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Global sensitivity analysis and Wasserstein spaces

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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 metamodelling 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

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

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

57 Nowadays, the computer code output is often no longer a real-valued multidimensional variable but
58 rather a function computed at various locations. In that sense, it can be considered as a functional
59 output. Some other times, the computer code is stochastic in the sense that the same inputs can lead
60 to different outputs. When the output of the computer code is a function (for instance, a cumulative
61 distribution function) or when the computer code is stochastic, Sobol indices are no longer well tailored.
62 It is then crucial to define indices adapted to the functional or random aspect of the output. When
63 the output is vectorial or valued in an Hilbert space, some generalizations of Sobol indices are available
64 [39, 24]. Nevertheless, these indices are still based on the Hoeffding decomposition of the output; so
65 that they only quantify the relative influence of an input through the variance. More recently, indices
66 based on the whole distribution have been developed [16, 9, 7]. In particular, the method relying on
67 Cramér-von-Mises distance [26] compares the conditionnal cumulative distribution function with the
68 unconditional one by considering the Hoeffding decomposition of half-space indicators (rather than the
69 Hoeffding decomposition of the output itself) and by integrating them. This method was then extend to
70 codes taking values in a Riemannian manifold [21] and then in general metric spaces [27].

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

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

97 2 Sensitivity indices for codes valued in general metric spaces

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

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

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

101 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
 103 probability distribution functions (p.d.f.) on \mathbb{R} or the space of cumulative distribution functions
 104 (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?

107 2.1 The general metric spaces sensitivity index

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

112 In [27], the authors performed GSA for codes f taking values in general metric spaces. To do so, they
 113 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

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

114 Roughly speaking, the previous indices divided into two parts. First, for any value of a , we consider the
 115 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
 116 of $T_a(Z)$. This part is called the Sobol part. Second, we integrate each part with respect to the measure
 117 $\mathbb{P}^{\otimes m}$; 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

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

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

121 • **First method - Pick-Freeze.** Introduced in [26], this procedure is based on a double Monte-Carlo
 122 scheme to estimate the Cramér-von-Mises (CVM) indices $S_{2,\text{CVM}}^{\mathbf{u}}$. More precisely, to estimate
 123 $S_{2,\text{GMS}}^{\mathbf{u}}$ in our context, we consider the following design of experiment consisting in

- 124 1. a classical Pick-Freeze N -sample, that is two N -samples of Z : $(Z_j, Z_j^{\mathbf{u}})$, $1 \leq j \leq N$;
- 125 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

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

while the one of the denominator is

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

126 For $\mathcal{X} = \mathbb{R}^k$, $m = 1$, and T_a given by $T_a(x) = \mathbb{1}_{x \leq a}$, the index $S_{2,\text{GMS,PF}}^{\mathbf{u}}$ is nothing more than
 127 the index $S_{2,\text{CVM}}^{\mathbf{u}}$ defined in [26] based on the Cramér-von-Mises distance and on the whole distri-
 128 bution of the output. Its estimator $\widehat{S}_{2,\text{CVM}}^{\mathbf{u}}$ defined as the ratio of $\widehat{N}_{2,\text{GMS,PF}}^{\mathbf{u}}$ and $\widehat{D}_{2,\text{GMS,PF}}^{\mathbf{u}}$ with
 129 $T_a(x) = \mathbb{1}_{x \leq a}$ has been proved to be asymptotically Gaussian [26, Theorem 3.8]. The proof relies
 130 on Donsker's theorem and the functional delta method [61, Theorem 20.8]. Analogously, in the
 131 general case of $S_{2,\text{GMS}}^{\mathbf{u}}$, the central limit theorem is still valid as soon as the collection $(T_a)_{a \in \mathcal{X}^m}$
 132 forms a Donsker's class of functions.

133 • **Second method - U-statistics.** As done in [27], this method allows the practitioner to get rid of the
 134 additional random variables $(W_{l,k})$ for $l \in \{1, \dots, m\}$ and $k \in \{1, \dots, N\}$. The estimator is now
 135 based on U-statistics and deals simultaneously with the Sobol part and the integration part with
 136 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 $l = 1, \dots, 4$,

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

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

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

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

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

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

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

146 More precisely, an i.i.d. sample of pairs of real-valued random variables $(X_{i,j}, Y_j)_{1 \leq j \leq N}$ ($i \in$
147 $\{1, \dots, p\}$) is considered, assuming for simplicity that the laws of X_i and Y are both diffuse (ties
148 are excluded). The pairs $(X_{i,(1)}, Y_{(1)}), \dots, (X_{i,(N)}, Y_{(N)})$ are rearranged in such a way that

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

149 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
150 is,

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

151 The new correlation coefficient is then given by

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

152 In [15], it is proved that $\xi_N(X_i, Y)$ converges almost surely to a deterministic limit $\xi(X_i, Y)$ which
153 is actually equal to $S_{2,\text{CVM}}^i$ when $Y = Z = f(X_1, \dots, X_p)$. Further, the author also proves a
154 central limit theorem when X_i and Y are independent, which is clearly not relevant in the context
155 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 $\widehat{D}_{2,\text{GMS},\text{Rank}}^i$

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

156 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
157 respect to X_i) in the Pick-Freeze estimation procedure.

158 Comparison of the estimation procedures

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

170 However, the Pick-Freeze estimators have two major drawbacks. First, they rely on a particular
 171 experimental design that may be unavailable in practice. Second, it can be unfortunately very time
 172 consuming in practice: the number of model calls to estimate all first-order Sobol indices grows linearly
 173 with the number of input parameters. For example, if we consider $p = 99$ input parameters and only
 174 $N = 1000$ calls are allowed, then only a sample of size $N/(p + 1) = 10$ is available to estimate each single
 175 first-order Sobol index.

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

180 Finally, embedding Chatterjee’s method in the GSA framework (called rank-based method in this
 181 framework) thereby eliminates the two drawbacks of the classical Pick-Freeze estimation. Indeed, the
 182 strength of the rank-based estimation procedure lies in the fact that only one N -sample of Z is required
 183 while $(m + 2)$ samples of size N are necessary in the Pick-Freeze estimation of a single index (worse,
 184 $(m + 1 + p)$ samples of size N are required when one wants to estimate p indices). Using a single sample
 185 of size N , it is now possible to estimate at the same time all the first-order Sobol indices, first-order
 186 Cramér-von-Mises indices, and other useful first-order sensitivity indices as soon as all inputs are real
 187 valued. More generally, the rank-based method allows for the estimation of a large class of GSA indices
 188 which includes the Sobol indices and the higher-order moment indices proposed by Owen [47, 49, 48].
 189 In addition, the rank-based estimator has nice theoretical properties. For instance, the estimator of the
 190 Sobol index S^i has been proved to be consistent and asymptotically Gaussian (see, e.g., Theorem 3.3 in
 191 [23]).

