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SENSITIVITY ANALYSIS WITH CORRELATED INPUTS: COMPARISON OF INDICES FOR THE LINEAR CASE.

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The objective of a global sensitivity analysis is to provide indices to rank the importance of each and every system inputs when considering the impact on a given system output. This paper discusses few of the methods proposed throughout the literature when dealing with a linear model for which part or all the input variable can not be considered independent. The aim is here to review methods from the late eighties in order to compare them to more recent developments, by investigating their underlying hypothesis, cost (in term of resources usage) and results. This paper focuses on the case where no assumption on the knowledge of the probability density functions, assuming that the analysis can be done from a provided sample, without the use of refined techniques which would require a dedicated surrogate model generation. After an introduction of the general problem, as often discussed in the independent approach, a review of solutions not solely relying on the variance decomposition is presented, along with their underlying hypothesis. A protocol is proposed, based on a statistical approach relying on random correlation matrix generation, to test and compare all methods with an increasing complexity, step-by-step procedure. Finally, dependencies with respect to parameters defining the problem, such as the input space size, the sample size, the nature of the input laws are tested before drawing conclusions on the methods and their usefulness.

KEY WORDS: *Uncertainty quantification, Stochastic sensitivity analysis, Random variables, Correlated models*

1. INTRODUCTION

Many research or engineering problems can be mathematically modelled as an input-output system structure linked together by a deterministic relation $f : \mathcal{X} \rightarrow \mathcal{Y}$, such as

$$\mathbf{Y} = f(\mathbf{X}) = f(X_1, \dots, X_{n_X}) \quad (1)$$

$$= \sum_{u \in \mathcal{S}} f_u(\mathbf{X}_u), \quad (2)$$

where x_i is the i th element of the input space \mathcal{X} whose dimension is set to be n_X ($\mathcal{X} \subseteq \mathbb{R}^{n_X}$). For the sake of simplicity, without loss of genericity, the output of this system is set to be a scalar (meaning that $\mathbf{Y} = Y \in \mathcal{Y} \in \mathbb{R}$). This relation can also be written as done in equation (2) using a multi-index of elements of $\llbracket 1, n_X \rrbracket$: considering \mathcal{S} the collection of subset of $\llbracket 1, n_X \rrbracket$ (and $\mathcal{S}^* = \mathcal{S} \setminus \{\emptyset\}$), for all $u \in \mathcal{S}$, one can write \mathbf{x}_u the variables in \mathbf{x} whose indices are in u . In order to complete this picture, \mathbf{x}_{-u} will be used to denote the complementary subset of \mathbf{x} whose variables are not in u while for all $i \in u$, \mathbf{x}_{u-i} will denote \mathbf{x}_u without its element x_i . Finally, the collection of subset of \mathcal{S} that does not include the i th input variable is written $\mathcal{S}_{-i} = \mathcal{S} \setminus \{i\}, \forall i \in \llbracket 1, n_X \rrbracket$.

Since there might be uncertainty about the true input values of the system structure, leading to potentially large fluctuations in the output response, it is common to treat the elements of the input space \mathcal{X} (the set of $\{X_i\}_{1 \leq i \leq n_X}$, called hereafter input variables, or inputs) as random variables. This can, for instance, be done in the probabilistic framework by associating a given (well chosen) probability density function (PDF) for each and every input variable. Even though this is not the only possible approach (one can consider imprecise probabilities [1], the theory of belief functions [2]...) it is a widespread one, that, along with all the others, turns the output response of our system into a random variable, later referred to as output variable, or the output. Characterising the empirical output distribution is the purpose of uncertainty analysis, while asserting the relative importance of each and every inputs on the system output is the sole objective of sensitivity analysis.

Unlike a local sensitivity analysis that focuses on the vicinity of a chosen “working point” \mathbf{x}_0 , the global sensitivity analysis (GSA) aims at establishing the rank of importance of inputs while being truthful in the full input space \mathcal{X} . To tackle this, it is common to consider variance-based methods, one of its most famous representative, in the uncertainty community, being the “so-called” Sobol indices. Its first version has been introduced by Sobol [3] and later completed by Homma and Saltelli [4] in order to form a couple of indices for every input, whose derivation is based on the analysis of variance (ANOVA) decomposition of the output variable’s variance. The main limitation of

1 this method, in order to ensure the uniqueness of the ANOVA decomposition, is a strong hypothesis on the the input
2 variables: they have to be independent.

3 Unfortunately, in many fields such as nuclear engineering [5], mechanical engineering [6], extinction risks as-
4 sessments in biology [7], just to name a few, input variables are dependent. The dependency can arise as the result
5 of constraints in the inputs space due to properties of inputs (*i.e.* composition constraints in material science for in-
6 stance) or because of the complex input structure where inputs may be themselves the output of some other model or
7 experiment [8]. In these cases the simple description of input uncertainty through independent marginal distribution
8 functions is not adequate. Correct procedures require sampling from the joint and conditional distribution functions
9 of inputs.

10 The purpose of this paper is to review and compare some ways to perform GSA when no information are known
11 on either the joint or the conditional probability density functions (for a more exhaustive review of GSA methods,
12 see [9]). In order to circumvent this, there have been many developments, in various fields of research, sometimes
13 limiting the investigation to the linear case for the sake of simplicity. This is the starting point of this paper: using
14 methods that allow estimation of sensitivity indices from a provided sample (disregarding whether it might arise
15 from simulation or experimental data) without any specific information on the inputs supposed behaviour but the
16 fact that our system response is well suited to be a linear combination of all the inputs (independent or not). To be
17 more generic, investigations are done on various parameters such as n_X the dimension of \mathcal{X} , the size of the provided
18 sample n_S . . . In order to be as generic as possible, to be able to probe low n_S cases for instance, only methods without
19 explicit construction of a dedicated surrogate model are considered.

