3))^2 + p_1(1 - p_2)^2 p_3(1 - p_3),$$

$$\text{Case 6} \quad \text{Var}(\mathbb{1}_{X_1=1}(p_2 - (1 - p_2)\mathbb{1}_{X_3=0})) = p_1(1 - p_1)(p_2 - (1 - p_2)(1 - p_3))^2 + p_1(1 - p_2)^2 p_3(1 - p_3),$$

$$\text{Case 11} \quad \text{Var}(\mathbb{1}_{X_1=1}(p_2 + (1 - 2p_2)\mathbb{1}_{X_3=1})) = p_1(1 - p_1)(p_2 + (1 - 2p_2)p_3)^2 + p_1(1 - 2p_2)^2 p_3(1 - p_3),$$

$$\text{Case 15} \quad \text{Var}(\mathbb{1}_{X_1=1}(p_2 + (1 - p_2)\mathbb{1}_{X_3=1})) = p_1(1 - p_1)(p_2 + (1 - p_2)p_3)^2 + p_1(1 - p_2)^2 p_3(1 - p_3).$$

350

**Direct representations of the indices  $S^{\mathbf{u}}(\mathbb{F})$  and  $S_{2,W_2}^{\mathbf{u}}$**  In Figure 1, we have represented the indices  $S^1(\mathbb{F})$ ,  $S^2(\mathbb{F})$ ,  $S^3(\mathbb{F})$ , and  $S^{1,3}(\mathbb{F})$  given by (26) with respect to the values of  $p_1$  and  $p_2$  varying from 0 to 1 for a fixed value of  $p_3$ . We have considered three different values of  $p_3$ :  $p_3 = 0.01$  (first row), 0.5, (second row) and 0.99 (third row). Analogously, the same kind of illustration for the indices  $S_{2,W_2}^1$ ,  $S_{2,W_2}^2$ ,  $S_{2,W_2}^3$ , and  $S_{2,W_2}^{1,3}$  given by (24) is provided in Figure 2. The analysis of Figures 1 and 2 shows that, although the Fréchet indices  $S^{\mathbf{u}}(\mathbb{F})$  differ from the Wasserstein indices  $S_{2,W_2}^{\mathbf{u}}$  as expected, they behave reassuringly similarly.

**Regions of predominance of the indices  $S^{\mathbf{u}}(\mathbb{F})$  and  $S_{2,W_2}^{\mathbf{u}}$**  In addition, the regions of predominance of each index  $S^{\mathbf{u}}(\mathbb{F})$  are plotted in Figure 3. The values of  $p_1$  and  $p_2$  still vary from 0 to 1 and the fixed values of  $p_3$  considered are:  $p_3 = 0.01$  (first row), 0.5, (second row) and 0.99 (third row). Finally, the same kind of illustration for the indices  $S_{2,W_2}^{\mathbf{u}}$  is given in Figure 4. Once again, we observe a global accordance of the predominance regions between the Fréchet indices  $S^{\mathbf{u}}(\mathbb{F})$  and the Wasserstein indices  $S_{2,W_2}^{\mathbf{u}}$ .

**Comparison of the estimation procedures (rank-based and Pick-Freeze)** In order to compare the accuracy of the Pick-Freeze method and the accuracy of the rank-based method at a fixed size, we assume that only 450 calls of the computer code are allowed to estimate the indices  $S^{\mathbf{u}}(\mathbb{F})$  and  $S_{2,W_2}^{\mathbf{u}}$  for  $\mathbf{u} = \{1\}$ ,  $\{2\}$ , and  $\{3\}$ . Hence, the sample size allowed in the rank-based procedure is  $N = 450$ . In the Pick-Freeze methodology, the estimation of the Fréchet indices  $S^{\mathbf{u}}(\mathbb{F})$  requires one initial output sample and three extra output samples to get the Pick-Freeze versions (one for each index) leading to an allowed sample size  $N = \lfloor 450/4 \rfloor = 112$  while it is  $N = \lfloor 450/6 \rfloor = 75$  for the Wasserstein indices  $S_{2,W_2}^{\mathbf{u}}$  ( $1 + 3 = 4$  output samples + two extra samples to handle the integration). We only focus on the first-order indices since, as explained previously, the rank-based procedure has not been developed yet for higher-order indices. We repeat the estimation procedure  $n_r = 200$  times. The boxplots of the mean square errors for the estimation of the Fréchet indices  $S^{\mathbf{u}}(\mathbb{F})$  and the Wasserstein indices  $S_{2,W_2}^{\mathbf{u}}$  have been plotted in Figure 5. We observe that, for a fixed total number of calls 450 to the code  $f$  (corresponding to a rank-based sample size  $N = 450$  and to a Pick-Freeze sample size  $N = 112$  for the Fréchet indices  $S^{\mathbf{u}}(\mathbb{F})$  and  $N = 74$  for the Wasserstein indices  $S_{2,W_2}^{\mathbf{u}}$ ), the rank-based estimation procedure performs much better than the Pick-Freeze method with significantly lower mean errors.

## 5 Sensitivity analysis for stochastic computer codes

This section deals with stochastic computer codes in the sense that two evaluations of the code for the same input lead to different outputs. Before performing a SA in this context, let us briefly describe the state of the art in this setting.

### 5.1 State of the art

A first natural way to handle stochastic computer codes is definitely to consider the expectation of the output code. Indeed, as mentioned in [10], previous works dealing with stochastic simulators together with robust design or optimization and SA consist mainly in approximating the mean and the variance

Case 1	$F_1 \sim \mathcal{U}([0, 1]), F_2 \sim \mathcal{U}([0, 1])$	Case 2	$F_1 \sim \mathcal{U}([0, 1]), F_2 \sim \mathcal{U}([0, 2])$
Prob.	$q_1^2$	Prob.	$q_1 q_2$
Num. 1	$p_1(1-p_1)(1-p_2)^2$	Num. 1	$p_1(1-p_1)(p_2+p_3-p_2 p_3)^2$
Num. 2	$(1-p_1)^2 p_2(1-p_2)$	Num. 2	$p_1^2 p_2(1-p_2)(1-p_3)^2$
Num. 3	0	Num. 3	$p_1^2(1-p_2)^2 p_3(1-p_3)$
Num. 1,3	$p_1(1-p_1)(1-p_2)^2$	Num. 1,3	$\text{Var}(\mathbb{1}_{X_1=1}(1-(1-p_2)\mathbb{1}_{X_3=0}))$
q Den.	$(1-p_1)(1-p_2)$	q Den.	$(1-p_1)+p_1(1-p_2)(1-p_3)$
Case 3	$F_1 \sim \mathcal{U}([0, 1]), F_2 \sim \mathcal{U}([0, 3])$	Case 4	$F_1 \sim \mathcal{U}([0, 1]), F_2 \sim \mathcal{U}([0, 4])$
Prob.	$q_1 q_3$	Prob.	$q_1 q_4$
Num. 1	$p_1(1-p_1)p_2^2 p_3^2$	Num. 1	0
Num. 2	$p_1^2 p_2(1-p_2)p_3^2$	Num. 2	0
Num. 3	$p_1^2 p_2^2 p_3(1-p_3)$	Num. 3	0
Num. 1,3	$p_1 p_2^2 p_3(1-p_1 p_3)$	Num. 1,3	0
q Den.	$1-p_1 p_2 p_3$	q Den.	0
Case 5	$F_1 \sim \mathcal{U}([0, 2]), F_2 \sim \mathcal{U}([0, 1])$	Case 6	$F_1 \sim \mathcal{U}([0, 2]), F_2 \sim \mathcal{U}([0, 2])$
Prob.	$q_1 q_2$	Prob.	$q_2^2$
Num. 1	$p_1(1-p_1)p_2^2 p_3^2$	Num. 1	$p_1(1-p_1)(p_2-(1-p_2)(1-p_3))^2$
Num. 2	$p_1^2 p_2(1-p_2)p_3^2$	Num. 2	$p_2(1-p_2)(p_1(1-p_3)-(1-p_1))^2$
Num. 3	$p_1^2 p_2^2 p_3(1-p_3)$	Num. 3	$p_1^2(1-p_2)^2 p_3(1-p_3)$
Num. 1,3	$p_1 p_2^2 p_3(1-p_1 p_3)$	Num. 1,3	$\text{Var}(\mathbb{1}_{X_1=1}(p_2-(1-p_2)\mathbb{1}_{X_3=0}))$
q Den.	$1-p_1 p_2 p_3$	q Den.	$(1-p_1)p_2+p_1(1-p_2)(1-p_3)$
Case 7	$F_1 \sim \mathcal{U}([0, 2]), F_2 \sim \mathcal{U}([0, 3])$	Case 8	$F_1 \sim \mathcal{U}([0, 2]), F_2 \sim \mathcal{U}([0, 4])$
Prob.	$q_2 q_3$	Prob.	$q_2 q_4$
Num. 1	$p_1(1-p_1)p_2^2 p_3^2$	Num. 1	0
Num. 2	$p_1^2 p_2(1-p_2)p_3^2$	Num. 2	0
Num. 3	$p_1^2 p_2^2 p_3(1-p_3)$	Num. 3	0
Num. 1,3	$p_1 p_2^2 p_3(1-p_1 p_3)$	Num. 1,3	0
q Den.	$1-p_1 p_2 p_3$	q Den.	0
Case 9	$F_1 \sim \mathcal{U}([0, 3]), F_2 \sim \mathcal{U}([0, 1])$	Case 10	$F_1 \sim \mathcal{U}([0, 3]), F_2 \sim \mathcal{U}([0, 2])$
Prob.	$q_1 q_3$	Prob.	$q_2 q_3$
Num. 1	0	Num. 1	$p_1(1-p_1)(1-p_2)^2$
Num. 2	0	Num. 2	$(1-p_1)^2 p_2(1-p_2)$
Num. 3	0	Num. 3	0
Num. 1,3	0	Num. 1,3	$p_1(1-p_1)(1-p_2)^2$
q Den.	0	q Den.	$(1-p_1)p_2+p_1$
Case 11	$F_1 \sim \mathcal{U}([0, 3]), F_2 \sim \mathcal{U}([0, 3])$	Case 12	$F_1 \sim \mathcal{U}([0, 3]), F_2 \sim \mathcal{U}([0, 4])$
Prob.	$q_3^2$	Prob.	$q_3 q_4$
Num. 1	$p_1(1-p_1)(p_2(1-p_3)+(1-p_2)p_3)^2$	Num. 1	$p_1(1-p_1)(1-p_2)^2$
Num. 2	$p_1^2 p_2(1-p_2)(2p_3-1)^2$	Num. 2	$(1-p_1)^2 p_2(1-p_2)$
Num. 3	$p_1^2(2p_2-1)^2 p_3(1-p_3)$	Num. 3	0
Num. 1,3	$\text{Var}(\mathbb{1}_{X_1=1}(p_2+(1-2p_2)\mathbb{1}_{X_3=1}))$	Num. 1,3	$p_1(1-p_1)(1-p_2)^2$
q Den.	$p_1(p_2(1-p_3)+(1-p_2)p_3)$	q Den.	$(1-p_1)p_2+p_1$
Case 13	$F_1 \sim \mathcal{U}([0, 4]), F_2 \sim \mathcal{U}([0, 1])$	Case 14	$F_1 \sim \mathcal{U}([0, 4]), F_2 \sim \mathcal{U}([0, 2])$
Prob.	$q_1 q_4$	Prob.	$q_2 q_4$
Num. 1	0	Num. 1	$p_1(1-p_1)(1-p_2)^2$
Num. 2	0	Num. 2	$(1-p_1)^2 p_2(1-p_2)$
Num. 3	0	Num. 3	0
Num. 1,3	0	Num. 1,3	$p_1(1-p_1)(1-p_2)^2$
q Den.	0	q Den.	$(1-p_1)p_2+p_1$
Case 15	$F_1 \sim \mathcal{U}([0, 4]), F_2 \sim \mathcal{U}([0, 3])$	Case 16	$F_1 \sim \mathcal{U}([0, 4]), F_2 \sim \mathcal{U}([0, 4])$
Prob.	$q_3 q_4$	Prob.	$q_4^2$
Num. 1	$p_1(1-p_1)(p_2+(1-p_2)p_3)^2$	Num. 1	$p_1(1-p_1)p_2^2 p_3^2$
Num. 2	$p_1^2 p_2(1-p_2)(1-p_3)^2$	Num. 2	$p_1^2 p_2(1-p_2)p_3^2$
Num. 3	$p_1^2(1-p_2)^2 p_3(1-p_3)$	Num. 3	$p_1^2 p_2^2 p_3(1-p_3)$
Num. 1,3	$\text{Var}(\mathbb{1}_{X_1=1}(p_2+(1-p_2)\mathbb{1}_{X_3=1}))$	Num. 1,3	$p_1 p_2^2 p_3(1-p_1 p_3)$
q Den.	$p_1(p_2+(1-p_2)p_3)$	q Den.	$p_1 p_2 p_3$