192 2.2 The universal sensitivity index

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

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

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

200 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 Ω 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

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

201 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
 202 Hoeffding decomposition of $T_a(Z)$. Hence, by construction, this index lies in $[0, 1]$ and shares the same
 203 properties as its Sobol counterparts, namely the two previously cited properties in (3) and (4).

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

- 206 • 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 Id the identity test function;
- 207 • the Cramér-von-Mises index $S_{2,\text{CVM}}^{\mathbf{u}}$ with respect to $X_{\mathbf{u}}$ is $S_{2,\text{Univ}}^{\mathbf{u}}(\mathbb{1}_{\cdot \leq a}, \mathbb{P}^{\otimes d})$ where $\mathcal{X} = \mathbb{R}^d$ and
 208 $\Omega = \mathcal{X}$;
- 209 • the general metric space sensitivity index $S_{2,\text{GMS}}^{\mathbf{u}}$ with respect to $X_{\mathbf{u}}$ is $S_{2,\text{Univ}}^{\mathbf{u}}(\mathbb{1}_{\cdot \leq a}, \mathbb{P}^{\otimes m})$ where
 210 $\Omega = \mathcal{X}^m$.

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

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

- 214 • First method - Pick-Freeze. We use the same design of experiment as in the first method of Section
 215 2.1 but instead of considering that the m additional N -samples $(W_{l,k})$ for $l \in \{1, \dots, m\}$ and
 216 $k \in \{1, \dots, N\}$ are drawn with respect to the distribution \mathbb{P} of the output, they are now drawn
 217 with respect to \mathbb{Q} . More precisely, we consider the following design of experiment consisting in
 - 218 1. a classical Pick-Freeze sample, that is two N -samples of Z : $(Z_j, Z_j^{\mathbf{u}})$, $1 \leq j \leq N$;
 - 219 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
 220 $(Z_j, Z_j^{\mathbf{u}})$ for $1 \leq j \leq N$.

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

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

while the one of the denominator is

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

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

- 224 • Second method - U-statistics. This method is not relevant in this case since $\mathbb{Q} \neq \mathbb{P}^{\otimes d}$.
- 225 • Third method - Rank-based. Here, the design of experiment reduces to
 - 226 1. a N -sample of Z : Z_j , $1 \leq j \leq N$;
 - 227 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 $\widehat{S}_{2,\text{Univ},\text{Rank}}^i$ of
 $S_{2,\text{Univ}}^i$ is then given by the ratio between

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

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

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

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

230 2.3 A sketch of answer to Questions 1 to 3

231 In the sequel, we discuss how pertinent choices of the metric, of the class of test functions T_a and of the
232 probability measure \mathbb{Q} can provide answers to Questions 1 to 3 raised at the beginning of Section 2. For
233 instance, in order to answer to Question 1, we can consider that $\mathcal{X} = \mathcal{M}_q(\mathbb{R})$ is the space of probability
234 measures μ on \mathbb{R} having finite q -moments that we endow with the Wasserstein metric W_q (see Section
235 3.1 for some recalls on Wasserstein metrics). We propose two possible approaches to define interesting
236 sensitivity indices in this framework.

- 237 • 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
238 the open ball defined by $\{\mu \in \mathcal{M}_q(\mathbb{R}), W_q(\mu, \mu_1) < W_q(\mu_1, \mu_2)\}$.
- 239 • In Section 4.2, we use the notion of Fréchet means on Wasserstein spaces (see Section 3.2) and the
240 index defined in (16) with appropriate choices of a , T_a , and \mathbb{Q} .

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

244 3 Wasserstein spaces and random distributions

245 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

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

246 where F^- and G^- are the generalized inverses of the increasing functions F and G and U is a random
247 variable uniformly distributed on $[0, 1]$. Of course, $F^-(U)$ and $G^-(U)$ have c.d.f.'s F and G . The
248 representation (19) of the q -Wasserstein distance when $p = 1$ can be generalized to a wider class of
249 "contrast functions". For more details on Wasserstein spaces, one can refer to [62] and [6] and the
250 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

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

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

252 For instance, $c(x, y) = -xy$ satisfies \mathcal{P} . If c satisfies \mathcal{P} , any function of the form $a(x) + b(y) + c(x, y)$
 253 also satisfies \mathcal{P} . If C is a convex real function, $c(x, y) = C(x - y)$ satisfies \mathcal{P} . In particular, $c(x, y) =$
 254 $(x - y)^2 = x^2 + y^2 - 2xy$ satisfies \mathcal{P} and actually so does $c(x, y) = |x - y|^q$ as soon as $q \geq 1$.

255 **Definition 3.2.** We define the *Skorokhod space* $\mathcal{D} := \mathcal{D}([0, 1])$ of all distribution functions as the space
 256 of all non-decreasing functions from \mathbb{R} to $[0, 1]$ that are right-continuous with left-hand limits with limit
 257 0 (resp. 1) in $-\infty$ (resp. $+\infty$) equipped with the supremum norm.

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

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

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

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

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

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

264 3.2 Extension of the Fréchet mean to contrast functions

265 In this section, we recall the classical definition of the notion of the Fréchet mean which is a natural
 266 extension of the classical mean for general metric spaces and then we extend this definition to the notion
 267 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

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

268 When \mathcal{M} is a metric space endowed with a distance d , the Fréchet feature with $l = d^2$ corresponds to
 269 the classical Fréchet mean (see [22]). In particular, $\mathcal{E}_{d^2}[X]$ minimizes $\mathbb{E}[d^2(X, \theta)]$ which is an extension
 270 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

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

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

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

274 **Theorem 3.6.** *Let c be a positive contrast function. Assume that the application defined by $(\omega, v) \in$
 275 $\Omega \times (0, 1) \mapsto \mathbb{F}^-(\omega, v) \in \mathbb{R}$ is measurable. In addition, assume that $\mathcal{E}_c[\mathbb{F}]$ exists and is unique. Then there
 276 exists a unique Fréchet mean of $\mathbb{E}[c(\mathbb{F}^-(v), s)]$ denoted by $\mathcal{E}_c[\mathbb{F}^-](v)$ and we have*

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

277 *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. □

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 α -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 α -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 α -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 σ 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 α -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

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

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

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

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

308 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
 309 computer code is then a c.d.f. denoted by

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

310 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
 311 handled analogously.

312 4.1 Sensitivity analysis using Equation (2) and Wasserstein balls

313 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

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

314 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
 315 decomposition of $T_a(\mathbb{F})$. Hence, by construction, this index lies in $[0, 1]$ and shares the two properties
 316 previously cited in (3) and (4).