20 After setting the mathematical conventions and notations that will be used throughout this paper in § 1.1, a
21 reminder of the concept of global sensitivity analysis from the high dimensional model representation (HDMR)
22 decomposition is provided in § 1.2. The methods chosen in this paper (Shapley value, the Lindeman, Merenda and
23 Gold or General Dominance indices, Johnson's Relative weight, the Structural and Correlative Sensitivity Analysis,
24 Sobol indices) are later introduced in § 2, bearing in mind that the resulting indices might be evaluated in different
25 ways given the context and the chosen algorithm. These methods are then tested in § 3, using a dedicated practical
26 protocol introduced in § 3.1, at first to throw a glance at the indices behaviour in § 3.2, but also to test their robustness
27 against n_S , n_X , few properties of the input PDF along with the resource consumption, in § 4. A discussion in which
28 these results are compared, both for their results and their implementation, is kept for § 5 before concluding this paper.

1 1.1 Mathematical conventions

2 The following notation conventions will be used when dealing with generic methodology description.

3 Upper case letters represent random variable, the output can then be written $Y = f(X)$, while upper case bold
4 letters represent matrices, so the following notation, $\mathbf{Y} = f(\mathbf{X})$, will now described an output sample generated from
5 an input design-of-experiments for instance.

6 Lower case letters are realisation of a random variable: $y = f(\mathbf{x})$ is a realisation of the output variable when
7 considering a specific realisation of the input vector \mathbf{x} . With the index, x_i represents the i th coordinate ($i = 1, \dots, n_X$)
8 of a realisation $\mathbf{x} = (x_1, \dots, x_{n_X})$. It is a realisation of the i th random variable X_i .

9 As already discussed, $\{X_i\}_{1 \leq i \leq n_X}$ are the input variables of our system, $Y = f(X)$ is its output variable, for
10 $f : \mathbb{R}^{n_X} \rightarrow \mathbb{R}$ a L^2 function, assuming $\text{Var}(Y) \neq 0$. Using the notation introduced previously for the subset $u \in \mathcal{S}$,
11 few more conventions are introduced:

- 12 • V_u is the variance of the expectation of Y conditioned to X_u , denoted

$$V_u = \text{Var}(\mathbb{E}(Y|X_u)). \quad (3)$$

- 13 • \mathbb{E}_u is the expectation of the variance of Y conditioned to X_u , denoted

$$\mathbb{E}_u = \mathbb{E}(\text{Var}(Y|X_u)). \quad (4)$$

- 14 • R_u^2 is the coefficient of determination of Y , when considered only as a function of X_u , denoted

$$R_u^2 = R_{y=f(X_u)}^2. \quad (5)$$

15 The underlying hypothesis used throughout this paper is the assumption that the system output can be written as
16 a linear combination of the input variables, so

$$Y = X\boldsymbol{\beta}, \quad (6)$$

17 where $\boldsymbol{\beta}$ is a vector of n_X -constant coefficients*. Finally, the theoretical correlation matrix of the (X, Y) system,
18 or the empirical one computed from a randomly-drawn sample (\mathbf{X}, \mathbf{Y}) , will be denoted $\boldsymbol{\Gamma}$ (respectively $\hat{\boldsymbol{\Gamma}}$) and two

*for the sake of simplicity, without genericity loss, $\beta_0 = \mathbb{E}(Y)$ can be set to 0

ways of splitting it by blocks will be used. On the one hand, the first one (first part of equation (7)), is splitting the input and output. On the other hand, the second one (second part of equation (7)) splits it into three parts: a subset u of the inputs ($u \in \mathcal{S}$), its complementary, denoted $-u$ and the output.

$$\mathbf{\Gamma} = \left(\begin{array}{c|c} \mathbf{\Gamma}_{XX} & \mathbf{\Gamma}_{XY} \\ \hline \mathbf{\Gamma}_{YX} & \mathbf{\Gamma}_{YY} \end{array} \right) = \left(\begin{array}{cc|c} \mathbf{\Gamma}_{uu} & \mathbf{\Gamma}_{u-u} & \mathbf{\Gamma}_{uY} \\ \mathbf{\Gamma}_{-uu} & \mathbf{\Gamma}_{-u-u} & \mathbf{\Gamma}_{-uY} \\ \hline \mathbf{\Gamma}_{Yu} & \mathbf{\Gamma}_{Y-u} & \mathbf{\Gamma}_{YY} \end{array} \right). \quad (7)$$

Finally, a large part of this paper will focus on a dichotomous approach, considering either the uncorrelated case, implying that $\mathbf{\Gamma}_{XX} = \mathbf{1}_{n_X}$ (there are no statistical correlation between all inputs two-by-two) or, on the contrary, the correlated case, when $\mathbf{\Gamma}_{XX} \neq \mathbf{1}_{n_X}$.

1.2 Decomposition of the system function

Many of the methods introduced later-on are using a decomposition of the system function, assuming that it is integrable in its definition domain, into an ensemble of sub-functions (hereafter referred to as summands) which can be written as such [10]

$$y = f_0 + \sum_{i=1}^{n_X} f_i(x_i) + \sum_{1 \leq i < j \leq n_X} f_{i,j}(x_i, x_j) + \dots + f_{x_1, x_2, \dots, x_{n_X}}(x_1, x_2, \dots, x_{n_X}). \quad (8)$$

Each and every terms are functions of the different interaction degrees of the inputs $\{x_i\}_{1 \leq i \leq n_X}$, leading to a total of $2^{n_X} - 1$ summands on top of the constant term f_0 . This decomposition is also referred to as the high dimensional model representation (HDMR [11]) and is not unique since there might be an infinity of choice to define the summands. Even though this approach has been combined as of 1948 by Hoeffding [10] with the analysis of variance approach (first introduced by Fisher [12] and commonly referred to as ANOVA, it has been popularised with the orthogonality constraints used to ensure its uniqueness. In 1993, Sobol [3] defined these orthogonality constraints (in its original case where $\mathcal{X} = [0, 1]^{n_X}$) as

$$\int f_u(\mathbf{x}_u) dx_i = 0 \quad \forall u \in \mathcal{S}, \quad \forall i \in u. \quad (9)$$