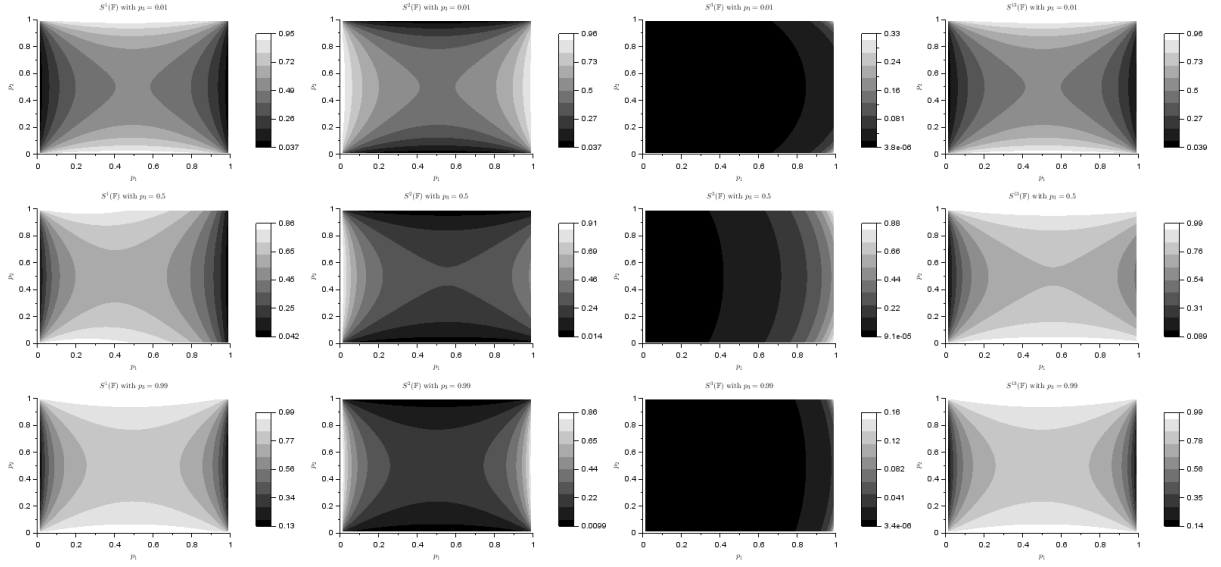


Figure 1: Model (30). Values of the indices  $S^1(\mathbb{F})$ ,  $S^2(\mathbb{F})$ ,  $S^3(\mathbb{F})$ , and  $S^{1,3}(\mathbb{F})$  given by (26) (from left to right) with respect to the values of  $p_1$  and  $p_2$  (varying from 0 to 1). In the first row (resp. second and third),  $p_3$  is fixed to  $p_3 = 0.01$  (resp. 0.5 and 0.99).

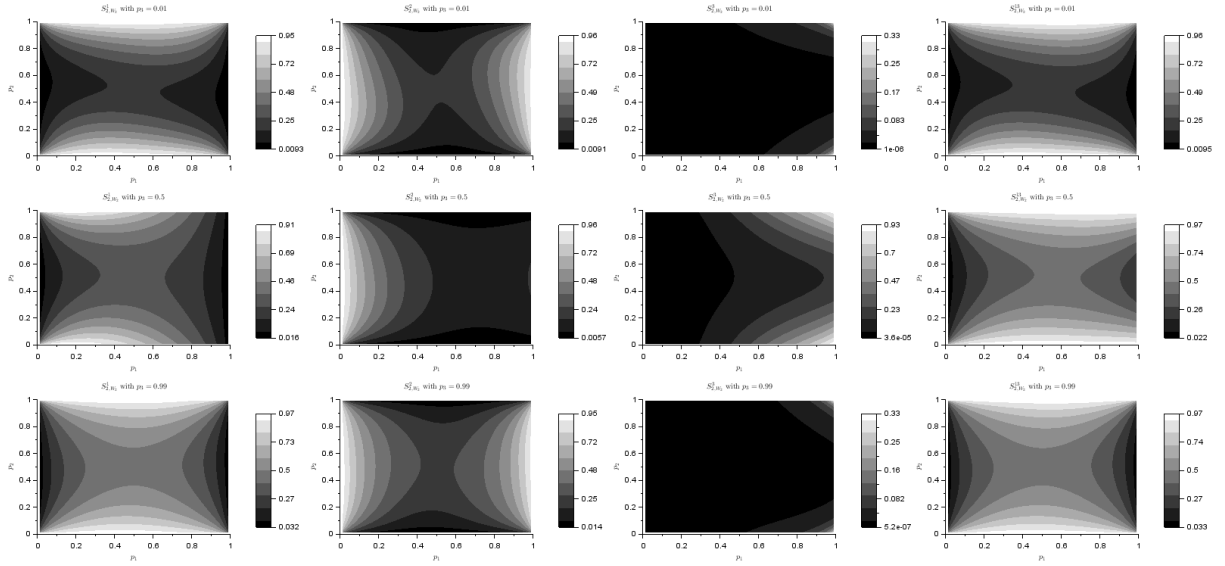


Figure 2: Model (30). Values of the indices  $S_{2,W_2}^1$ ,  $S_{2,W_2}^2$ ,  $S_{2,W_2}^3$ , and  $S_{2,W_2}^{1,3}$  given by (24) (from left to right) with respect to the values of  $p_1$  and  $p_2$  (varying from 0 to 1). In the first row (resp. second and third),  $p_3$  is fixed to  $p_3 = 0.01$  (resp. 0.5 and 0.99).

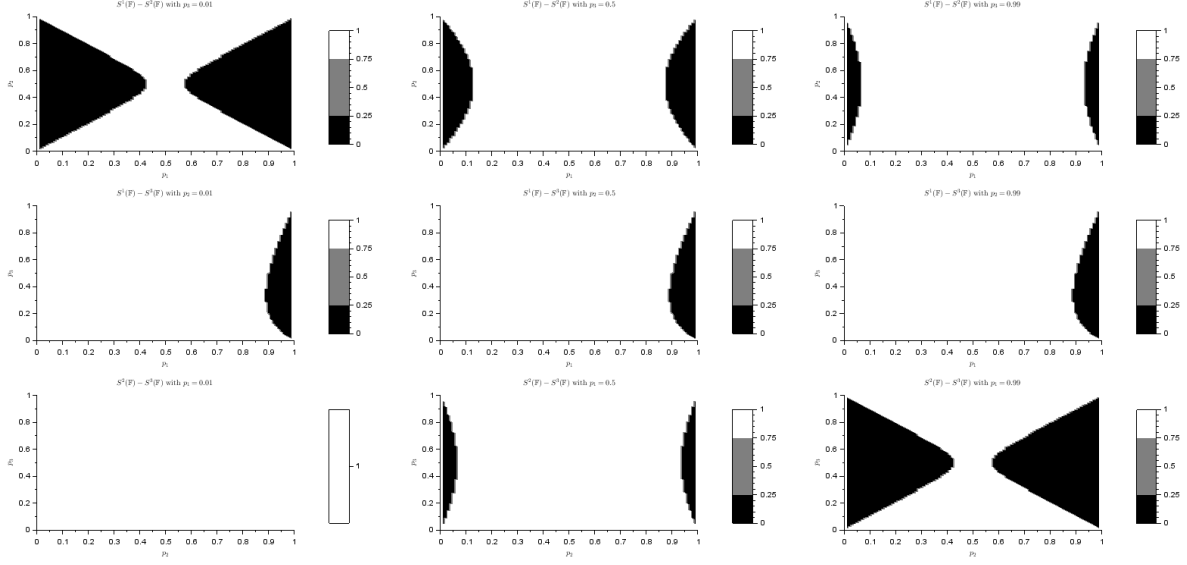


Figure 3: Model (30). In the first row of the figure, regions where  $S^1(\mathbb{F}) \geq S^2(\mathbb{F})$  (black),  $S^1(\mathbb{F}) \leq S^2(\mathbb{F})$  (white), and  $S^1(\mathbb{F}) = S^2(\mathbb{F})$  (gray) with respect to  $p_1$  and  $p_2$  varying from 0 to 1 and, from left to right,  $p_3 = 0.01, 0.5$ , and  $0.99$ . Analogously, the second (resp. last) row considers the regions with  $S^1(\mathbb{F})$  and  $S^3(\mathbb{F})$  (resp.  $S^2(\mathbb{F})$  and  $S^3(\mathbb{F})$ ) with respect to  $p_1$  and  $p_3$  (resp.  $p_2$  and  $p_3$ ) varying from 0 to 1 and, from left to right,  $p_2 = 0.01, 0.5$ , and  $0.99$  (resp.  $p_1 = 0.01, 0.5$ , and  $0.99$ ).

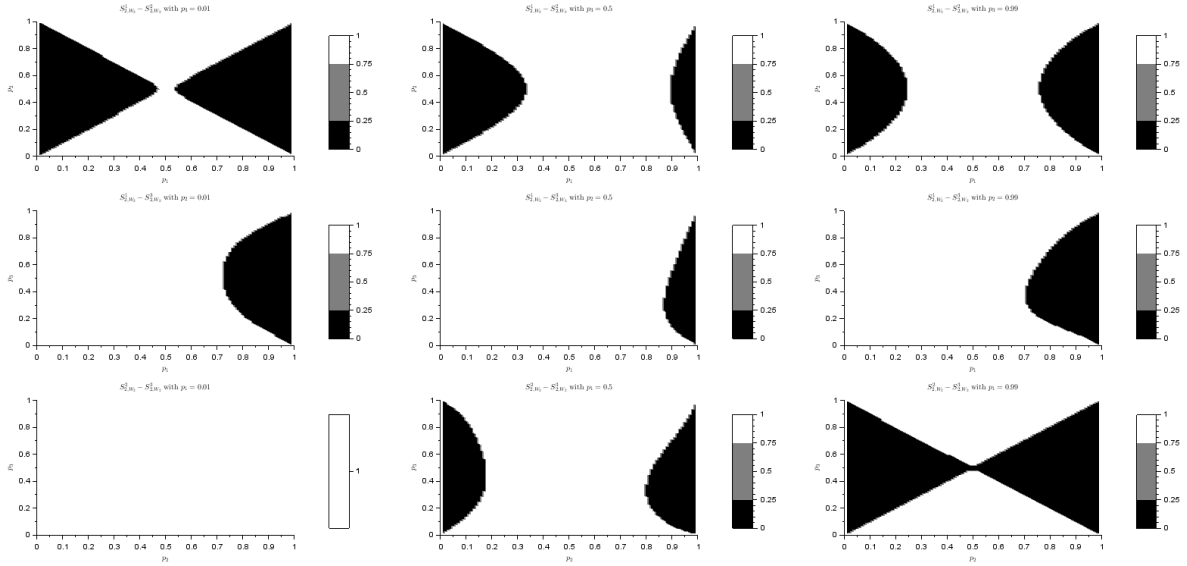


Figure 4: Model (30). In the first row of the figure, regions where  $S^1_{2,W_2} \geq S^2_{2,W_2}$  (black),  $S^1_{2,W_2} \leq S^2_{2,W_2}$  (white), and  $S^1_{2,W_2} = S^2_{2,W_2}$  (gray) with respect to  $p_1$  and  $p_2$  varying from 0 to 1 and, from left to right,  $p_3 = 0.01, 0.5$ , and  $0.99$ . Analogously, the second (resp. last) row considers the regions with  $S^1_{2,W_2}$  and  $S^3_{2,W_2}$  (resp.  $S^2_{2,W_2}$  and  $S^3_{2,W_2}$ ) with respect to  $p_1$  and  $p_3$  (resp.  $p_2$  and  $p_3$ ) varying from 0 to 1 and, from left to right,  $p_2 = 0.01, 0.5$ , and  $0.99$  (resp.  $p_1 = 0.01, 0.5$ , and  $0.99$ ).