317 4.2 Sensitivity analysis using Equation (16) and Fréchet means

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

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

320 by the property of the conditional expectation. On the one hand, we extend this formula to the framework
 321 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

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

322 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

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

323 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
324 two properties previously cited in (3) and (4).

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

327 4.3 Estimation procedure

328 As noticed in the previous section, both

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

329 with T_a defined in (23) and

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

330 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

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

331 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
332 the estimations based on U-statistics together on the Pick-Freeze design of experiment. Thirdly, it is also
333 possible and easy to obtain rank-based estimations in the vein of (12).

334 4.4 Numerical comparison of both indices

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

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

337 so that

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

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 $S_{2,W_2}^{\mathbf{u}}$

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

349 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

351 **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
 352 $S^1(\mathbb{F})$, $S^2(\mathbb{F})$, $S^3(\mathbb{F})$, 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
 353 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
 354 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 ,
 355 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
 356 the Fréchet indices $S^{\mathbf{u}}(\mathbb{F})$ differ from the Wasserstein indices $S_{2,W_2}^{\mathbf{u}}$ as expected, they behave reassuringly
 357 similarly.

358 **Regions of predominance of the indices $S^{\mathbf{u}}(\mathbb{F})$ and $S_{2,W_2}^{\mathbf{u}}$** In addition, the regions of predominance
 359 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
 360 values of p_3 considered are: $p_3 = 0.01$ (first row), 0.5, (second row) and 0.99 (third row). Finally, the
 361 same kind of illustration for the indices $S_{2,W_2}^{\mathbf{u}}$ is given in Figure 4. Once again, we observe a global
 362 accordance of the predominance regions between the Fréchet indices $S^{\mathbf{u}}(\mathbb{F})$ and the Wasserstein indices
 363 $S_{2,W_2}^{\mathbf{u}}$.

364 **Comparison of the estimation procedures (rank-based and Pick-Freeze)** In order to compare
 365 the accuracy of the Pick-Freeze method and the accuracy of the rank-based method at a fixed size, we
 366 assume that only 450 calls of the computer code are allowed to estimate the indices $S^{\mathbf{u}}(\mathbb{F})$ and $S_{2,W_2}^{\mathbf{u}}$
 367 for $\mathbf{u} = \{1\}$, $\{2\}$, and $\{3\}$. Hence, the sample size allowed in the rank-based procedure is $N = 450$.
 368 In the Pick-Freeze methodology, the estimation of the Fréchet indices $S^{\mathbf{u}}(\mathbb{F})$ requires one initial output
 369 sample and three extra output samples to get the Pick-Freeze versions (one for each index) leading to
 370 an allowed sample size $N = \lfloor 450/4 \rfloor = 112$ while it is $N = \lfloor 450/6 \rfloor = 75$ for the Wasserstein indices
 371 $S_{2,W_2}^{\mathbf{u}}$ ($1 + 3 = 4$ output samples + two extra samples to handle the integration). We only focus on the
 372 first-order indices since, as explained previously, the rank-based procedure has not been developed yet
 373 for higher-order indices. We repeat the estimation procedure $n_r = 200$ times. The boxplots of the mean
 374 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
 375 plotted in Figure 5. We observe that, for a fixed total number of calls 450 to the code f (corresponding
 376 to a rank-based sample size $N = 450$ and to a Pick-Freeze sample size $N = 112$ for the Fréchet indices
 377 $S^{\mathbf{u}}(\mathbb{F})$ and $N = 74$ for the Wasserstein indices $S_{2,W_2}^{\mathbf{u}}$), the rank-based estimation procedure performs
 378 much better than the Pick-Freeze method with significantly lower mean errors.

379 5 Sensitivity analysis for stochastic computer codes

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

383 5.1 State of the art

384 A first natural way to handle stochastic computer codes is definitely to consider the expectation of the
 385 output code. Indeed, as mentioned in [10], previous works dealing with stochastic simulators together
 386 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	$p_1(1-p_1)(p_2+p_3-p_2p_3)^2$
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.	$p_1 p_2 p_3$

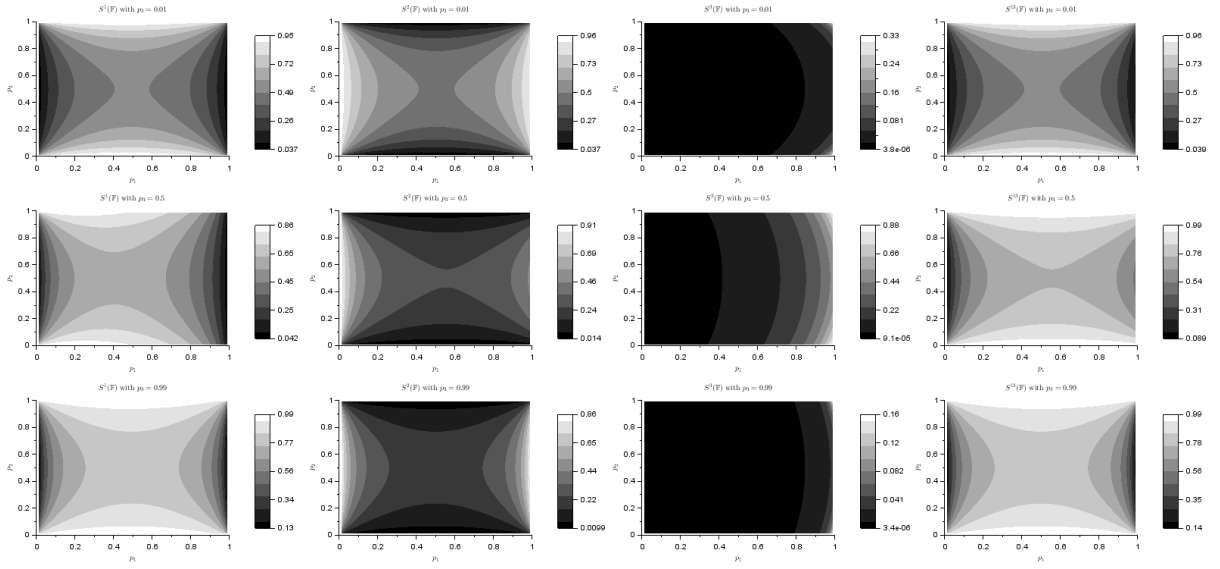


Figure 1: Model (30). Values of the indices $S^1(\mathbb{F})$, $S^2(\mathbb{F})$, $S^3(\mathbb{F})$, and $S^{1,3}(\mathbb{F})$ given by (26) (from left to right) with respect to the values of p_1 and p_2 (varying from 0 to 1). In the first row (resp. second and third), p_3 is fixed to $p_3 = 0.01$ (resp.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