As a direct consequence, all the summands are orthogonal, meaning that

$$\mathbb{E}[f_u(\mathbf{x}_u) f_v(\mathbf{x}_v)] = 0, \quad \forall u \neq v \in \mathcal{S}. \quad (10)$$

1 Finally, if the function f is square integrable ($f \in L^2$), Sobol [3] introduces the following quantities denoted D_u ,
2 defined as:

$$D_u = \int f_u^2(\mathbf{x}_u) d\mathbf{x}_u, \quad \forall u \in \mathcal{S}, \quad (11)$$

3 and shows that they are all finite. Once this procedure is applied to all summands of equation (8), on both sides, it
4 leads in the functional ANOVA decomposition, written as

$$\text{Var}(f(\mathbf{x})) = \mathbb{E}[(f(\mathbf{x}) - f_0)^2] = \sum_{u \in \mathcal{S}^*} \mathbb{E}[f_u(\mathbf{x}_u)^2] = \sum_{u \in \mathcal{S}^*} \text{Var}(f_u(\mathbf{x}_u)). \quad (12)$$

5 Suppose now that $(\mathbb{R}^{n_x}, \mathcal{B}(\mathbb{R}^{n_x}), \mu)$ is a probability space where \mathbb{R}^{n_x} is the sample space, $\mathcal{B}(\mathbb{R}^{n_x})$ is the
6 Borel σ -algebra and μ the probability measure with $d\mu = p(\mathbf{x})d\mathbf{x}$, where $p_{\mathbf{x}}$ is the probability density function of
7 \mathbf{x} . This decomposition has been further investigated and generalised by Li *et al.* [13] with the introduction of the
8 hierarchical orthogonal condition (based on the work from Stone [14] and Hooker [15]), providing a criterion to
9 state that the HDMR component functions are uniquely determined. The existence of this decomposition is formally
10 demonstrated, under suitable conditions on the joint distribution function of the input variables, by Chastaing *et*
11 *al.* [16] resulting in the HOFD: the hierarchically orthogonal functional decomposition. The functional expansion
12 introduced in equation (2) is then still valid, with the summands being defined as

$$f_u(\mathbf{x}_u) = \int f(\mathbf{x}) p_{-u}(\mathbf{x}_{-u}) d\mathbf{x}_{-u} - \sum_{v \subset u} f_v(\mathbf{x}_v) - \sum_{\substack{u \not\subset v \in \mathcal{S} \\ u \cap v \neq \emptyset}} \int f_v(\mathbf{x}_v) p_{-u}(\mathbf{x}_{-u}) d\mathbf{x}_{-u}, \quad u \in \mathcal{S}. \quad (13)$$

13 This definition is given providing that all summands fulfil the relaxed vanishing condition

$$\int f_u(\mathbf{x}_u) p_u(\mathbf{x}_u) dx_i = 0, \quad \forall u \in \mathcal{S}^* \quad \text{and} \quad i \in u, \quad (14)$$

14 or equivalently the hierarchical orthogonal condition

$$\mathbb{E}[f_u(\mathbf{x}_u) f_v(\mathbf{x}_v)] = 0, \quad \forall u \in \mathcal{S}^* \quad \text{and} \quad \forall v \subset u. \quad (15)$$

15 This statement means that a higher order component function is only required to be orthogonal to all nested lower
16 order component functions whose variables are a subset of those in the higher order component function. Further
17 details (or ways to introduce this decomposition) can be found in the literature [17–19].

1 Since the HDMR component functions with correlated variables are not mutually orthogonal, the standard vari-
 2 ance decomposition of the unconditional variance of the output does not hold. A new covariance decomposition of
 3 the unconditional variance of the output was introduced [16,17]

$$\begin{aligned}
 \text{Var}(f(\mathbf{x})) &= \mathbb{E}[(f(\mathbf{x}) - f_0)^2] = \mathbb{E}\left[\sum_{u \in \mathcal{S}^*} f_u(\mathbf{x}_u)(f(\mathbf{x}) - f_0)\right] \\
 &= \sum_{u \in \mathcal{S}^*} \text{Cov}(f_u(\mathbf{x}_u), f(\mathbf{x})) = \sum_{u \in \mathcal{S}^*} \text{Cov}\left(f_u(\mathbf{x}_u), \sum_{v \in \mathcal{S}^*} f_v(\mathbf{x}_v)\right) \\
 &= \sum_{u \in \mathcal{S}^*} \left[\text{Var}(f_u(\mathbf{x}_u)) + \text{Cov}\left(f_u(\mathbf{x}_u), \sum_{\substack{v \in \mathcal{S}^* \\ u \neq v}} f_v(\mathbf{x}_v)\right) \right]. \tag{16}
 \end{aligned}$$

4 This summarises briefly the theoretical development on the breakdown of a function into a finite number of
 5 summands, from a very specific decomposition in 1948 [10] to its more recent generalised presentation even in
 6 dependent case. Several of the methods tested in this paper partly rely on the equation introduced beforehand.

7 1.3 Independent variables

8 This last section is briefly reminding concepts of global sensitivity analysis used in the independent case. It is not
 9 meant to be neither a reference nor an exhaustive list, as many articles and books are compiling and discussing these
 10 aspects [20–24], but some of these quantities are mentioned later-on in § 2.