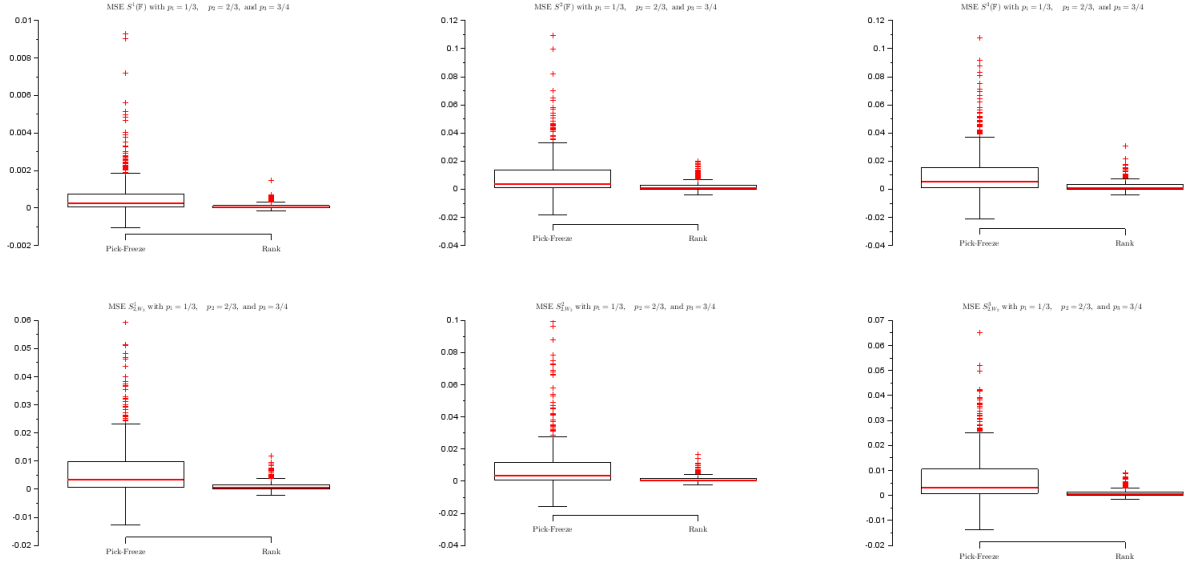


Figure 5: Model (30) with  $p_1 = 1/3$ ,  $p_2 = 2/3$ , and  $p_3 = 3/4$ . Boxplots of the mean square errors of the estimation of the Fréchet indices  $S^{\mathbf{u}}(\mathbb{F})$  (top row) and the Wasserstein indices  $S_{2,W_2}^{\mathbf{u}}$  (bottom row) with a fixed sample size  $N$  and  $n_r = 200$  replications. The indices with respect to  $\mathbf{u} = \{1\}$ ,  $\{2\}$ , and  $\{3\}$  are displayed from left to right. The results of the Pick-Freeze estimation procedure with  $N = 112$  for the Fréchet indices  $S^{\mathbf{u}}(\mathbb{F})$  and  $N = 75$  for the Wasserstein indices  $S_{2,W_2}^{\mathbf{u}}$  are provided in the left side of each graphic. The results of the rank-based methodology with  $N = 450$  are provided in the right side of each graphic.

of the stochastic output [18, 11, 37, 2] and then performing a GSA on the expectation of the output code [42].

As pointed out by [35], another approach amounts to consider that the stochastic code is of the form  $f(X, D)$  where the random element  $X$  contains the classical input variables and the variable  $D$  is an extra unobserved random input. Such an idea was exploited in [36] to compare the estimation of the Sobol indices in an “exact” model to the estimation of the Sobol indices in an associated metamodel. In this framework, the metamodel is considered as a random perturbation of the “exact” model and the perturbation is a function of the inputs and of an extra independent random variable. Analogously, the author of [43] assumes the existence of an extra random variable  $D$  which is not chosen by the practitioner but rather generated at each computation of the output independently of  $X$ . In this setting, the author builds two different indices. The first index is obtained by substituting  $f(X, D)$  for  $f(X)$  in the classical definition of the first-order Sobol index  $S^i = \text{Var}(\mathbb{E}[f(X)|X_i])/\text{Var}(f(X))$ . In this case,  $D$  is considered as another input, even though it is not observable. The second index is obtained by substituting  $\mathbb{E}[f(X, D)|X]$  for  $f(X)$  in the Sobol index. The noise is then smoothed out. Similarly, the authors of [31] traduce the randomness of the computer code using such an extra random variable. In practice, they approximate the statistical properties of the first-order Sobol indices by using a sample of the extra random variable and the associated sample of estimates of the Sobol indices. In [63], the expectation of these random Sobol indices is investigated in the case of stochastic simulator and generalized lambda models. In the same vein, the authors of [3] propose to deal with the differential entropy of the output of a stochastic simulator.

## 5.2 The space $\mathcal{W}_q$ as an ideal version of stochastic computer codes

When dealing with stochastic computer codes, the practitioner is generally interested in the distribution  $\mu_x$  of the output for a given input  $x$ . As previously seen, one can translate this type of codes in terms of a deterministic code by considering an extra input which is not chosen by the practitioner himself but which is a latent variable generated randomly by the computer code and independently of the classical input. As usual in the framework of SA, one considers the input as a random variable. All the random

variables (the one chosen by the practitioner and the one generated by the computer code) are built on the same probability space, leading to the function  $f_s$

$$\begin{aligned} f_s : E \times \mathcal{D} &\rightarrow \mathbb{R} \\ (x, D) &\mapsto f_s(x, D), \end{aligned} \quad (32)$$

where  $D$  is the extra random variable lying in some space  $\mathcal{D}$ . We naturally denote the output random variable  $f_s(x, \cdot)$  by  $f_s(x)$ .

Hence, one may define another (deterministic) computer code associated with  $f_s$  for which the output associated to  $x$  is the probability measure  $\mu_x$

$$\begin{aligned} f : E &\rightarrow \mathcal{W}_q(E) \\ x &\mapsto \mu_x. \end{aligned} \quad (33)$$

The framework of (33) is exactly the one of Section 4.1 and has already been handled. Obviously, in practice, one does not assess the output of the code  $f$  but one can only obtain an empirical approximation of the measure  $\mu_x$  given by  $n$  evaluations of  $f_s$  at  $x$ , namely,

$$\mu_{x,n} = \frac{1}{n} \sum_{k=1}^n \delta_{f_s(x, D_k)}$$

where  $\delta$  is the Dirac function. Further, (33) can be seen as an ideal version of (32). Concretely, for a single random input  $\vec{X} = (X_1, \dots, X_p) \in E = E_1 \times \dots \times E_p$ , we will evaluate  $n$  times the code  $f_s$  defined by (32) (so that the code will generate independently  $n$  hidden variables  $D_1, \dots, D_n$ ) and one may observe

$$f_s(\vec{X}, D_1), \dots, f_s(\vec{X}, D_n)$$

leading to the measure  $\mu_{\vec{X},n} = \sum_{k=1}^n \delta_{f_s(\vec{X}, D_k)} / n$  that approximates the distribution  $\mu_x$  of  $f_s(\vec{X})$ . We emphasize on the fact that the random variables  $D_1, \dots, D_n$  are not observed.

### 5.3 Sensitivity analysis

Let us now present the methodology we adopt in the sequel. In order to study the sensitivity of the distribution  $\mu_x$ , one can use the framework introduced in Section 4.1 and the index  $S_{2,W_q}^u$  given by (24).

In an ideal scenario which corresponds to the framework of (33), one may assess the probability measure  $\mu_x$  for any  $x$ . Then following the estimation procedure of Section 4.3, one gets an estimation of the sensitivity index  $S_{2,W_q}^u$  with good asymptotic properties [27, Theorem 2.4].

In the more realistic framework presented above in (32), we only have access to the approximation  $\mu_{x,n}$  of  $\mu_x$  rendering more complex the estimation procedure and the study of the asymptotic properties. In this case, the general design of experiments is the following

$$\begin{aligned} (\vec{X}_1, D_{1,1}, \dots, D_{1,n}) &\rightarrow f_s(\vec{X}_1, D_{1,1}), \dots, f_s(\vec{X}_1, D_{1,n}), \\ (\vec{X}_1^u, D'_{1,1}, \dots, D'_{1,n}) &\rightarrow f_s(\vec{X}_1^u, D'_{1,1}), \dots, f_s(\vec{X}_1^u, D'_{1,n}), \\ &\vdots \\ (\vec{X}_N, D_{N,1}, \dots, D_{N,n}) &\rightarrow f_s(\vec{X}_N, D_{N,1}), \dots, f_s(\vec{X}_N, D_{N,n}), \\ (\vec{X}_N^u, D'_{N,1}, \dots, D'_{N,n}) &\rightarrow f_s(\vec{X}_N^u, D'_{N,1}), \dots, f_s(\vec{X}_N^u, D'_{N,n}), \end{aligned}$$

where  $\vec{X}_j$  is the  $j$ -th realization of  $\vec{X}$  with  $j = 1, \dots, N$ ,  $\vec{X}_j^u$  is the associated Pick-Freeze version, and  $2 \times N \times n$  is the total number of evaluations of the stochastic computer code (32). Then, we construct the approximations  $\mu_{\vec{X}_j,n}$  of  $\mu_{\vec{X}_j}$  for any  $j = 1, \dots, N$  given by

$$\mu_{\vec{X}_j,n} = \frac{1}{n} \sum_{k=1}^n \delta_{f_s(\vec{X}_j, D_{j,k})}. \quad (34)$$

From there, one may use one of the three estimation procedures presented in Section 2.1.

- First method - Pick-Freeze. It suffices to plug the empirical version  $\mu_n$  of each measure  $\mu$  under concern in (28) to get  $\widehat{S}_{2,W_q,\text{PF},n}^{\mathbf{u}}$ .
- Second method - U-statistics. For  $l = 1, \dots, 4$ , let

$$U_{l,N,n} = \binom{N}{m(l)}^{-1} \sum_{1 \leq i_1 < \dots < i_{m(l)} \leq N} \Phi_l^s(\mu_{i_1,n}, \dots, \mu_{i_{m(l)},n}) \quad (35)$$

where as previously seen  $\Phi^s$  is the symmetrized version of  $\Phi$ . defined in (8) and  $\boldsymbol{\mu} = (\mu, \mu^{\mathbf{u}})$ . Then, we estimate  $S_{2,W_q}^{\mathbf{u}}$  by

$$\widehat{S}_{2,W_q,\text{Ustat},n}^{\mathbf{u}} = \frac{U_{1,N,n} - U_{2,N,n}}{U_{3,N,n} - U_{4,N,n}}. \quad (36)$$

- Third method - Rank-based. The rank-based estimation procedure may also easily be extended to this context by using the empirical version  $\mu_n$  of each measure  $\mu$  under concern instead of the true one  $\mu$ , as explained into more details in the numerical study developed in Section 5.5. This procedure leads to  $\widehat{S}_{2,W_q,\text{Rank},n}^{\mathbf{u}}$ .