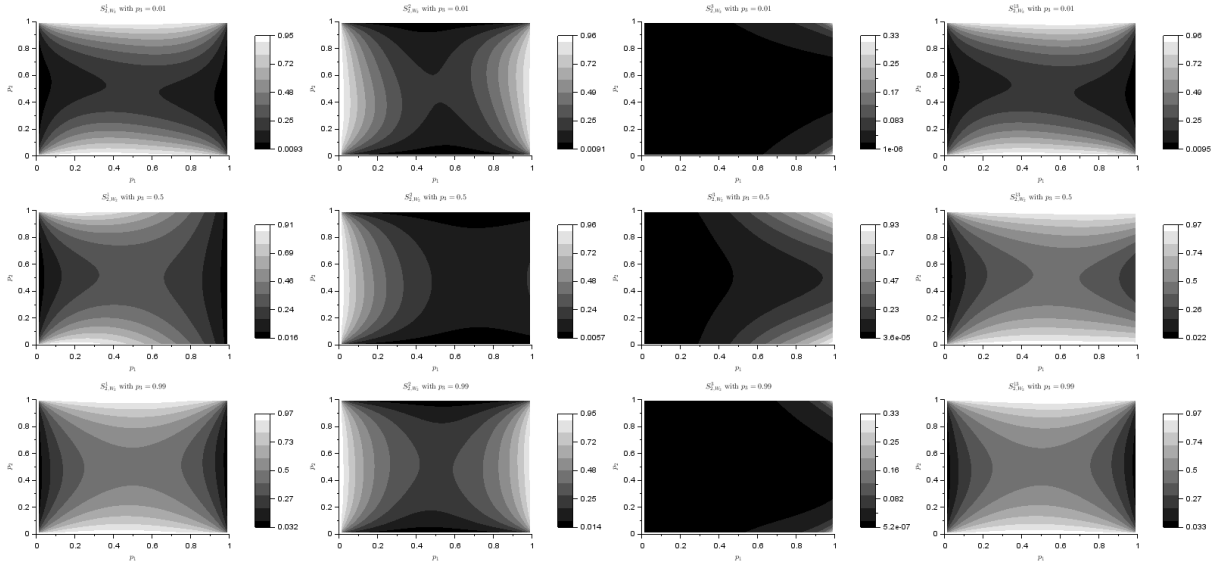


Figure 2: Model (30). Values of the indices S_{2,W_2}^1 , S_{2,W_2}^2 , S_{2,W_2}^3 , and $S_{2,W_2}^{1,3}$ given by (24) (from left to right) with respect to the values of p_1 and p_2 (varying from 0 to 1). In the first row (resp. second and third), p_3 is fixed to $p_3 = 0.01$ (resp. 0.5 and 0.99).

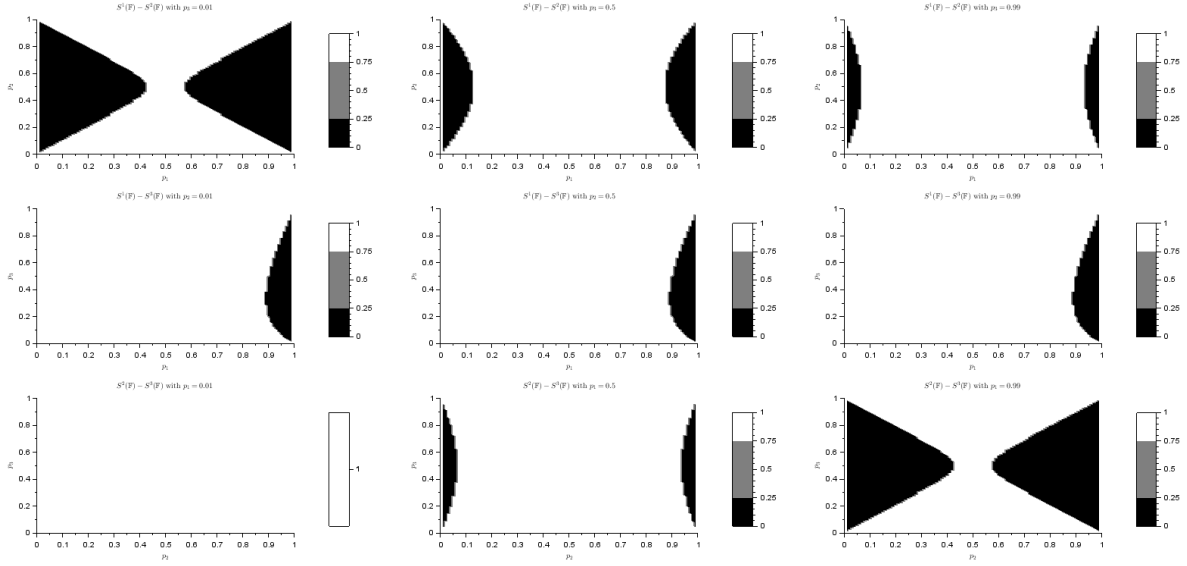


Figure 3: Model (30). In the first row of the figure, regions where $S^1(\mathbb{F}) \geq S^2(\mathbb{F})$ (black), $S^1(\mathbb{F}) \leq S^2(\mathbb{F})$ (white), and $S^1(\mathbb{F}) = S^2(\mathbb{F})$ (gray) with respect to p_1 and p_2 varying from 0 to 1 and, from left to right, $p_3 = 0.01, 0.5,$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