11 In the general independent case, two common sensitivity indices can be defined, $\forall i \in \llbracket 1, n_X \rrbracket$, as

$$S_i^S = \frac{\text{Var}(E(Y|X_i))}{\text{Var}(Y)} \quad \text{and} \quad S_{T_i} = 1 - \frac{\text{Var}(E(Y|X_{\sim i}))}{\text{Var}(Y)}, \tag{17}$$

12 where $\sim i$ represents all the input variables but the i th one. These indices are respectively called the *first-order*
 13 *sensitivity index* $S_i^{S^\dagger}$ and the *total-order sensitivity index* S_{T_i} (but it is not unusual to see names like *first-order Sobol*
 14 *index* and *total-order Sobol index*). The former one has been introduced by Sobol [3], as it ensues from equation (12),
 15 once both sides are divided by $\text{Var}(f(\mathbf{x}))$, transforming it into

$$1 = \sum_{u \in \mathcal{S}^*} S_u^S = \sum_{u \in \mathcal{S}^*} \frac{\text{Var}(f_u(\mathbf{x}_u))}{\text{Var}(Y)}, \tag{18}$$

[†]the superscript S stands for Sobol and is used here to prevent from any misleading in order not to state that one index should be written as S_i that might be understood as a premium index.

1 where the f_u are expressed as $f_u = \mathbb{E}(Y|\mathbf{X}_u) - \sum_{v \subset u} f_v$. The *first-order* index only describes the impact of the
 2 input X_i on the output, it does not take into account the possible interaction between inputs. This name implies that
 3 there might be higher-order indices coping for the crossed impact of X_i with any other set of inputs. Once all these
 4 higher-order indices are considered, meaning the full set of $2^{n_X} - 1$ values to be computed (the cardinal of \mathcal{S}^*), it
 5 provides a perfect breakdown of the output variance. A general form for these indices can be written as

$$S_u^S = \frac{1}{\text{Var}(Y)} \sum_{v \subseteq u} (-1)^{|u|-|v|} V_v, \quad \forall u \in \mathcal{S}^*. \quad (19)$$

6 where $|u|$ and $|v|$ represent respectively the cardinal of u and the cardinal of any of its subset v . Even though it is
 7 possible to find another general form for the Sobol indices, sometimes referred to as “closed Sobol indices” [25],
 8 defined by $S_u^{cl} = V_u/\text{Var}(Y)$ which assess the total impact of the inputs $(X_i)_{i \in u}$, this paper will focus on the one
 9 written in equation (19). In order to prevent from having to estimate all these indices, Homma and Saltelli introduce
 10 the *total-order* index [4], shown as the right-hand part of equation (17), which is equivalent to sum all the indices that
 11 would include the input i in consideration, so in the general form:

$$S_{T_i} = \sum_{u \subseteq (\{i\} \cap \mathcal{S} \setminus \{i\})} S_u^S. \quad (20)$$

12 1.3.1 Special case of the linear model

13 Whatever the problem may be, it is possible to measure the linear correlation coefficient of the i th input with the
 14 given output, also named *Pearson*, or *Bravais-Pearson* coefficient [26], defined, $\forall i \in \llbracket 1, n_X \rrbracket$, as

$$\rho_i = \rho(X_i, Y) = \frac{\text{Cov}(X_i, Y)}{\sqrt{\text{Var}(X_i) \text{Var}(Y)}}. \quad (21)$$

15 Another estimator currently used is the standard regression coefficient (*SRC*), also called the standardised coef-
 16 ficient [27], which is computed using the β coefficients (the regression coefficients that multiply the input variables
 17 in the linear regression form introduced in equation (6)). It can indeed be written, $\forall i \in \llbracket 1, n_X \rrbracket$ as

$$SRC_i = SRC(X_i, Y) = \beta_i \sqrt{\frac{\text{Var}(X_i)}{\text{Var}(Y)}}. \quad (22)$$

1 In the simple linear and independent case, it is possible to link all these coefficients by the following relation

$$\rho_i^2 = SRC_i^2 = S_i^S = S_{T_i}, \quad \forall i \in \llbracket 1, n_X \rrbracket. \quad (23)$$

2 Since the same quantity can be estimated in various ways, following Occam's razor principle implies that the simplest
3 method is the best solution. If the independence hypothesis has to be dropped, meaning in the context of this paper
4 that $\Gamma_{XX} \neq \mathbf{1}_{n_X}$ but is nonetheless invertible, the ANOVA decomposition as introduced in equation (18) can not
5 hold. New sensitivity indices should be found in this general case.

6 2. THEORETICAL DESCRIPTION OF THE CONSIDERED METHODS

7 This section is providing a description of the methods proposed in order to get a quantitative estimation of the impact
8 of an input variable on the output of the system, in a linear-dependent case. To prevent from drawing any conclusion
9 on their usefulness, they are discussed in order of first appearance in the scientific literature.

10 2.1 Shapley value

11 2.1.1 Historical formulation

12 The concept of Shapley value has been introduced in the game theory context, when considering the case of a coalitional game, *i.e.* a couple (n_X, c) where

- 14 • n_X is the number of players;
- 15 • c is the characteristic function, $c : \mathcal{S} \rightarrow \mathbb{R}$ with $c(\emptyset) = 0$ and $\forall A \subset B, c(A) \leq c(B)$.