Actually, these estimators are easy to compute since, for two discrete measures supported on a same number of points and given by

$$\nu_1 = \frac{1}{n} \sum_{k=1}^n \delta_{x_k}, \quad \nu_2 = \frac{1}{n} \sum_{k=1}^n \delta_{y_k},$$

the Wasserstein distance between  $\nu_1$  and  $\nu_2$  simply writes

$$W_q^q(\nu_1, \nu_2) = \frac{1}{n} \sum_{k=1}^n (x_{(k)} - y_{(k)})^q, \quad (37)$$

where  $z_{(k)}$  is the  $k$ -th order statistics of  $z$ .

## 5.4 Central limit theorem for the estimator based on U-statistics

In this section, we focus on the computationnally less expensive estimator: the one based on U-statistics. For statistical purposes, we establish a central limit theorem for  $\widehat{S}_{2,W_q,\text{Ustat},n}^{\mathbf{u}}$  inspired from [27]. In addition, we consider several examples and study when the conditions of Proposition 5.1 hold.

**Proposition 5.1.** *Consider three i.i.d. copies  $X_1$ ,  $X_2$  and  $X_3$  of a random variable  $X$ . Let  $\delta(N)$  be a sequence tending to 0 as  $N$  goes to infinity and such that*

$$\mathbb{P}(|W_q(\mu_{X_1}, \mu_{X_3}) - W_q(\mu_{X_1}, \mu_{X_2})| \leq \delta(N)) = o\left(\frac{1}{\sqrt{N}}\right).$$

Let  $n$  be such that  $\mathbb{E}[W_q(\mu_X, \mu_{X,n})] = o(\delta(N)/\sqrt{N})$ . Under the assumptions of Theorem 2.4 in [27], we get, for any  $\mathbf{u} \subset \{1, \dots, p\}$ ,

$$\sqrt{N} \left( \widehat{S}_{2,W_q,\text{Ustat},n}^{\mathbf{u}} - S_{2,W_q}^{\mathbf{u}} \right) \xrightarrow[n \rightarrow +\infty]{\mathcal{L}} \mathcal{N}(0, \sigma^2) \quad (38)$$

where the asymptotic variance  $\sigma^2$  is given by (13) in the proof of Theorem 2.4 in [27].

In some particular frameworks, one may derive easily a suitable value of  $\delta(N)$ . Two examples are given in the following.

**Example 5.2.** If the inverse of the random variable  $W = |W_q(\mu_{X_1}, \mu_{X_3}) - W_q(\mu_{X_1}, \mu_{X_2})|$  has a finite expectation, then, by Markov inequality,

$$\mathbb{P}(W \leq \delta(N)) = \mathbb{P}(W^{-1} \geq \delta(N)^{-1}) \leq \frac{1}{\delta(N)} \mathbb{E} \left[ \frac{1}{W} \right]$$

and it suffices to choose  $\delta(N)$  so that  $\delta(N)^{-1} = o(N^{-1/2})$  as  $N$  goes to infinity.

**Example 5.3** (Uniform example). Assume that  $X$  is uniformly distributed on  $[0, 1]$  and that  $\mu_X$  is a Gaussian distribution centered at  $X$  with unit variance. Then the Wasserstein distance  $W_2(\mu_{X_1}, \mu_{X_2})$  rewrites as  $(X_1 - X_2)^2$  so that the random variable  $W = |W_2(\mu_{X_1}, \mu_{X_3}) - W_2(\mu_{X_1}, \mu_{X_2})|$  is given by

$$|(X_1 - X_3)^2 - (X_1 - X_2)^2| = |(X_3 - X_2)(X_2 + X_3 - 2X_1)|.$$

Consequently,

$$\mathbb{P}(W \leq \delta(N)) \leq \mathbb{P}(|X_3 - X_2| \leq \sqrt{\delta(N)}) + \mathbb{P}(|X_2 + X_3 - 2X_1| \leq \sqrt{\delta(N)}).$$

Notice that  $|X_3 - X_2|$  is triangularly distributed with parameter  $a = 0$ ,  $b = 1$ , and  $c = 0$  leading to

$$\mathbb{P}(|X_3 - X_2| \leq \alpha) = \alpha(2 - \alpha), \quad \text{for all } \alpha \in [0, 1].$$

In addition,

$$\begin{aligned} \mathbb{P}(|X_2 + X_3 - 2X_1| \leq \sqrt{\delta(N)}) &\leq \mathbb{P}(|X_2 - X_1| - |X_3 - X_1| \leq \sqrt{\delta(N)}) \\ &= \int_0^1 \mathbb{P}(|X_2 - u| - |X_3 - u| \leq \sqrt{\delta(N)}) du. \end{aligned}$$

Now,  $X_2 - u$  and  $X_3 - u$  are two independent random variables uniformly distributed on  $[-u, -u]$ . Then (see Figure 6), one has

$$\mathbb{P}(|X_2 - u| - |X_3 - u| \leq \alpha) \leq 4\alpha,$$

whence

$$\mathbb{P}(|X_2 + X_3 - 2X_1| \leq \sqrt{\delta(N)}) \leq 4\sqrt{\delta(N)}.$$

Thus it turns out that  $\mathbb{P}(W \leq \delta(N)) = O(\sqrt{\delta(N)})$ . Consequently, a suitable choice for  $\delta(N)$  is  $\delta(N) = o(1/N)$ .

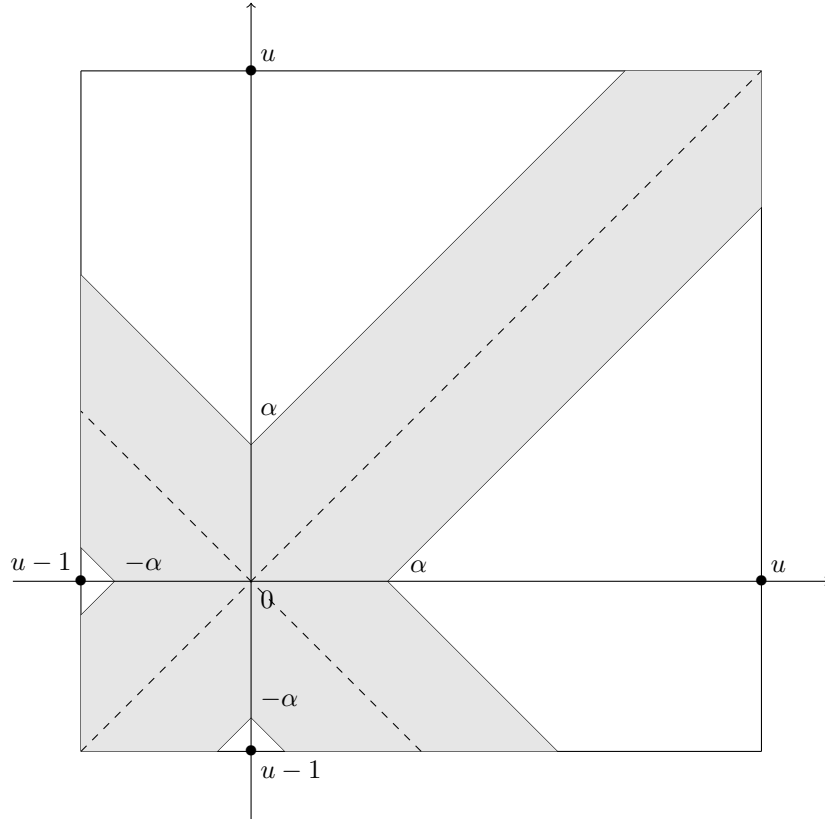


Figure 6: Domain  $\Gamma_{u, \alpha} = \{(x_1, x_2) \in [0, 1]; |x_1 - u| - |x_2 - u| \leq \alpha\}$  (in grey).

Analogously, one may derive suitable choices for  $n$  in some particular cases. For instance, we refer the reader to [6] to get upper bounds on  $\mathbb{E}[W_q(\mu_X, \mu_{X, n})]$  for several values of  $q \geq 1$  and several assumptions on the distribution on  $\mu_X$ : general, uniform, Gaussian, beta, log concave, etc. Here are some results.

473 • In the general framework, the upper bound for  $q \geq 1$  relies on the functional

$$J_q(\mu_X) = \int_{\mathbb{R}} \frac{(F_{\mu_X}(x)(1 - F_{\mu_X}(x)))^{q/2}}{f_{\mu_X}(x)^{q-1}} dx$$

474 where  $F_{\mu_X}$  is the c.d.f. associated to  $\mu_X$  and  $f_{\mu_X}$  its p.d.f. See Cf. [6, Theorems 3.2, 5.1 and 5.3].

475 • Assume that  $\mu_X$  is uniformly distributed on  $[0, 1]$ . Then by [6, Theorems 4.7, 4.8 and 4.9], for any  
476  $n \geq 1$ ,

$$\mathbb{E}[W_2(\mu_X, \mu_{X,n})^2] \leq \frac{1}{6n},$$

477 for any  $q \geq 1$  and for any  $n \geq 1$ ,

$$\mathbb{E}[W_q(\mu_X, \mu_{X,n})^q]^{1/q} \leq (Const) \sqrt{\frac{q}{n}}.$$

478 and for any  $n \geq 1$ ,

$$\mathbb{E}[W_{\infty}(\mu_X, \mu_{X,n})] \leq \frac{(Const)}{n}.$$

479 E.g.  $(Const) = \sqrt{\pi/2}$ .

480 • Assume that  $\mu_X$  is a log-concave distribution with standard deviation  $\sigma$ . Then by [6, Corollaries  
481 6.10 and 6.12], for any  $1 \leq q < 2$  and for any  $n \geq 1$ ,

$$\mathbb{E}[W_q(\mu_X, \mu_{X,n})^q] \leq \frac{(Const)}{2-q} \left( \frac{\sigma}{\sqrt{n}} \right)^q,$$

482 for any  $n \geq 1$ ,

$$\mathbb{E}[W_2(\mu_X, \mu_{X,n})^2] \leq \frac{(Const)\sigma^2 \log n}{n},$$

483 and for any  $q > 2$  and for any  $n \geq 1$ ,

$$\mathbb{E}[W_q(\mu_X, \mu_{X,n})^q] \leq \frac{C_q \sigma^q}{n},$$

484 where  $C_q$  depends on  $q$ , only. Furthermore, if  $\mu_X$  supported on  $[a, b]$ , then for any  $n \geq 1$ ,

$$\mathbb{E}[W_2(\mu_X, \mu_{X,n})^2] \leq \frac{(Const)(b-a)^2}{n+1}.$$

485 E.g.  $(Const) = 4/\ln 2$ . Cf. [6, Corollary 6.11].

486 **Example 5.3 - continued.** We consider that  $X$  is uniformly distributed on  $[0, 1]$  and  $\mu_X$  is a Gaussian  
487 distribution centered at  $X$  with unit variance. Then, by [6, Corollary 6.14], we have, for any  $n \geq 3$ ,

$$\mathbb{E}[W_2(\mu_X, \mu_{X,n})^2] \leq \frac{(Const) \log \log n}{n},$$

488 and for any  $q > 2$  and for any  $n \geq 3$ ,

$$\mathbb{E}[W_q(\mu_X, \mu_{X,n})^q] \leq \frac{C_q}{n(\log n)^{q/2}},$$

489 where  $C_q$  depends only on  $q$ . Since we have already chosen  $\delta(N) = o(N^{-1})$ , it remains to take  $n$  so that  
490  $\log \log n/n = o(N^{-2})$  to fulfill the condition  $\mathbb{E}[W_2(\mu_X, \mu_{X,n})] = o(\delta(N)/\sqrt{N})$ .