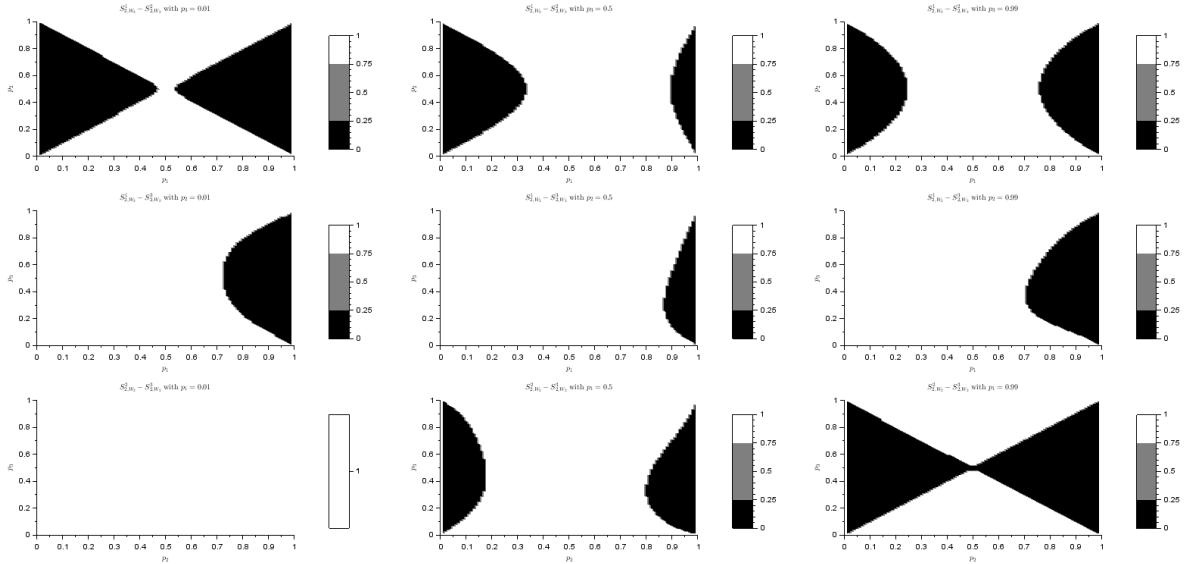


Figure 4: Model (30). In the first row of the figure, regions where $S_{2,W_2}^1 \geq S_{2,W_2}^2$ (black), $S_{2,W_2}^1 \leq S_{2,W_2}^2$ (white), and $S_{2,W_2}^1 = S_{2,W_2}^2$ (gray) with respect to p_1 and p_2 varying from 0 to 1 and, from left to right, $p_3 = 0.01, 0.5,$ and 0.99 . Analogously,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

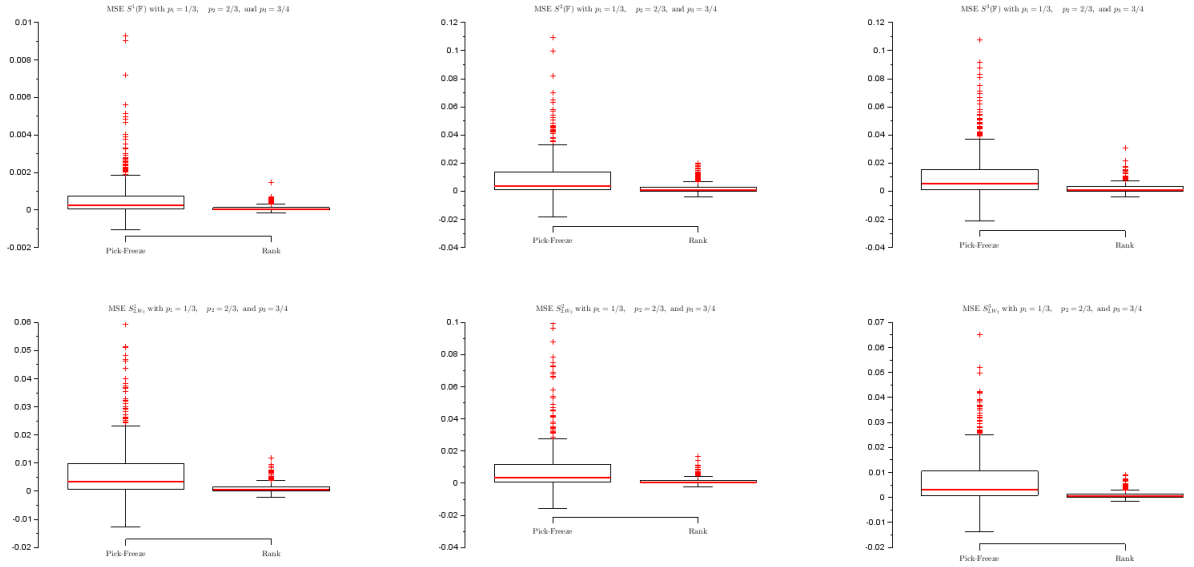


Figure 5: Model (30) with $p_1 = 1/3$, $p_2 = 2/3$, and $p_3 = 3/4$. Boxplots of the mean square errors of the estimation of the Fréchet indices $S^{\mathbf{u}}(\mathbb{F})$ (top row) and the Wasserstein indices $S_{2,W_2}^{\mathbf{u}}$ (bottom row) with a fixed sample size N and $n_r = 200$ replications. 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.

387 of the stochastic output [18, 11, 37, 2] and then performing a GSA on the expectation of the output code
388 [42].

389 As pointed out by [35], another approach amounts to consider that the stochastic code is of the form
390 $f(X, D)$ where the random element X contains the classical input variables and the variable D is an
391 extra unobserved random input. Such an idea was exploited in [36] to compare the estimation of the
392 Sobol indices in an “exact” model to the estimation of the Sobol indices in an associated metamodel.
393 In this framework, the metamodel is considered as a random perturbation of the “exact” model and
394 the perturbation is a function of the inputs and of an extra independent random variable. Analogously,
395 the author of [43] assumes the existence of an extra random variable D which is not chosen by the
396 practitioner but rather generated at each computation of the output independently of X . In this setting,
397 the author builds two different indices. The first index is obtained by substituting $f(X, D)$ for $f(X)$ in
398 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
399 is considered as another input, even though it is not observable. The second index is obtained by substituting
400 $\mathbb{E}[f(X, D)|X]$ for $f(X)$ in the Sobol index. The noise is then smoothed out. Similarly, the authors of
401 [31] traduce the randomness of the computer code using such an extra random variable. In practice,
402 they approximate the statistical properties of the first-order Sobol indices by using a sample of the extra
403 random variable and the associated sample of estimates of the Sobol indices. In [63], the expectation
404 of these random Sobol indices is investigated in the case of stochastic simulator and generalized lambda
405 models. In the same vein, the authors of [3] propose to deal with the differential entropy of the output
406 of a stochastic simulator.

407 5.2 The space \mathcal{W}_q as an ideal version of stochastic computer codes

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

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

$$f_s : E \times \mathcal{D} \rightarrow \mathbb{R} \quad (32)$$

$$(x, D) \mapsto f_s(x, D),$$

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

417 Hence, one may define another (deterministic) computer code associated with f_s for which the output
 418 associated to x is the probability measure μ_x

$$f : E \rightarrow \mathcal{W}_q(E) \quad (33)$$

$$x \mapsto \mu_x.$$

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

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

422 where δ is the Dirac function. Further, (33) can be seen as an ideal version of (32). Concretely, for
 423 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
 424 defined by (32) (so that the code will generate independently n hidden variables D_1, \dots, D_n) and one
 425 may observe

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

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

428 5.3 Sensitivity analysis

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

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

434 In the more realistic framework presented above in (32), we only have access to the approximation
 435 $\mu_{x,n}$ of μ_x rendering more complex the estimation procedure and the study of the asymptotic properties.
 436 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

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

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

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

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

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

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

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

446 Actually, these estimators are easy to compute since, for two discrete measures supported on a same
447 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 ν_1 and ν_2 simply writes

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

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

449 5.4 Central limit theorem for the estimator based on U-statistics

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

453 **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
454 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 $\mathbf{u} \subset \{1, \dots, p\}$,

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

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

456 In some particular frameworks, one may derive easily a suitable value of $\delta(N)$. Two examples are
457 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,