16 The characteristic function c has the following meaning: if u is a coalition of players, then $c(u)$, called the
17 worth of coalition u , describes the total expected sum of payoffs the members of u can obtain through cooperation.
18 Shapley [28] proposed a way to distribute the total gains to the players, assuming that they all collaborate. It is a "fair"
19 distribution in the sense that it is the only distribution with certain desirable properties listed below. According to the
20 Shapley value, the amount received by player i , in a coalitional game (n_X, c) , is

$$\varphi_i := \frac{1}{n_X} \sum_{u \subset \mathcal{S}_i} \binom{n_X - 1}{|u|}^{-1} (c(u \cup \{i\}) - c(u)). \quad (24)$$

21 The main properties of the Shapley values are the following ones:

- 1 • efficiency: $\sum_{i=1}^{n_X} \varphi_i = c(\mathcal{S})$
- 2 • symmetry: if i and j are two equivalent players, meaning $c(u \cup \{i\}) = c(u \cup \{j\}), \forall u \subset \mathcal{S} \setminus \{i, j\}$, then
- 3 $\varphi_i = \varphi_j$
- 4 • additivity: combining two coalitional games (n_X, c) and (n_X, d) , results in a new coalitional game $(n_X, c + d)$
- 5 where $(c + d)(u) = c(u) + d(u), \forall u \subset \mathcal{S}$ and $\varphi_i(c + d) = \varphi_i(c) + \varphi_i(d), \forall i \in \llbracket 1, n_X \rrbracket$.
- 6 • nullity: $\varphi_i = 0$ for a null player. A player i is null if $c(u \cup \{i\}) = c(u), \forall u \subset \mathcal{S}_{-i}$
- 7

8 The concept of Shapley value has been used in economy for sometimes [29–31] but has only recently been

9 brought up in the uncertainty community.

10 2.1.2 Formulation for sensitivity analysis

11 Given the convention above and bearing in mind the general formula for Sobol indices given in equation (19),

12 Owen [32] has defined the Shapley value, in the sensitivity analysis framework, for a given input $i \in \llbracket 1, n_X \rrbracket$,

13 as:

$$\eta_i := \frac{1}{n_X \text{Var}(Y)} \sum_{u \subset \mathcal{S}_{-i}} \binom{n_X - 1}{|u|}^{-1} (V_{u \cup \{i\}} - V_u). \quad (25)$$

14 Based on this definition, Shapley values have been exhibited as proper sensitivity indices in [25] when the inputs are

15 dependent. There is indeed only one value for each input variable, this value always lies in $[0, 1]$ and their sum equals

16 to one, once all input variables are considered (even with correlation).

17 2.1.3 Linear Gaussian case

18 In the case where $X \sim \mathcal{N}(\mu, \mathbf{\Gamma}_{XX})$, assuming $\mu = 0$, for the sake of simplicity without genericity loss, one can

19 rewrite the sensitivity indices, as they can be calculated explicitly. Sobol' indices, for instance, can be expressed with

20 expectations of conditional variances [33], as done below:

$$S_u^S := \frac{(-1)^{|u|}}{\text{Var}(Y)} \sum_{v \subset u} (-1)^{|v|+1} \mathbb{E}_v, \forall u \neq \emptyset, \quad (26)$$

1 which leads to a new expression for the i th Shapley value [34]:

$$\eta_i := \frac{1}{n_X \text{Var}(Y)} \sum_{u \subset C-i} \binom{n_X - 1}{|u|}^{-1} (\mathbb{E}_u - \mathbb{E}_{u \cup \{i\}}). \quad (27)$$

Using the Gaussian framework, one can express the conditional variance as shown here [35]:

$$\begin{aligned} V_u &= \text{Var}(X_{-u} \beta_{-u} | X_u) \\ &= \beta_{-u}^T (\Gamma_{-u,-u} - \Gamma_{-u,u} \Gamma_{u,u}^{-1} \Gamma_{u,-u}) \beta_{-u}. \end{aligned} \quad (28)$$

2 This expression is constant for a given subset u , so it is equal to its expectation which provide a way to compute
3 all Shapley values. A step-by-step procedure, called *LG-Shapley*, is proposed by Broto *et al.* in [33].

4 **2.2 LMG or General Dominance indices**

5 Another way to quantify the impact of correlated inputs seemed to have arisen in a book by Lindeman, Merenda
6 and Gold (LMG) [36] (but as stated in [35], this reference is very difficult to obtain). The rest of this paper uses
7 the formalism provided by Budescu *et al.* [37,38] that defines the General Dominance (GD) indices as the average
8 increment in the coefficient of determination associated with the predictor X_i in all possible sub-models. Bearing in
9 mind that this method is also discussed as the LMG one (*c.f.* [36]), the resulting indices will hereafter be called the
10 LMG-GDI.

11

12 The idea is to call D_i^k the average increase in the coefficient of determination due to adding X_i to the $\binom{n_X-1}{k}$
13 different sub-models, each with k variables, $k = 0, \dots, (n_X - 1)$; thus

$$D_i^k = \sum_{u \subseteq S-i, |u|=k} \binom{n_X - 1}{k}^{-1} (R_{u \cup i}^2 - R_u^2). \quad (29)$$

14 Then, another coefficient D_i is obtained by averaging the D_i^k across all S sub-model sizes. This can be written as

$$\begin{aligned} D_i &= \frac{1}{n_X} \sum_{k=0}^{n_X-1} D_i^k \\ &= \frac{1}{n_X} \sum_{u \subset C-i} \binom{n_X - 1}{|u|}^{-1} (R_{u \cup i}^2 - R_u^2). \end{aligned} \quad (30)$$

1 Finally the coefficient of determination can be computed through the multiple correlation equation, which is
 2 shown below when considering, for illustration purpose, the full model (under linear Gaussian hypothesis):

$$R^2 = \mathbf{\Gamma}_{YX} \mathbf{\Gamma}_{XX}^{-1} \mathbf{\Gamma}_{XY}. \quad (31)$$

3 One can also express the R_u^2 formula (*c.f.* equation (5)) using the second form of the correlation matrix by block
 4 introduced in equation (7), which represents the quality of the regression if it were to be done only using input
 5 variables in the subset $u, \forall u \subset \mathcal{S}$.

$$R_u^2 = \mathbf{\Gamma}_{Yu} \mathbf{\Gamma}_{uu}^{-1} \mathbf{\Gamma}_{uY}. \quad (32)$$

6 The complexity in terms of number of configurations is exactly the same as the one for the Shapley value.

7 **2.3 The relative weight method**

8 The idea here is very similar to the standard regression coefficients introduced in § 1.3, as one will use orthogonal
 9 transformation to represent our data, with dependent inputs. The method has been introduced by Johnson [39] and its
 10 principle can be split into three steps:

- 11 • transform the dependent input variables X through a linear transformation into Z so that $Z^T Z = \mathbf{1}_{n_X}$;
- 12 • compute sensitivity index of the output Y with respect to Z ;
- 13 • reconstruct the sensitivity index of the output Y with respect to the component of X .