## 5.5 Numerical study

**Example 4.1 - continued.** Here, we consider again the code given by (30) and we set  $\vec{X} = (X_1, X_2, X_3)$  and  $p = 3$ . Having in mind the notation of Section 5.2, we consider the ideal code

$$\begin{aligned} f : \quad E &\rightarrow \mathcal{W}_q(E) \\ (X_1, X_2, X_3) &\mapsto \mu_{(X_1, X_2, X_3)} \end{aligned}$$

where  $\mu_{(X_1, X_2, X_3)}$  is the uniform distribution on  $[0, 1 + X_1 + X_2 + X_1 X_3]$  for which the c.d.f. is  $\mathbb{F}$  given by (30) and its stochastic counterpart

$$\begin{aligned} f_s : \quad E \times D &\rightarrow \mathbb{R} \\ (X_1, X_2, X_3, D) &\mapsto f_s(X_1, X_2, X_3, D) \end{aligned} \tag{39}$$

where  $f_s(X_1, X_2, X_3, D)$  is a realization of  $\mu_{(X_1, X_2, X_3)}$ .

Hence, we no longer assume that one may observe  $N$  realizations of  $\mathbb{F}$  associated to the  $N$  initial realizations of  $(X_1, X_2, X_3)$ . Instead, for any of the  $N$  initial realizations of  $(X_1, X_2, X_3)$ , we assess  $n$  realizations of a uniform random variable on  $[0, 1 + X_1 + X_2 + X_1 X_3]$ .

In order to compare the estimation accuracy of the Pick-Freeze method and the rank-based method at a fixed size, we assume once again that only 450 calls of the computer code  $f$  are allowed to estimate the Fréchet indices  $S^{\mathbf{u}}(\mathbb{F})$  and the Wasserstein indices  $S_{2, W_2}^{\mathbf{u}}$  for  $\mathbf{u} = \{1\}$ ,  $\{2\}$ , and  $\{3\}$ . As in Example 4.1 of Section 4.4, the sample size allowed in the rank-based procedure is then  $N = 450$  while, in the Pick-Freeze methodology, it is only  $N = 112$  for the Fréchet indices  $S^{\mathbf{u}}(\mathbb{F})$  and  $N = 75$  for the Wasserstein indices  $S_{2, W_2}^{\mathbf{u}}$ . We only focus on the first-order indices since, as explained previously, the rank-based procedure has not been developed yet for higher-order indices. The empirical c.d.f. based on the empirical measures  $\mu_{X_j, n}$  for  $j = 1, \dots, N$  in (34) are constructed with  $n = 500$  evaluations. We repeat the estimation procedure  $n_r = 200$  times. The boxplots of the mean square errors for the estimation of the Fréchet indices  $S^{\mathbf{u}}(\mathbb{F})$  and the Wasserstein indices  $S_{2, W_2}^{\mathbf{u}}$  have been plotted in Figure 7. We observe that, for a fixed total number of calls 450 to the code  $f$  (corresponding to a rank-based sample size  $N = 450$  and to a Pick-Freeze sample size  $N = 112$  for the Fréchet indices  $S^{\mathbf{u}}(\mathbb{F})$  and  $N = 74$  for the Wasserstein indices  $S_{2, W_2}^{\mathbf{u}}$ ), the rank-based estimation procedure performs much better than the Pick-Freeze method with significantly lower mean errors.

Another numerical study, in the particular setting of stochastic computer codes and inspired by [32], is considered in Section 6.3.

## 6 Sensitivity analysis with respect to the law of the inputs

This section deals with what is called second-level analysis and that corresponds to the SA with respect to the input distributions (rather than the inputs themselves). Before explaining our contributions in this framework, let us briefly describe its state of the art.

### 6.1 State of the art

The paper [44] is devoted to second-level uncertainty which corresponds to the uncertainty on the input distributions and/or on the parameters of the input distributions. As mentioned by the authors, such uncertainties can be handled in two different manners: (1) aggregating them with no distinction [13, 14] or (2) separating them [44]. In [13], the uncertainty concerns the parameters of the input distributions. The authors study the expectation with respect to the distribution of the parameters of the conditional output. In [14], the second-level uncertainties are transformed into first-level uncertainties considering the aggregated vector containing the input random variables vector together with the vector of uncertain parameters. Alternatively, in [44], the uncertainty brought by the lack of knowledge of the input distributions and the uncertainty of the random inputs are treated separately. A double Monte-Carlo algorithm is first considered. In the outer loop, a Monte-Carlo sample of input distribution is generated, while the inner loop proceeds to a GSA associated to each distribution. A more efficient algorithm is also proposed with a unique Monte-Carlo loop. The SA is then performed using the so-called Hilbert-Schmidt dependence measures (HSIC indices) on the input distributions rather than the input random variables themselves. See, e.g., [29] for the definition of the HSIC indices and more details on the algorithms.



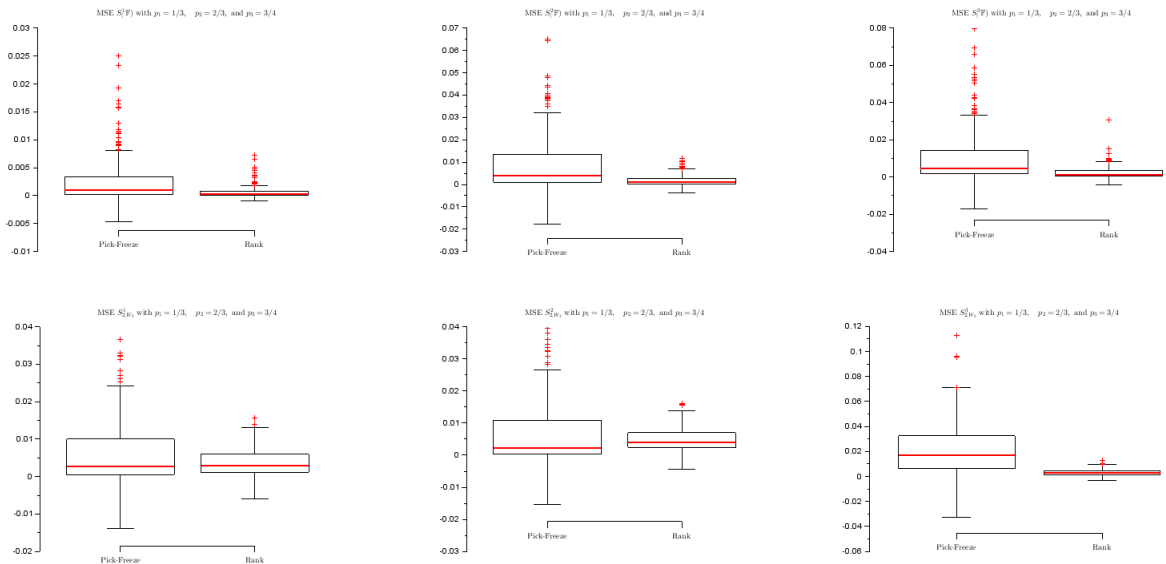


Figure 7: Model (39) with  $p_1 = 1/3$ ,  $p_2 = 2/3$ , and  $p_3 = 3/4$ . Boxplot of the mean square errors of the estimation of the Fréchet indices  $S^u(\mathbb{F})$  (top row) and the Wasserstein indices  $S^u_{2,W_2}$  (bottom row) with a fixed sample size  $N$ , an approximation size  $n$  fixed at  $n = 500$ , and a number  $n_r = 200$  of replications. The indices with respect to  $\mathbf{u} = \{1\}$ ,  $\{2\}$ , and  $\{3\}$  are displayed from left to right. The results of the Pick-Freeze estimation procedure with  $N = 112$  for the Fréchet indices  $S^u(\mathbb{F})$  and  $N = 75$  for the Wasserstein indices  $S^u_{2,W_2}$  are provided in the left side of each graphic. The results of the rank-based methodology with  $N = 450$  are provided in the right side of each graphic.

In [45], a different approach is adopted. A failure probability is studied while the uncertainty concerns the parameters of the input distributions. An algorithm with low computational cost is proposed to handle such uncertainty together with the rare event setting. A single initial sample allows to compute the failure probabilities associated to different parameters of the input distributions. A similar idea is exploited in [41] in which the authors consider input perturbations and Perturbed-Law based Indices that are used to quantify the impact of a perturbation of an input p.d.f. on a failure probability. Analogously, the authors of [30, 32] are interested in (marginal) p.d.f. perturbations and the aim is to study the “robustness of the Sobol indices to distributional uncertainty and to marginal distribution uncertainty” which correspond to second-level uncertainty. For instance, the basic idea of the approach proposed in [30] is to view the total Sobol index as an operator which inputs the p.d.f. and returns the Sobol index. Then the analysis of robustness is done computing and studying the Fréchet derivative of this operator. The same principle is used in [32] to treat the robustness with respect to the marginal distribution uncertainty. Recently, [59] proposes a very clever approach of second-level SA when some moments of the distribution of the inputs are fixed. Its approach characterizes among all compactly supported input distribution with fixed first moments the range of variability of the Sobol indices.

Note that the “ $p$ -box” framework in the sense it is used by [55] presents some similarities with the example provided in Section 3.3 (in the context of random distributions and Fréchet means). It is also worth mentioning the classical approach of epistemic GSA of Dempster-Shafer theory (see, e.g., [56, 1]). This theory describes the random variables together with an epistemic uncertainty traduced in terms of an associated epistemic variable  $Z$  on a set  $A$ , a mass function representing a probability measure on the set  $\mathbb{P}(A)$  of all subsets  $A$ . This lack of knowledge leads to an upper bound and a lower bound of the c.d.f. and can be viewed as second-level uncertainty.

## 6.2 Link with stochastic computer codes

We propose a new procedure that stems from the methodology in the context of stochastic computer codes described in Section 5. We denote by  $\eta_i$  ( $i = 1, \dots, p$ ) the distribution of the input  $X_i$  ( $i = 1, \dots, p$ ) in the model given by (1). There are several ways to model the uncertainty with respect to the choice of

each  $\eta_i$ . Here we adopt the following framework. We assume that each  $\eta_i$  belongs to some family  $\mathcal{P}_i$  of probability measures endowed with the probability measure  $\mathbb{P}_{\eta_i}$ . In general, there might be measurability issues and the question of how to define a  $\sigma$ -field on some general spaces  $\mathcal{P}_i$  can be tricky. We will restrict our study to the simple case where the existence of the probability measure  $\mathbb{P}_{\eta_i}$  on  $\mathcal{P}_i$  is given by the construction of the set  $\mathcal{P}_i$ . More precisely, we proceed as follows.