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

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

459 **Example 5.3** (Uniform example). Assume that X is uniformly distributed on $[0, 1]$ and that μ_X is a
 460 Gaussian distribution centered at X with unit variance. Then the Wasserstein distance $W_2(\mu_{X_1}, \mu_{X_2})$
 461 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,

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

462 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,

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

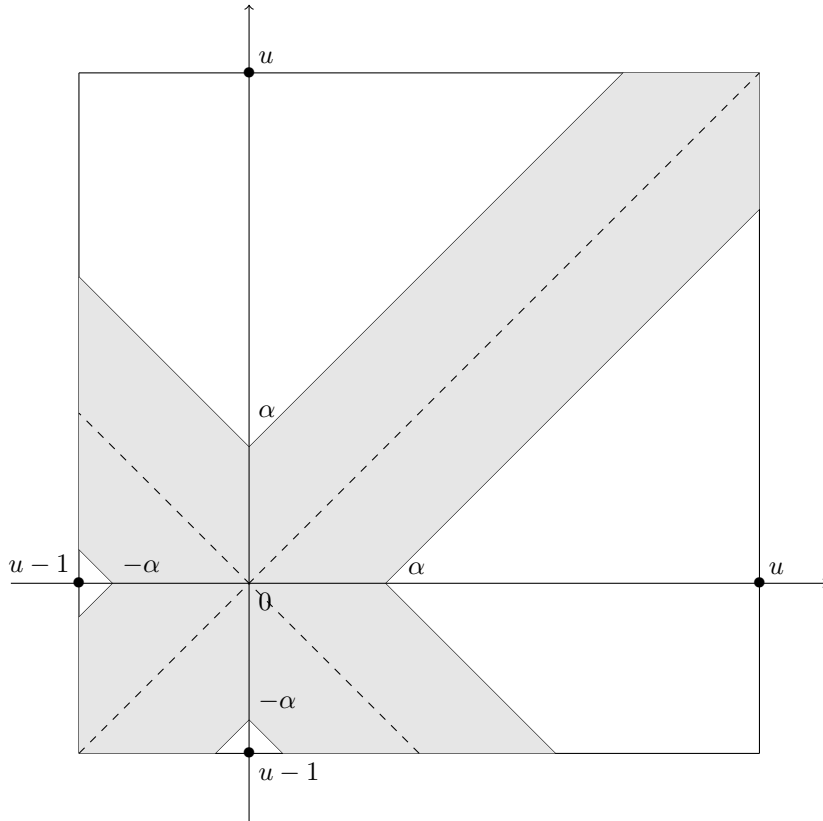
463 Now, $X_2 - u$ and $X_3 - u$ are two independent random variables uniformly distributed on $[-u, -u]$. Then
 464 (see Figure 6), one has

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

465 whence

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

466 Thus it turns out that $\mathbb{P}(W \leq \delta(N)) = O(\sqrt{\delta(N)})$. Consequently, a suitable choice for $\delta(N)$ is $\delta(N) =$
 467 $o(1/N)$.



468

469

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

470

471

472

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 μ_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_{μ_X} is the c.d.f. associated to μ_X and f_{μ_X} its p.d.f. See Cf. [6, Theorems 3.2, 5.1 and 5.3].

475 • Assume that μ_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 μ_X is a log-concave distribution with standard deviation σ . 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 μ_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 μ_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 $\mathbb{E}[W_2(\mu_X, \mu_{X,n})] = o(\delta(N)/\sqrt{N})$.

491 5.5 Numerical study

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

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

494 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
 495 by (30) and its stochastic counterpart

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

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

497 Hence, we no longer assume that one may observe N realizations of \mathbb{F} associated to the N initial
 498 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
 499 realizations of a uniform random variable on $[0, 1 + X_1 + X_2 + X_1 X_3]$.

500 In order to compare the estimation accuracy of the Pick-Freeze method and the rank-based method at
 501 a fixed size, we assume once again that only 450 calls of the computer code f are allowed to estimate the
 502 Fréchet indices $S^u(\mathbb{F})$ and the Wasserstein indices S_{2, W_2}^u for $\mathbf{u} = \{1\}$, $\{2\}$, and $\{3\}$. As in Example 4.1 of
 503 Section 4.4, the sample size allowed in the rank-based procedure is then $N = 450$ while, in the Pick-Freeze
 504 methodology, it is only $N = 112$ for the Fréchet indices $S^u(\mathbb{F})$ and $N = 75$ for the Wasserstein indices
 505 S_{2, W_2}^u . We only focus on the first-order indices since, as explained previously, the rank-based procedure
 506 has not been developed yet for higher-order indices. The empirical c.d.f. based on the empirical measures
 507 $\mu_{X_j, n}$ for $j = 1, \dots, N$ in (34) are constructed with $n = 500$ evaluations. We repeat the estimation
 508 procedure $n_r = 200$ times. The boxplots of the mean square errors for the estimation of the Fréchet
 509 indices $S^u(\mathbb{F})$ and the Wasserstein indices S_{2, W_2}^u have been plotted in Figure 7. We observe that, for a
 510 fixed total number of calls 450 to the code f (corresponding to a rank-based sample size $N = 450$ and to
 511 a Pick-Freeze sample size $N = 112$ for the Fréchet indices $S^u(\mathbb{F})$ and $N = 74$ for the Wasserstein indices
 512 S_{2, W_2}^u), the rank-based estimation procedure performs much better than the Pick-Freeze method with
 513 significantly lower mean errors.