14 Practically, the method proposed in [39] relies on the singular value decomposition of \mathbf{X} , written as $\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$
 15 for which \mathbf{U} contains the eigenvectors of $\mathbf{X}\mathbf{X}^T$, \mathbf{V} contains the eigenvectors of $\mathbf{X}^T\mathbf{X}$ and $\mathbf{\Sigma}$ is a diagonal matrix
 16 containing the singular values of \mathbf{X} (the squared form of the singular values corresponds to the eigenvalues of $\mathbf{X}^T\mathbf{X}$).
 17 From there, the best-fitting orthogonal approximation of \mathbf{X} can be obtained (see Johnson [40] for the demonstration)
 18 as

$$\mathbf{Z} = \mathbf{U}\mathbf{V}^T. \quad (33)$$

The second steps consists in regressing \mathbf{Y} onto \mathbf{Z} , which is obtained by

$$\begin{aligned}\beta^* &= (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T \mathbf{Y} = (\mathbf{V} \mathbf{U}^T \mathbf{U} \mathbf{V}^T)^{-1} \mathbf{V} \mathbf{U}^T \mathbf{Y} \\ &= \mathbf{V} \mathbf{U}^T \mathbf{Y}.\end{aligned}\quad (34)$$

The squared elements of β^* represent the proportion of predictable variance in Y accounted for by the $(Z_i)_{i=1, \dots, p}$, but in the case where two or more original variables are highly correlated, the Z variables are not a close representation of the X ones. To take this into account, Johnson propose to regress \mathbf{X} onto \mathbf{Z} , leading to another set of weights defined as:

$$\begin{aligned}\Lambda^* &= (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T \mathbf{X} = (\mathbf{V} \mathbf{U}^T \mathbf{U} \mathbf{V}^T)^{-1} \mathbf{V} \mathbf{U}^T \mathbf{U} \Sigma \mathbf{V}^T \\ &= \mathbf{V} \Sigma \mathbf{V}^T.\end{aligned}\quad (35)$$

1 From there, the variance of Y explained by X_i can be denoted as Δ_i^2 and estimated from the following formula

$$\Delta_i^2 = \sum_{j=1}^{n_X} \lambda_{ij}^{*2} \beta_j^{*2}, \quad (36)$$

2 where $\lambda_{ij}^* = (\Lambda^*)_{ij}$, $\forall i, j \in \llbracket 1, n_X \rrbracket$ and bearing in mind that

$$\text{Var}(Y) = \sum_{i=1}^{n_X} \Delta_i^2 = \sum_{i=1}^{n_X} \beta_i^{*2}. \quad (37)$$

3 The resulting sensitivity indices are written

$$\Delta_i^* = \frac{\Delta_i^2}{\text{Var}(Y)}, \quad 1 \leq i \leq n_X, \quad (38)$$

4 and are commonly referred to as relative weights, or Johnson's relative weights.

5 2.4 The variance-covariance approach

6 As stated in § 1.2, the decomposition into a finite set of summands can be generalised, (as long as $f \in \mathcal{L}^2$) and leads
7 to the decomposition of the system output variance as shown in equation (16), where the breakdown is done as the
8 sum of the covariance of all summands with respect to every summands of the original function. As for the Sobol

1 indices, this decomposition can be written as a sum equals to 1 by dividing both sides as done below:

$$1 = \sum_{u \in \mathcal{S}^*} \left[\frac{\text{Var}(f_u(\mathbf{x}_u))}{\text{Var}(f(\mathbf{x}))} + \frac{\text{Cov}\left(f_u(\mathbf{x}_u), \sum_{\substack{v \in \mathcal{S}^* \\ u \neq v}} f_v(\mathbf{x}_v)\right)}{\text{Var}(f(\mathbf{x}))} \right] \quad (39)$$

$$= \sum_{u \in \mathcal{S}^*} [S_u^{Cu} + S_u^{Cc}] = \sum_{u \in \mathcal{S}^*} S_u^C. \quad (40)$$

2 Even though the decomposition of the variance remains very general as written in equation (39), a choice has
 3 been made mixing the original notation from [17] and the one from [41] mainly to prevent any kind of confusion
 4 while discussing the indices. The resulting indices are written S_u^C where the superscript C stands for covariance,
 5 implying covariance-based measurements, this notation has been added on top of the notation from the structural and
 6 correlative sensitivity analysis method (SCSA) [13,17,18] to prevent from introducing confusions with the general
 7 form of Sobol indices.

8 This sensitivity index is further split into two contribution: S_u^{Cu} and S_u^{Cc} . The former term ensues from the
 9 structural independent contribution, meaning related to $f_u(\mathbf{x}_u)$ and the marginal probability density function $p_u(\mathbf{x}_u)$
 10 only. On the other hand, the latter arises from the correlative contribution, meaning the relation between $f_u(\mathbf{x}_u)$ and
 11 the other functions along with the joint probability density function $p(\mathbf{x})$. The superscripts have been modified to Cu
 12 and Cc standing respectively for covariance-uncorrelated and covariance-correlated parts (this notation are inspired
 13 from [41] since this convention is far more transparent than the a and b ones from [13]).