- First, for  $1 \leq i \leq p$ , let  $d_i$  be an integer and let  $\Theta_i \subset \mathbb{R}^{d_i}$ . Then consider the probability space  $(\Theta_i, \mathcal{B}(\Theta_i), \nu_{\Theta_i})$  where  $\mathcal{B}(\Theta_i)$  is the Borel  $\sigma$ -field and  $\nu_{\Theta_i}$  is a probability measure on  $(\Theta_i, \mathcal{B}(\Theta_i))$ .
- Second, for  $1 \leq i \leq p$ , we consider an identifiable parametric set of probability measure  $\mathcal{P}_i$  on  $E_i$ :  $\mathcal{P}_i := \{\eta_\theta, \theta \in \Theta_i\}$ . Let us denote by  $\pi_i$  the one-to-one mapping from  $\Theta_i$  to  $\mathcal{P}_i$  defined by  $\pi_i(\theta) := \eta_\theta \in \mathcal{P}_i$  and define the  $\sigma$ -field  $\mathcal{F}_i$  on  $\mathcal{P}_i$  by

$$A \in \mathcal{F}_i \iff \exists B \in \mathcal{B}(\Theta_i), A = \pi_i(B).$$

Then we endow this measurable space with the probability  $\Pi_i$  defined, for any  $A \in \mathcal{F}_i$ , by

$$\Pi_i(A) = \nu_{\Theta_i}(\pi_i^{-1}(A)).$$

- Third, in order to perform a second-level SA on (1), we introduce the stochastic mapping  $f_s$  from  $\mathcal{P}_1 \times \dots \times \mathcal{P}_p$  to  $\mathcal{X}$  defined by

$$f_s(\eta_1, \dots, \eta_p) = f(X_1, \dots, X_p) \quad (40)$$

where  $(X_1, \dots, X_p)$  is a random vector distributed as  $\mu_1 \otimes \dots \otimes \mu_p$ . Hence  $f_s$  is a stochastic computer code from  $\mathcal{P}_1 \times \dots \times \mathcal{P}_p$  to  $\mathcal{X}$  and once the probability measures  $\mathbb{P}_{\eta_i}$  on each  $\mathcal{P}_i$  are defined, we can perform SA using the framework of Section 5.

### 6.3 Numerical study

As in [32], let us consider the synthetic example defined on  $[0, 1]^3$  by

$$f(X_1, X_2, X_3) = 2X_2e^{-2X_1} + X_3^2. \quad (41)$$

We are interested in the uncertainty in the support of the random variables  $X_1$ ,  $X_2$ , and  $X_3$ . To do so, we follow the notation and framework of [32]. For  $i = 1, 2$ , and  $3$ , we assume that  $X_i$  is uniformly distributed on the interval  $[A_i, B_i]$ , where  $A_i$  and  $B_i$  are themselves uniformly distributed on  $[0, 0.1]$  and  $[0.9, 1]$  respectively. As remarked in [32], it seems natural that  $f$  will vary more in the  $X_2$ -direction when  $X_1$  is close to 0 and less when  $X_1$  is close to 1.

As mentioned in Section 6.1, the authors of [32] view the total Sobol index as an operator which inputs the p.d.f. and returns the total Sobol index. Then they study the Fréchet derivative of this operator and determine the most influential p.d.f., which depends on a parameter denoted by  $\delta$ . Finally, they make the parameter  $\delta$  vary.

Here, we adopt the methodology explained in the previous section (Section 6.2). Namely, we consider the stochastic computer code given by

$$f_s(\eta_1, \eta_2, \eta_3) = 2X_2e^{-2X_1} + X_3^2, \quad (42)$$

where the  $X_i$ 's are independently drawn according to the uniform measure  $\eta_i$  on  $[A_i, B_i]$  with  $A_i$  and  $B_i$  themselves uniformly distributed on  $[0, 0.1]$  and  $[0.9, 1]$  respectively. Then to estimate the indices  $S_{2, W_2}^u$ , for  $\mathbf{u} = \{1\}$ ,  $\{2\}$ ,  $\{3\}$ ,  $\{1, 2\}$ ,  $\{1, 3\}$ , and  $\{2, 3\}$ , we proceed as follows.

1. For  $i = 1, 2$ , and  $3$ ,
  - (a) we produce a  $N$ -sample  $([A_{i,j}, B_{i,j}])_{j=1, \dots, N}$  of intervals  $[A_i, B_i]$ .
  - (b) for  $j = 1, \dots, N$ ,
    - i. we generate a  $n$ -sample  $(X_{i,j,k})_{k=1, \dots, n}$  of  $X_i$ , where  $X_{i,j,k}$  is uniformly distributed on  $[A_{i,j}, B_{i,j}]$ .

ii. we compute the  $n$ -sample  $(Z_{j,k})_{k=1,\dots,n}$  of the output using

$$Z = f(X_1, X_2, X_3) = 2X_2e^{-2X_1} + X_3^2.$$

Thus we get a  $N$ -sample of the empirical measures of the distribution of the output  $Z$  given by

$$\mu_{Z_j,n} := \frac{1}{n} \sum_{k=1}^n \delta_{Z_{j,k}}, \quad \text{for } j = 1, \dots, N.$$

(c) We order the intervals  $([A_{i,j}, B_{i,j}])_{j=1,\dots,N}$  and we get the Pick-Freeze versions of  $Z$  to treat the SA regarding the input  $\mathbf{u}$ .

2. Finally, it remains to compute the indicators of the empirical version of (28) using (37) and their means to get the Pick-Freeze estimators of  $S_{2,W_2}^{\mathbf{u}}$ .

Notice that we only consider the estimators based on the Pick-Freeze method since we allow for both bounds of the interval to vary and, as explained previously, the rank-based procedure has not been developed yet, neither for higher-order indices nor in higher dimensions.

**Simulations** First, we compute the estimators of  $S_{2,W_2}^{\mathbf{u}}$  following the previous procedure with a sample size  $N = 500$  and an approximation size  $n = 500$ . The results are displayed in Table 1 (first row). We also perform another batch of simulations allowing for higher variability on the bounds: for  $i = 1, 2$ , and 3,  $A_i$  is now uniformly distributed on  $[0, 0.45]$  while  $B_i$  is now uniformly distributed on  $[0.55, 1]$ . The results are displayed in Table 1 (second row).

	$\mathbf{u}$	$\{1\}$	$\{2\}$	$\{3\}$	$\{1, 2\}$	$\{1, 3\}$	$\{2, 3\}$
$A_i \in [0, 0.1]$ $B_i \in [0.9, 1]$	$\hat{S}_{2,W_2}^{\mathbf{u}}$	0.07022	0.08791	0.09236	0.14467	0.21839	0.19066
$A_i \in [0, 0.45]$ $B_i \in [0.55, 1]$	$\hat{S}_{2,W_2}^{\mathbf{u}}$	0.11587	0.06542	0.169529	0.22647	0.40848	0.34913

Table 1: Model (41). GSA on the parameters of the input distributions. Estimations of  $S_{2,W_2}^{\mathbf{u}}$  with a sample size  $N = 500$  and an approximation size  $n = 500$ . In the first row, for  $i = 1, 2$ , and 3,  $A_i$  is uniformly distributed on  $[0, 0.1]$  while  $B_i$  is uniformly distributed on  $[0.9, 1]$ . In the second row, we allow for more variability: for  $i = 1, 2$ , and 3,  $A_i$  is uniformly distributed on  $[0, 0.45]$  while  $B_i$  is uniformly distributed on  $[0.55, 1]$ .

Second, we run another simulation allowing for more variability on the upper bound related to the third input  $X_3$  only:  $B_3$  is uniformly distributed on  $[0.5, 1]$  (instead of  $[0.9, 1]$ ). For  $i = 1$  and 2,  $A_i$  is still uniformly distributed on  $[0, 0.1]$  while  $B_i$  is still uniformly distributed on  $[0.9, 1]$ . The results are displayed in Table 2. We still use a sample size  $N = 500$  and an approximation size  $n = 500$ .

$\mathbf{u}$	$\{1\}$	$\{2\}$	$\{3\}$	$\{1, 2\}$	$\{1, 3\}$	$\{2, 3\}$
$\hat{S}_{2,W_2}^{\mathbf{u}}$	0.01196	0.06069	0.56176	-0.01723	0.63830	0.59434

Table 2: Model (41). GSA on the parameters of the input distributions. Estimations of  $S_{2,W_2}^{\mathbf{u}}$  with a sample size  $N = 500$  and an approximation size  $n = 500$  and more variability on  $B_3$ , now uniformly distributed on  $[0.5, 1]$ . For  $i = 1$  and 2,  $A_i$  is still uniformly distributed on  $[0, 0.1]$  while  $B_i$  is still uniformly distributed on  $[0.9, 1]$ .

Third, the aim is to highlight the fact that performing a classical GSA differs from performing a second-level SA. In that view, we perform a classical GSA on the inputs rather than on the parameters of their distributions (corresponding to a second-level analysis). Namely, we consider the index  $S_{2,\text{CVM}}^{\mathbf{u}}$  and proceed to its estimation with a sample size  $N = 10^4$ . The reader is referred to [26, Section 3] for the definition of this index  $S_{2,\text{CVM}}^{\mathbf{u}}$  and its Pick-Freeze estimator together with their properties. The results are displayed in Table 3.

$\mathbf{u}$	$\{1\}$	$\{2\}$	$\{3\}$	$\{1, 2\}$	$\{1, 3\}$	$\{2, 3\}$
$\hat{S}_{2,\text{CVM}}^{\mathbf{u}}$	0.13717	0.15317	0.33889	0.33405	0.468163	0.53536

Table 3: Model (41). Direct GSA on the inputs. Estimations of  $S_{2,\text{CVM}}^{\mathbf{u}}$  with a sample size  $N = 10^4$ . The reader is referred to [26, Section 3] for the definition of the index  $S_{2,\text{CVM}}^{\mathbf{u}}$  and its Pick-Freeze estimator together with their properties.

**Comments** When one is interested in the choice of the input distributions of  $X_1$ ,  $X_2$ , and  $X_3$ , the first row in Table 1 shows that each choice is equally important. Now, if we give more freedom to the space where the distribution lives, the relative importance may change as one can see in Table 1 (second row) and in Table 2. More precisely, in Table 2, the variability of the third input distribution (namely, the variability of its upper bound) is five times larger than the other variabilities. Not surprisingly, it results that the importance of the choice of the third input distribution is then much more important than the choices of the distributions of the two first inputs.

As said in the previous paragraph, when one is interested in the choice of the input distributions of  $X_1$ ,  $X_2$ , and  $X_3$ , the first row in Table 1 shows that each choice is equally important. Nevertheless, performing a classical GSA on the inputs using the Cramér-von-Mises index for example, we see, in Table 3, that the index related to  $X_3$  is more than twice as important as  $X_1$  and  $X_2$  (when considering only first-order effects). Hence, here, the classical GSA largely differs numerically from a second-level SA as expected.

## 7 Synthesis and practical advices

In this short section, we give a “road map” to help the practitioners. We restrict our study to the case of order-one indices; for higher indices, the road map remains the same except that the rank statistics can not be used to estimate the several indices.

### 7.1 First-level sensitivity analysis for the practitioners

#### 7.1.1 The road map

Here, the input distributions are fixed and we aim at performing SA for a deterministic or a stochastic code. In the sections above, we have presented several indices that depend on the nature of the code/inputs/outputs, on the choice of the family of test functions  $T_a$ , and on the integrating probability measure  $\mathbb{Q}$ . The choice of  $(T_a, \mathbb{Q})$  is still an open question that is beyond the scope of this work. We present in Figure 8 a classification tree giving the practitioners the algorithm to be used in order to estimate the index he is interested in. The several algorithms are described in Section 7.1.2.