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

516 6 Sensitivity analysis with respect to the law of the inputs

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

520 6.1 State of the art

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

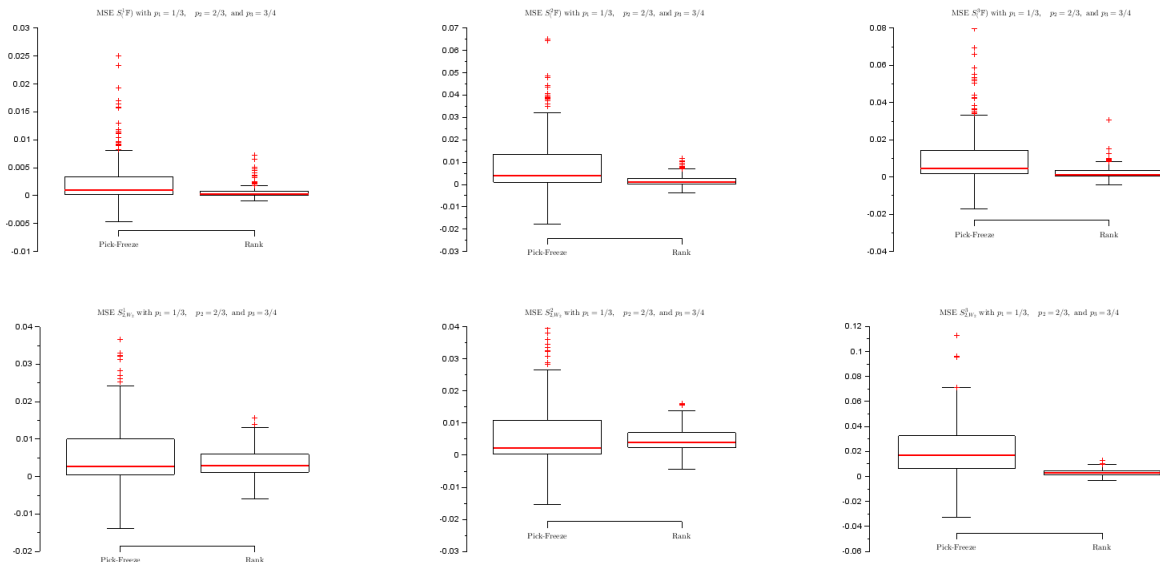


Figure 7: Model (39) with $p_1 = 1/3$, $p_2 = 2/3$, and $p_3 = 3/4$. Boxplot of the mean square errors of the estimation of the Fréchet indices $S^{\mathbf{u}}(\mathbb{F})$ (top row) and the Wasserstein indices $S_{2,W_2}^{\mathbf{u}}$ (bottom row) with a fixed sample size N , an approximation size n 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 $S^{\mathbf{u}}(\mathbb{F})$ 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.

535 In [45], a different approach is adopted. A failure probability is studied while the uncertainty concerns
536 the parameters of the input distributions. An algorithm with low computational cost is proposed to handle
537 such uncertainty together with the rare event setting. A single initial sample allows to compute the failure
538 probabilities associated to different parameters of the input distributions. A similar idea is exploited in
539 [41] in which the authors consider input perturbations and Perturbed-Law based Indices that are used to
540 quantify the impact of a perturbation of an input p.d.f. on a failure probability. Analogously, the authors
541 of [30, 32] are interested in (marginal) p.d.f. perturbations and the aim is to study the “robustness of the
542 Sobol indices to distributional uncertainty and to marginal distribution uncertainty” which correspond
543 to second-level uncertainty. For instance, the basic idea of the approach proposed in [30] is to view the
544 total Sobol index as an operator which inputs the p.d.f. and returns the Sobol index. Then the analysis
545 of robustness is done computing and studying the Fréchet derivative of this operator. The same principle
546 is used in [32] to treat the robustness with respect to the marginal distribution uncertainty. Recently,
547 [59] proposes a very clever approach of second-level SA when some moments of the distribution of the
548 inputs are fixed. Its approach characterizes among all compactly supported input distribution with fixed
549 first moments the range of variability of the Sobol indices.

550 Note that the “ p -box” framework in the sense it is used by [55] presents some similarities with the
551 example provided in Section 3.3 (in the context of random distributions and Fréchet means). It is also
552 worth mentioning the classical approach of epistemic GSA of Dempster-Shafer theory (see, e.g., [56, 1]).
553 This theory describes the random variables together with an epistemic uncertainty traduced in terms of
554 an associated epistemic variable Z on a set A , a mass function representing a probability measure on the
555 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.
556 and can be viewed as second-level uncertainty.

557 6.2 Link with stochastic computer codes

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

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

- 566 • 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
 567 $(\Theta_i, \mathcal{B}(\Theta_i), \nu_{\Theta_i})$ where $\mathcal{B}(\Theta_i)$ is the Borel σ -field and ν_{Θ_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 π_i the one-to-one mapping from Θ_i to \mathcal{P}_i defined by
 $\pi_i(\theta) := \eta_\theta \in \mathcal{P}_i$ and define the σ -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 Π_i defined, for any $A \in \mathcal{F}_i$, by

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

- 568 • Third, in order to perform a second-level SA on (1), we introduce the stochastic mapping f_s from
 569 $\mathcal{P}_1 \times \dots \times \mathcal{P}_p$ to \mathcal{X} defined by

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

570 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
 571 code from $\mathcal{P}_1 \times \dots \times \mathcal{P}_p$ to \mathcal{X} and once the probability measures \mathbb{P}_{η_i} on each \mathcal{P}_i are defined, we can
 572 perform SA using the framework of Section 5.

573 6.3 Numerical study

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

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

574 We are interested in the uncertainty in the support of the random variables X_1 , X_2 , and X_3 . To do
 575 so, we follow the notation and framework of [32]. For $i = 1, 2$, and 3 , we assume that X_i is uniformly
 576 distributed on the interval $[A_i, B_i]$, where A_i and B_i are themselves uniformly distributed on $[0, 0.1]$ and
 577 $[0.9, 1]$ respectively. As remarked in [32], it seems natural that f will vary more in the X_2 -direction when
 578 X_1 is close to 0 and less when X_1 is close to 1.

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

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

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

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

- 586 1. For $i = 1, 2$, and 3 ,
 - 587 (a) we produce a N -sample $([A_{i,j}, B_{i,j}])_{j=1, \dots, N}$ of intervals $[A_i, B_i]$.
 - 588 (b) for $j = 1, \dots, N$,
 - 589 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
 590 $[A_{i,j}, B_{i,j}]$.

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

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

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

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

594 (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
595 the SA regarding the input \mathbf{u} .

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

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

601 **Simulations** First, we compute the estimators of $S_{2,W_2}^{\mathbf{u}}$ following the previous procedure with a sample
602 size $N = 500$ and an approximation size $n = 500$. The results are displayed in Table 1 (first row). We
603 also perform another batch of simulations allowing for higher variability on the bounds: for $i = 1, 2$, and
604 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 $[0.55, 1]$.

605 Second, we run another simulation allowing for more variability on the upper bound related to the
606 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
607 still uniformly distributed on $[0, 0.1]$ while B_i is still uniformly distributed on $[0.9, 1]$. The results are
608 displayed in Table 2. We still use a sample size $N = 500$ and an approximation size $n = 500$.
609

\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 $[0.9, 1]$.

610 Third, the aim is to highlight the fact that performing a classical GSA differs from performing a
611 second-level SA. In that view, we perform a classical GSA on the inputs rather than on the parameters
612 of their distributions (corresponding to a second-level analysis). Namely, we consider the index $S_{2,CVM}^{\mathbf{u}}$
613 and proceed to its estimation with a sample size $N = 10^4$. The reader is referred to [26, Section 3] for the
614 definition of this index $S_{2,CVM}^{\mathbf{u}}$ and its Pick-Freeze estimator together with their properties. The results
615 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.