14 The first interesting thing to notice about these new definitions is the fact that as soon as independent case is
 15 considered, the correlative contribution $S_u^{Cc} = 0$ leading back to $S_u^C = S_u^{Cu} = S_u^S$, which makes Sobol indices a
 16 special case of the decomposition introduced in equation (39). If the system is dependent, as discussed by Chastaing *et*
 17 *al.* [42], the value of S_i^C is the sum of two contributions which can compensate one-another leading to five possible
 18 configurations:

- 19 • when X_i has importance mainly through its dependence with other variables, it can lead to a positive or negative
 20 S_i^C value. In the former case, the other variables are reinforcing the influence of the input under consideration
 21 while in the latter case, it is relevant to wonder about its significance.
- 22 • when X_i has a significant importance on its own, it can be either reinforced or weakened by the contribution
 23 induced by the dependence;
- 24 • when S_i^C is null, either coming from negligible direct and indirect contribution, or by a complete compensation

1 of them. The former case is simple as the input can be ruled out, but on the other hand, the interpretation of the
2 latter remains an open problem.

3 As this paper focuses on the linear dependent case, the simple estimation proposed in [43] is used to provide a
4 accurate values for all contributions $(S_i^C, S_i^{Cu}, S_i^{Cv})$ which are then used as reference guides when comparing the
5 results of other methods. There are other techniques available to estimate these coefficients in the general approach:
6 Li *et al.* [17] propose to approximate these summands expanded on a suitable basis, bypassing some technical prob-
7 lem of degenerate design matrix by using a continuous descent technique through the D-MORPH algorithm. More
8 recently, Chastaing *et al.* [42] propose an alternative to directly construct a hierarchical orthogonal basis, by recur-
9 sively constructing for each summand a multidimensional basis that satisfies the hierarchical orthogonal conditions,
10 leading to a procedure named hierarchically orthogonal Gram–Schmidt (HOGS).

11 2.5 The weighted first last method

12 This method has been proposed by Wallard in his PhD manuscript [44], which also provides a far more extensive
13 review on linear dependent sensitivity analysis than this paper (however it is written in french). It is called weifila,
14 whose name stands for *weighted first last*, and it combines two measurements:

- 15 • the *first* sensitivity index, is the squared Bravais–Pearson coefficient, called ρ_i^2 in this paper (*c.f.* equation (21));
- 16 • the *last* sensitivity index, called I_i^{last} and defined as $I_i^{last} = R_{\mathcal{X}}^2 - R_{\mathcal{X}_{-i}}^2$ which quantifies the impact of X_i on
17 the coefficient of determination when added last in the model.

18 Summing each of these indices over the number of input variables leads to the definition of the first and last
19 effects, shown below

$$F = \sum_i \rho_i^2 \quad \text{and} \quad L = \sum_i I_i^{last}, \quad (41)$$

20 The weifila index ensues from these effects, so when considering a specific input variable: definition of the weifila
21 index as

$$W_i = I_i^{last} \left(\frac{|F - R^2|}{|F - L|} \right) + \rho_i^2 \left(\frac{|R^2 - L|}{|F - L|} \right). \quad (42)$$

22 This very simple index should yield $\sum_i W_i = R^2$ and should provide, according to [44], results very close to the
23 Shapley values. It might be useful to state that for an independent linear model (meaning when $R^2 = 1$), both first
24 and last index are equivalent, so are their sum, respectively F and L , both equal to 1. This shed an interesting light
25 on the weifila index for this peculiar case.

1 3. DEFINING THE PROTOCOL AND LOOKING AT DISTRIBUTIONS

2 This section introduces the framework used to test the sensitivity indices, by means of random correlation matrix
 3 generation. The procedure is discussed in § 3.1 testing different configurations in order to robustify the results and a
 4 glimpse on obtained data is shown in § 3.2 for few given configurations in order to compare the indices values.

5 3.1 Randomly-drawn correlation matrices

6 The protocol used in this paper to test all the sensitivity indices consists in generating a large number of random
 7 correlation matrices, designed not be singular[‡], in order to cover as much realistic configurations as possible. The
 8 idea behind this is to be estimate all sensitivity indices introduced previously and compared them, the covariance-
 9 based ones being used as references (since in the linear dependent case, their estimation is simple and is a perfect
 10 breakdown of the system output variance, *c.f.* § 2.4).

11 3.1.1 The Gram approach

12 The first implemented way to do this is by using a given number of centred-reduced Gaussian input variables, which
 13 can be written as fixing $X \sim \mathcal{N}(0, \Gamma_{XX})$ and $Y = \sum_i X_i$. The correlation matrix of the input variables is defined
 14 by generating a random matrix $\mathbf{A}(p, p)$ where every coefficient is drawn from a centred-reduced Gaussian law. A
 15 $\mathbf{G}(p, p)$ matrix is then generated as $\mathbf{G} = p^{-1} \mathbf{A} \mathbf{A}^T$ and from there, once the following diagonal matrix \mathbf{S} is defined
 16 as $\mathbf{S}(p, p) = \text{diag}(1./\sqrt{\mathbf{G}_{ii}})$, the random correlation matrix is obtained as:

$$\Gamma_{XX} = \mathbf{S} \mathbf{G} \mathbf{S}. \quad (43)$$

17 This procedure, sometimes referred to as the Gram one, ensures that the resulting correlation matrix is non-singular
 18 while creating dependence between the input variables, as stated by Marsaglia *et al.* [45]. Apart from the diagonal
 19 elements (always set to 1), the marginal distributions of all the correlation coefficient are the same, following a beta
 20 distribution of the form

$$\rho_{ij} \sim \beta\left(\frac{n_X - 1}{2}, \frac{n_X - 1}{2}, -1, 1\right), \quad \forall i, j \in \llbracket 1, n_X \rrbracket, i \neq j, \quad (44)$$

[‡]no input variable $i, \forall i \llbracket 1, n_X \rrbracket$ should be fully defined as a function of the other inputs, so no function g should exist so that $X_i = g(X_1, \dots, X_{i-1}, X_{i+1}, \dots, X_{n_X})$.