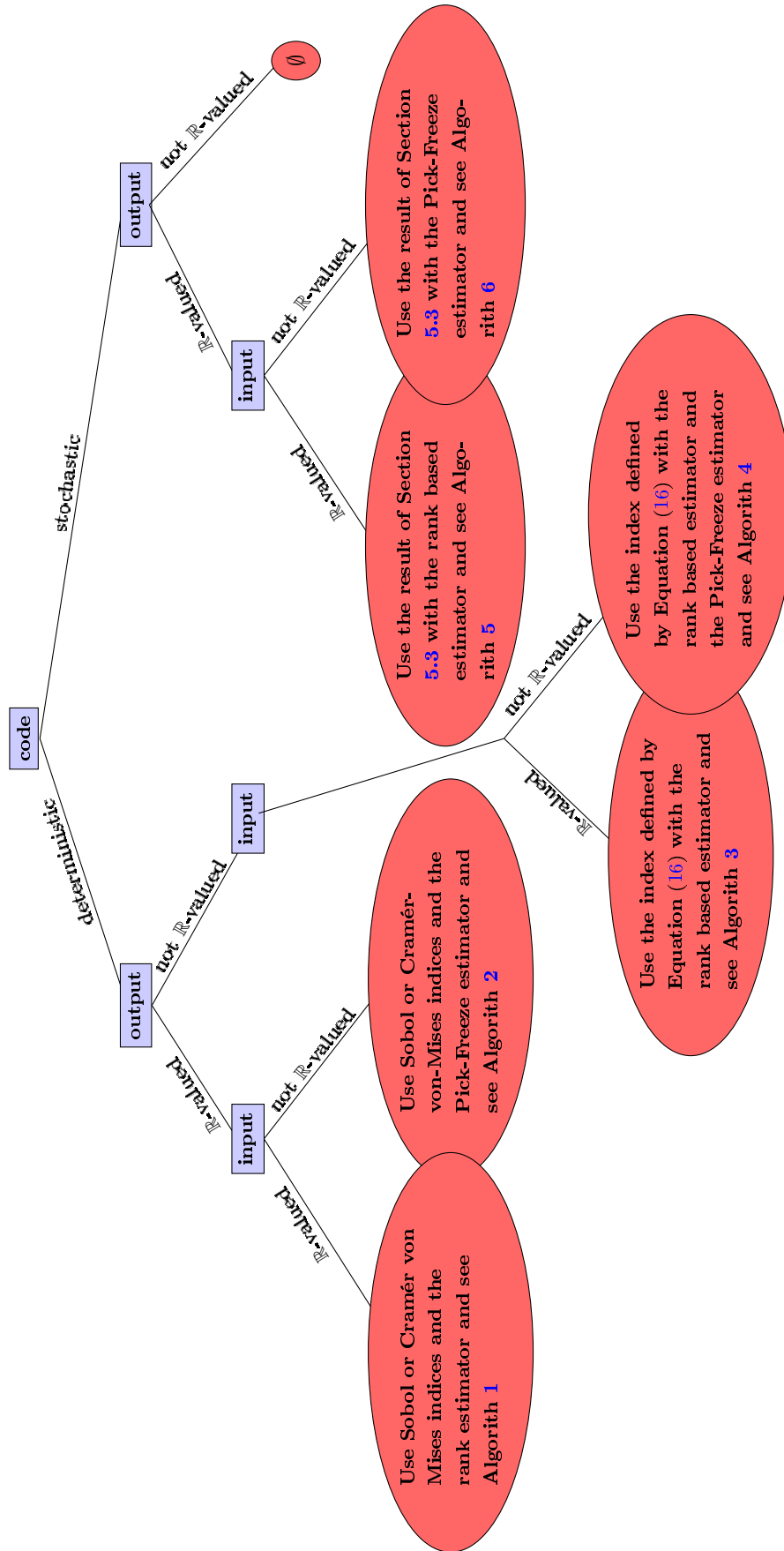


Figure 8: Road map for the practitioners

### 643 7.1.2 Algorithms

644 We assume in the following that our only aim is to estimate the order-one index with respect to  $X_1$  and we present the different simulation algorithms depending on the nature of the computer code.

---

**Algorithm 1** Estimating the order-one Sobol index  $S^1$  for a  $\mathbb{R}$ -valued deterministic code with  $\mathbb{R}$ -valued inputs

---

Enter  $N$  the total number of calls to the computer code  
 Simulate a  $N$ -sample of the inputs  $(X_{1,j}, \dots, X_{p,j})$  for  $j = 1, \dots, N$   
 Compute the  $N$  corresponding outputs  $Z_j = f(X_{1,j}, \dots, X_{p,j})$  for  $j = 1, \dots, N$   
 Rearrange the pairs  $(X_{1,j}, Z_j)$  for  $j = 1, \dots, N$  by increasing order according to the first coordinate  
 Denote by  $(X_{1,(j)}, Z_{(j)})$  for  $j = 1, \dots, N$  the reordered pairs  
**return**  $\hat{S}_{\text{Rank}}^1 = \frac{\frac{1}{N} \sum_{j=1}^{N-1} Z_{(j)} Z_{(j+1)} - \left(\frac{1}{N} \sum_{j=1}^N Z_j\right)^2}{\frac{1}{N} \sum_{j=1}^{N-1} Z_j^2 - \left(\frac{1}{N} \sum_{j=1}^N Z_j\right)^2}$ .

---

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**Algorithm 2** Estimating the order-one Sobol index  $S^1$  for a  $\mathbb{R}$ -valued deterministic code with general inputs (not necessarily  $\mathbb{R}$ -valued)

---

Enter  $N$  the total number of calls to the computer code  
 Simulate a Pick-Freeze  $N^*$ -sample of the inputs  $(X_{1,j}, \dots, X_{p,j})$  for  $j = 1, \dots, N^*$  with  $N^* = \lfloor N/2 \rfloor$   
 Compute the  $N^*$  corresponding outputs  $(Z_j, Z_j^{(1)})$  for  $j = 1, \dots, N^*$   
**return**  $\hat{S}_{\text{PF}}^1 = \frac{\frac{1}{N^*} \sum_{j=1}^{N^*} Z_j Z_j^{(1)} - \left(\frac{1}{N^*} \sum_{j=1}^{N^*} (Z_j + Z_j^{(1)})/2\right)^2}{\frac{1}{2N^*} \sum_{j=1}^{N^*} (Z_j^2 + (Z_j^{(1)})^2) - \left(\frac{1}{2N^*} \sum_{j=1}^{N^*} (Z_j + Z_j^{(1)})\right)^2}$ .

---



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**Algorithm 3** Estimating the order-one universal index  $S_{2,\text{Univ}}^1$  for a metric space-valued deterministic code with  $\mathbb{R}$ -valued inputs

---

Choose a class of functions  $T_a$   
 Choose a probability measure  $\mathbb{Q}$   
 Enter  $N$  the total number of calls to the computer code  
 Simulate a  $N$ -sample of the inputs  $(X_{1,j}, \dots, X_{p,j})$  for  $j = 1, \dots, N$   
 Compute the  $N$  corresponding outputs  $Z_j = f(X_{1,j}, \dots, X_{p,j})$  for  $j = 1, \dots, N$   
 Rearrange the pairs  $(X_{1,j}, Z_j)$  for  $j = 1, \dots, N$  by increasing order according to the first coordinate  
 Denote by  $(X_{1,(j)}, Z_{(j)})$  for  $j = 1, \dots, N$  the reordered pairs  
**if**  $\mathbb{Q} = \mathbb{P}$  **then**  
   Compute  $\hat{N}_{2,\text{GMS},\text{Rank}}^1$  as in (14) and  $\hat{D}_{2,\text{GMS},\text{Rank}}^1$  as in (15)  
   **return**  $\hat{S}_{2,\text{GMS},\text{Rank}}^1 = \frac{\hat{N}_{2,\text{GMS},\text{Rank}}^1}{\hat{D}_{2,\text{GMS},\text{Rank}}^1}$   
**else**  
   Simulate a  $N$ -sample  $(W_1, \dots, W_N)$  of a  $\mathbb{Q}$ -distributed random variable  
   Compute  $\hat{N}_{2,\text{Univ},\text{Rank}}^1$  as in (17) and  $\hat{D}_{2,\text{Univ},\text{Rank}}^1$  as in (18)  
   **return**  $\hat{S}_{2,\text{Univ},\text{Rank}}^1 = \frac{\hat{N}_{2,\text{Univ},\text{Rank}}^1}{\hat{D}_{2,\text{Univ},\text{Rank}}^1}$   
**end if**

---

---

**Algorithm 4** Estimating the order-one universal index  $S_{2,\text{Univ}}^1$  for a metric space-valued deterministic code with general inputs (not necessarily  $\mathbb{R}$ -valued)

---

Choose a class of functions  $T_a$  with  $\dim(a) = m$   
Choose a probability measure  $\mathbb{Q}$   
Enter  $N$  the total number of calls to the computer code  
**if**  $\mathbb{Q} = \mathbb{P}$  **then**  
    Replace the  $N$ -sample of the output in Algorithm 3 by the Pick-Freeze  $N_m$ -sample of Algorithm 2 with  $N_m = \lfloor N/(m+2) \rfloor$   
    Simulate  $m$  new samples of size  $N_m$  of the output  
    Proceed as in Algorithm 3  
    **return**  $\hat{S}_{2,\text{GMS},\text{PF}}^1$   
**else**  
    Replace the  $N$ -sample of the output in Algorithm 3 by the Pick-Freeze  $N^*$ -sample of Algorithm 2 with  $N^* = \lfloor N/2 \rfloor$   
    Proceed as in Algorithm 3  
    **return**  $\hat{S}_{2,\text{Univ},\text{PF}}^1$   
**end if**

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**Algorithm 5** Estimating the order-one universal index  $S_{2,\text{Univ}}^1$  for a  $\mathbb{R}$ -valued stochastic code with  $\mathbb{R}$ -valued inputs

---

Choose the class of functions  $T_a$  as in (23)  
Enter  $N$  the total number of calls to the computer code  
Enter  $n$  the approximation size  
Simulate a  $N_n$ -sample of the inputs  $(X_{1,j}, \dots, X_{p,j})$  for  $j = 1, \dots, N_n$  with  $N_n = \lfloor N/n \rfloor$   
**for**  $j = 1, \dots, N_n$  **do**  
    Compute  $n$  times the random value of  $f(X_{1,j}, \dots, X_{p,j})$  denoted by  $Z_{j,k}$  for  $k = 1, \dots, n$   
**end for**  
Proceed as in Algorithm 3 with output the empirical measure  $\mu_{Z_j,n} = \frac{1}{n} \sum_{k=1}^n \delta_{Z_{j,k}}$   
**return**  $\hat{S}_{2,W_2,\text{Rank},n}^1$

---



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**Algorithm 6** Estimating the order-one universal index  $S_{2,\text{Univ}}^1$  for a  $\mathbb{R}$ -valued stochastic code with general inputs (not necessarily  $\mathbb{R}$ -valued)

---

Choose the class of functions  $T_a$  as in (23) with  $\dim(a) = m$   
Enter  $N$  the total number of calls to the computer code  
Enter  $n$  the approximation size  
Simulate a  $N_{m,n}$ -sample of the inputs  $(X_{1,j}, \dots, X_{p,j})$  for  $j = 1, \dots, N_n$  with  $N_{m,n} = \lfloor N/(n(m+2)) \rfloor$   
**for**  $j = 1, \dots, N_{m,n}$  **do**  
    Compute  $n$  times the random value of  $f(X_{1,j}, \dots, X_{p,j})$  denoted by  $Z_{j,k}$  for  $k = 1, \dots, n$   
**end for**  
Proceed as in Algorithm 4 with output the empirical measure  $\mu_{Z_j,n} = \frac{1}{n} \sum_{k=1}^n \delta_{Z_{j,k}}$   
**return**  $\hat{S}_{2,W_2,\text{PF},n}^1$

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## 7.2 Second-level sensitivity analysis for the practitioners

In this section, we present the algorithms to be used in second-level SA.