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

623 As said in the previous paragraph, when one is interested in the choice of the input distributions of
624 X_1 , X_2 , and X_3 , the first row in Table 1 shows that each choice is equally important. Nevertheless,
625 performing a classical GSA on the inputs using the Cramér-von-Mises index for example, we see, in Table
626 3, that the index related to X_3 is more than twice as important as X_1 and X_2 (when considering only
627 first-order effects). Hence, here, the classical GSA largely differs numerically from a second-level SA as
628 expected.

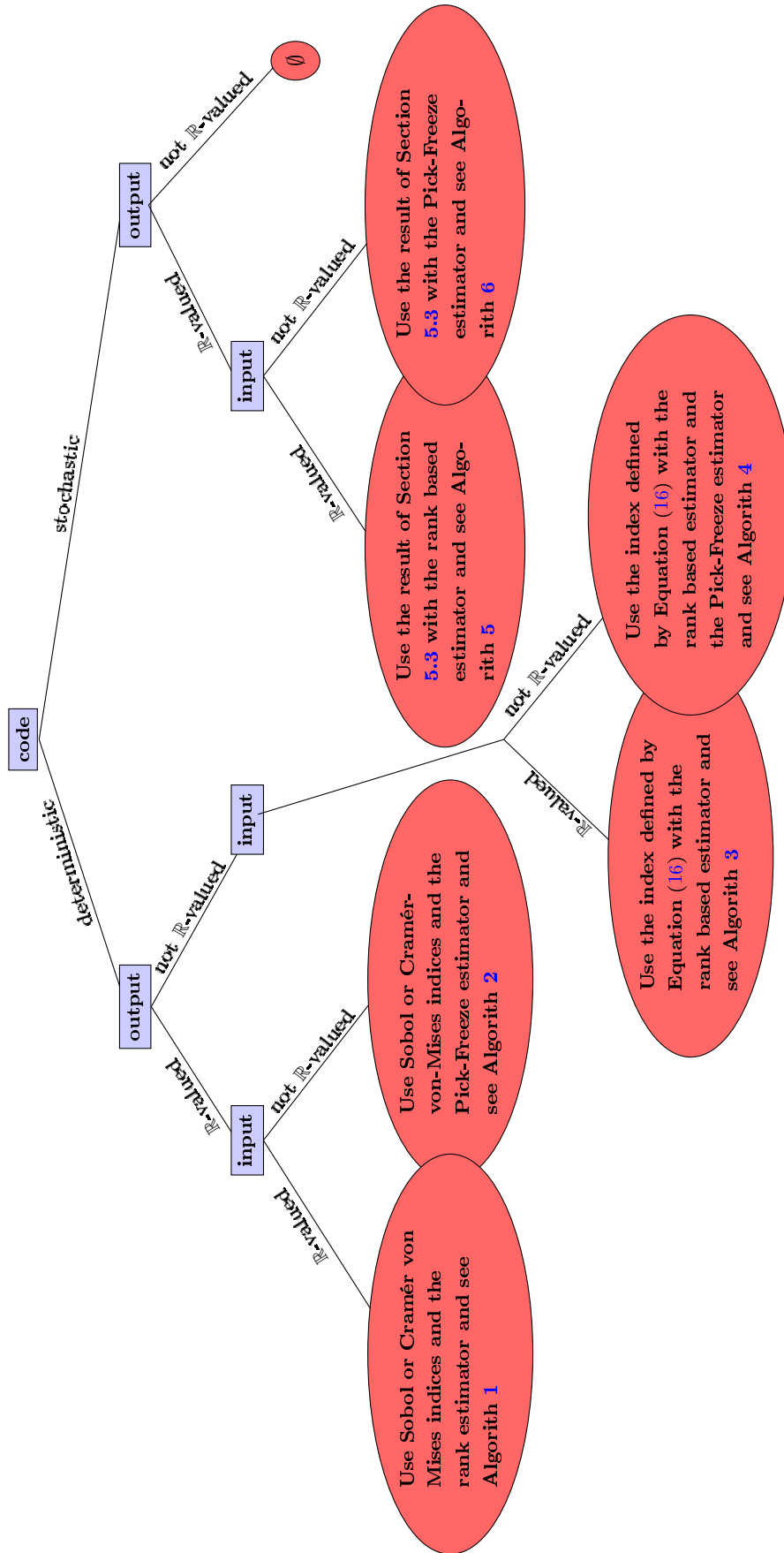
629 7 Synthesis and practical advices

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

633 7.1 First-level sensitivity analysis for the practitioners

634 7.1.1 The road map

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



641

642

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 $\hat{S}_{\text{Rank}}^1 = \frac{\frac{1}{N} \sum_{j=1}^{N-1} Z_{(j)} Z_{(j+1)} - (\frac{1}{N} \sum_{j=1}^N Z_j)^2}{\frac{1}{N} \sum_{j=1}^{N-1} Z_j^2 - (\frac{1}{N} \sum_{j=1}^N Z_j)^2}$.

645

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 $\hat{S}_{\text{PF}}^1 = \frac{\frac{1}{N^*} \sum_{j=1}^{N^*} Z_j Z_j^{(1)} - (\frac{1}{N^*} \sum_{j=1}^{N^*} (Z_j + Z_j^{(1)})/2)^2}{\frac{1}{2N^*} \sum_{j=1}^{N^*} (Z_j^2 + (Z_j^{(1)})^2) - (\frac{1}{2N^*} \sum_{j=1}^{N^*} (Z_j + Z_j^{(1)})^2)}$.

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 $\hat{S}_{2,\text{GMS,PF}}^1$
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 $\hat{S}_{2,\text{Univ,PF}}^1$
end if

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 $\hat{S}_{2,W_2,\text{Rank},n}^1$

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 $\hat{S}_{2,W_2,\text{PF},n}^1$

646 7.2 Second-level sensitivity analysis for the practitioners

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

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 $\hat{S}_{2,W_2,\text{PF},n}^1$

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 $\hat{S}_{2,W_2,\text{PF},n}^1$

648 8 Conclusion

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

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

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666 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 ,

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

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

669 *Proof of Proposition 5.1.* One has

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

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

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

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

Since $(U_{l,N,n} - U_{l,N,n})$, 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

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

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

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

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 Ω . 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:

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

676 It remains to choose first, $\delta(N)$ so that $\mathbb{P}(\Delta(N)^c) = o\left(\frac{1}{\sqrt{N}}\right)$ and second, n such that $\mathbb{E}[W_q(\mu_{X_1}, \mu_{X_{1,n}})] =$
677 $o(\delta(N)/\sqrt{N})$. Consequently, $\sqrt{N}(U_{1,N,n} - U_{1,N}) = o_{\mathbb{P}}(1)$. Analogously, one gets $\sqrt{N}(U_{l,N,n} - U_{l,N}) =$
678 $o_{\mathbb{P}}(1)$ for $l=2, 3$ and 4 . □

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