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**Algorithm 7** Estimating the order-one universal index  $S_{2,\text{Univ}}^1$  for a  $\mathbb{R}$ -valued deterministic code with  $\mathbb{R}$ -valued inputs

---

```

Choose the class of functions  $T_a$  as in (23)
Enter  $N$  the total number of simulations
Enter  $n$  the approximation size
Simulate a  $N$ -sample of the distribution parameters of the inputs  $(\theta_{1,j}, \dots, \theta_{p,j})$  for  $j = 1, \dots, N$ 
for  $j = 1, \dots, N$  do
    Simulate a  $N$ -sample of the inputs  $(X_{1,j}, \dots, X_{p,j})$ 
    Simulate a  $n$ -sample of inputs distributed following  $(\mu_{\theta_{1,j}}, \dots, \mu_{\theta_{p,j}})$  denoted by  $(X_{1,j,k}, \dots, X_{p,j,k})$ 
    for  $k = 1, \dots, n$ 
        Compute the  $n$  corresponding outputs  $Z_{j,k} = f(X_{1,j,k}, \dots, X_{p,j,k})$  for  $k = 1, \dots, n$ 
    end for
Proceed as in Algorithm 5 with output the empirical measure  $\mu_{Z_j,n} = \frac{1}{n} \sum_{k=1}^n \delta_{Z_{j,k}}$ 
return  $\hat{S}_{2,W_2,\text{PF},n}^1$ 

```

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**Algorithm 8** Estimating the order-one universal index  $S_{2,\text{Univ}}^1$  for a  $\mathbb{R}$ -valued deterministic code with general inputs (not necessarily  $\mathbb{R}$ -valued) for second-level SA

---

```

Choose the class of functions  $T_a$  as in (23)
Enter  $N$  the total number of simulations
Enter  $n$  the approximation size
Simulate a  $N$ -sample of the distribution parameters of the inputs  $(\theta_{1,j}, \dots, \theta_{p,j})$  for  $j = 1, \dots, N$ 
for  $j = 1, \dots, N$  do
    Simulate a  $N$ -sample of the inputs  $(X_{1,j}, \dots, X_{p,j})$ 
    Simulate a  $n$ -sample of inputs distributed following  $(\mu_{\theta_{1,j}}, \dots, \mu_{\theta_{p,j}})$  denoted by  $(X_{1,j,k}, \dots, X_{p,j,k})$ 
    for  $k = 1, \dots, n$ 
        Compute the  $n$  corresponding outputs  $Z_{j,k} = f(X_{1,j,k}, \dots, X_{p,j,k})$  for  $k = 1, \dots, n$ 
    end for
Proceed as in Algorithm 6 with output the empirical measure  $\mu_{Z_j,n} = \frac{1}{n} \sum_{k=1}^n \delta_{Z_{j,k}}$ 
return  $\hat{S}_{2,W_2,\text{PF},n}^1$ 

```

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## 8 Conclusion

In this article, we present a very general way to perform SA when the output  $Z$  of a computer code lives in a metric space. The main idea is to consider real-valued squared integrable test functions  $(T_a(Z))_{a \in \Omega}$  parameterized by a finite number of elements of a probability space. Then Hoeffding decomposition of the test functions  $T_a(Z)$  is computed and integrated with respect to the parameter  $a$ . This very general and flexible definition allows, on the one hand, to recover a lot of classical indices (namely, the Sobol indices and the Cramér-von-Mises indices) and, on the other hand, to perform a well tailored and interpretable SA. Furthermore, a SA is also made possible for computer codes for which the output is a c.d.f. and for stochastic computer codes (that are seen as an approximation of c.d.f.-valued computer codes). Last, it enables also to perform second-level SA by embedding second-level SA as a particular case of stochastic computer codes.

As already seen, a clear limitation comes from the dimensions. On the one hand, the metric based on Wasserstein balls is well-suited in dimension one for its nice theoretical properties and its easy-to-implement estimation. In higher dimension, things become more tricky. On the other hand, the rank-based estimation has not been developed yet in dimension higher than one. A nice perspective is then to tackle the estimation beyond the dimension one.



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## A Proof of Proposition 5.1

**Notation** It is convenient to have short expressions for terms that converge in probability to zero. We follow [61]. The notation  $o_{\mathbb{P}}(1)$  (respectively  $O_{\mathbb{P}}(1)$ ) stands for a sequence of random variables that converges to zero in probability (resp. is bounded in probability) as  $n \rightarrow \infty$ . More generally, for a sequence of random variables  $R_n$ ,

$$\begin{aligned} X_n = o_{\mathbb{P}}(R_n) & \text{ means } X_n = Y_n R_n \text{ with } Y_n \xrightarrow{\mathbb{P}} 0 \\ X_n = O_{\mathbb{P}}(R_n) & \text{ means } X_n = Y_n R_n \text{ with } Y_n = O_{\mathbb{P}}(1). \end{aligned}$$

For deterministic sequences  $X_n$  and  $R_n$ , the stochastic notation reduce to the usual  $o$  and  $O$ . Finally,  $c$  stands for a generic constant that may differ from one line to another.

*Proof of Proposition 5.1.* One has

$$\sqrt{N} \left( \hat{S}_{2,W_q,Ustat,n}^u - S_{2,GMS}^u \right) = \sqrt{N} \left( \hat{S}_{2,W_q,Ustat,n}^u - \hat{S}_{2,GMS,Ustat}^u \right) + \sqrt{N} \left( \hat{S}_{2,GMS,Ustat}^u - S_{2,GMS}^u \right).$$

By [27, Theorem 2.4], the second term in the right-hand side of the previous equation is asymptotically Gaussian. If we prove that the first term in the right-hand side is  $o_{\mathbb{P}}(1)$ , then by Slutsky's Lemma [61, Lemma 2.8],  $\sqrt{N} \left( \hat{S}_{2,GMS,Ustat,n}^u - S_{2,GMS}^u \right)$  is asymptotically Gaussian.

Now we prove that  $\sqrt{N} \left( \hat{S}_{2,GMS,Ustat,n}^u - \hat{S}_{2,GMS,Ustat}^u \right) = o_{\mathbb{P}}(1)$ . We write

$$\begin{aligned} \hat{S}_{2,W_q,Ustat,n}^u - \hat{S}_{2,GMS,Ustat}^u &= \Psi(U_{1,N,n}, U_{2,N,n}, U_{3,N,n}, U_{4,N,n}) - \Psi(U_{1,N}, U_{2,N}, U_{3,N}, U_{4,N}) \\ &= \frac{[(U_{1,N,n} - U_{1,N}) - (U_{2,N,n} - U_{2,N})](U_{3,N} - U_{4,N})}{[(U_{3,N,n} - U_{3,N}) - (U_{4,N,n} - U_{4,N}) + (U_{3,N} - U_{4,N})](U_{3,N} - U_{4,N})} \\ &\quad - \frac{[(U_{3,N,n} - U_{3,N}) - (U_{4,N,n} - U_{4,N})](U_{1,N} - U_{2,N})}{[(U_{3,N,n} - U_{3,N}) - (U_{4,N,n} - U_{4,N}) + (U_{3,N} - U_{4,N})](U_{3,N} - U_{4,N})}. \end{aligned}$$

Since  $(U_{l,N,n} - U_{l,N})$ , for  $l = 3$  and  $4$  and  $(U_{3,N} - U_{4,N})$  converges almost surely respectively to  $0$  and  $I(\Phi_3) - I(\Phi_4)$ , the denominator converges almost surely. Thus it suffices to prove that the numerator is  $o_{\mathbb{P}}(1/\sqrt{N})$  which reduces to prove that  $\sqrt{N}(U_{l,N,n} - U_{l,N}) = o_{\mathbb{P}}(1)$  for  $l = 1, \dots, 4$ , where  $U_{l,N,n}$  (respectively  $U_{l,N}$ ) has been defined in (35) (resp. (11)). Let  $l = 1$  for example. The other terms can be treated analogously. Here,  $m(1) = 3$ . We write

$$\begin{aligned} &\mathbb{E}[|U_{1,N,n} - U_{1,N}|] \\ &\leq \binom{N}{3}^{-1} (3!)^{-1} \sum_{\substack{1 \leq i_1 < i_2 < i_3 \leq N \\ \tau \in \mathcal{S}_3}} \mathbb{E} \left[ \left| \Phi_1(\mu_{X_{\tau(i_1)},n}, \mu_{X_{\tau(i_2)},n}, \mu_{X_{\tau(i_3)},n}) - \Phi_1(\mu_{X_{\tau(i_1)}}, \mu_{X_{\tau(i_2)}}, \mu_{X_{\tau(i_3)}}) \right| \right] \\ &= \mathbb{E} \left[ \left| \Phi_1(\mu_{X_1,n}, \dots, \mu_{X_2,n}, \mu_{X_3,n}) - \Phi_1(\mu_{X_1}, \mu_{X_2}, \mu_{X_3}) \right| \right] \\ &\leq 2\mathbb{E} \left[ \left| \mathbb{1}_{W_q(\mu_{X_1}, \mu_{X_3}) \leq W_q(\mu_{X_1}, \mu_{X_2})} - \mathbb{1}_{W_q(\mu_{X_1,n}, \mu_{X_3,n}) \leq W_q(\mu_{X_1,n}, \mu_{X_2,n})} \right| \right] \\ &=: 2\mathbb{E}[B_n] \end{aligned}$$

where the random variable  $B_n$  in the expectation in the right-hand side of the previous inequality is a Bernoulli random variable whose distribution does not depend on  $(\mu_{X_1}, \mu_{X_2}, \mu_{X_3})$ . Let  $\Delta(N)$  be the following event

$$\Delta(N) = \left\{ \left| W_q(\mu_{X_{\tau(1)}}, \mu_{X_{\tau(3)}}) - W_q(\mu_{X_{\tau(1)}}, \mu_{X_{\tau(2)}}) \right| \geq \delta(N) \right\}.$$

Obviously, we get  $\mathbb{E}[B_n \mathbb{1}_{\Delta(N)^c}] \leq \mathbb{P}(\Delta(N)^c)$ , where  $A^c$  stands for the complementary of  $A$  in  $\Omega$ . Furthermore,

$$\begin{aligned} \mathbb{E}[B_n \mathbb{1}_{\Delta(N)}] &\leq \mathbb{E}[B_n | \Delta(N)] = \mathbb{P}(B_n = 1 | \Delta(N)) \\ &\leq \sum_{r=1}^3 \mathbb{P}\left(W_q(\mu_{X_r}, \mu_{X_{r,n}}) \geq \frac{\delta(N)}{4}\right) \\ &\leq \frac{12}{\delta(N)} \mathbb{E}[W_q(\mu_{X_1}, \mu_{X_{1,n}})]. \end{aligned}$$

Finally, we introduce  $\varepsilon > 0$  and we study:

$$\begin{aligned} \mathbb{P}\left(\sqrt{N}|U_{1,N,n} - U_{1,N}| \geq \varepsilon\right) &\leq \frac{\sqrt{N}}{\varepsilon} \mathbb{E}[|U_{1,N,n} - U_{1,N}|] \\ &\leq 2 \frac{\sqrt{N}}{\varepsilon} \mathbb{E}[B_n] \\ &\leq \frac{\sqrt{N}}{\varepsilon} \frac{24}{\delta(N)} \mathbb{E}[W_q(\mu_{X_1}, \mu_{X_{1,n}})] + 2 \frac{\sqrt{N}}{\varepsilon} \mathbb{P}(\Delta(N)^c). \end{aligned}$$

It remains to choose first,  $\delta(N)$  so that  $\mathbb{P}(\Delta(N)^c) = o\left(1/\sqrt{N}\right)$  and second,  $n$  such that  $\mathbb{E}[W_q(\mu_{X_1}, \mu_{X_{1,n}})] = o(\delta(N)/\sqrt{N})$ . Consequently,  $\sqrt{N}(U_{1,N,n} - U_{1,N}) = o_{\mathbb{P}}(1)$ . Analogously, one gets  $\sqrt{N}(U_{l,N,n} - U_{l,N}) = o_{\mathbb{P}}(1)$  for  $l=2, 3$  and  $4$ .  $\square$

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