1 whose mean value is 0 and whose standard deviation is known to be $\sigma_\rho = n_X^{-2}$. This introduces an issue in the rep-
 2 resentativity of the possible correlation coefficients since, with increasing dimension n_X , the correlation coefficient
 3 distribution is shrinking and leaves large fraction of the possible space empty. This is illustrated in Figure 1, for four
 4 values of input space ($n_X = 4, 8, 12, 16$), with the marginal distribution on top and the bi-variate representation of
 ($\rho_{0,1}, \rho_{0,2}$).

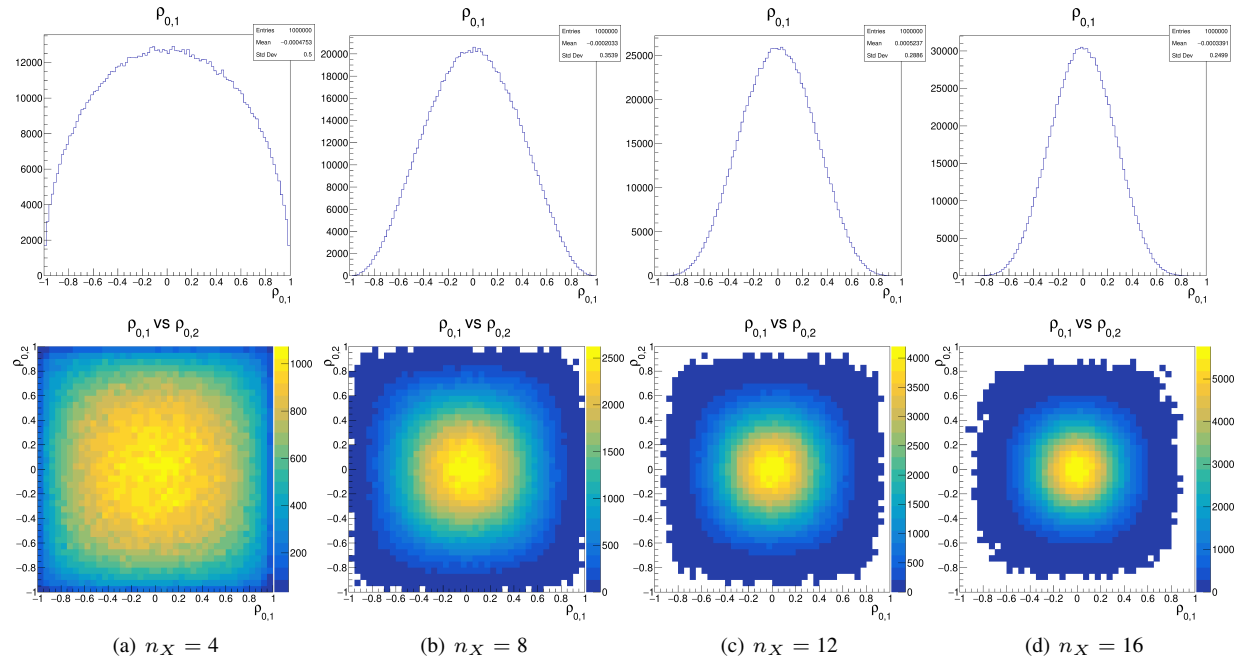


FIG. 1: Marginal distribution of the correlation coefficient (top) and bi-variate representation of $(\rho_{0,1}, \rho_{0,2})$ (bottom), when drawn with the Gram procedure with n_X is set to 4 (a), 8 (b), 12 (c) and 16 (d).

5

6 3.1.2 The Archakov-Hansen approach

7 In order to circumvent this issue, another procedure is used, referred to as the Archakov-Hansen one [46], based on the
 8 fact that there is a one-to-one correspondence between the set of $n_X \times n_X$ non-singular correlation matrices, denoted
 9 \mathcal{C}_{n_X, n_X} and \mathbb{R}^d for $d = n_X(n_X - 1)/2$. In other words, any vector $\gamma \in \mathbb{R}^d$ corresponds to a unique correlation
 10 matrix $C(\gamma) \equiv g^{-1}(\gamma)$, where this g function has been introduced in [46] as $\gamma = g(C) := \text{vecl}(\log C)$ given that the
 11 operator $\text{vecl}(\cdot)$ vectorises the lower off-diagonal elements and $\log C$ is the matrix logarithm of C . The proposal is to
 12 draw the vector of \mathbb{R}^d as a multivariate normal distribution whose dimension is wisely chosen to get a d -size sample.
 13 This can be written as $\gamma \sim \mathcal{N}(\gamma_0, I\omega_0)$ where γ_0 is a vector of constant mean value and ω_0 is a weight that is used to
 14 multiply the identity matrix I . For illustration purpose, one value of the input space has been chosen ($n_X = 12$) while

1 four values have been used both for γ_0 ($\gamma_0 = -0.6, -0.3, 0, 0.15$) and for ω_0 ($\omega_0 = 1, 1/2, 1/5, 1/25$) in order to
 2 produce a matrix of bi-variate representation of $(\rho_{0,1}, \rho_{0,2})$ gathered in Figure 2. All these distributions should be
 3 balanced with those from the Gram method, shown in Figure 1(c).

4 By varying both the γ_0 and ω_0 parameters, it is possible to change the marginal distribution of the correlation
 5 coefficient by impacting respectively its central value and its spread. From Figure 2 and comparing these distributions
 6 to the one of interest in Figure 1(c), it is fair to conclude that, even though results drawn from the Gram method should
 7 not be discarded, they should be at least completed and reinforced by the use of the Archakov-Hansen approach. It
 8 could indeed, on the one hand, ensure a better coverage of the correlation phase space and also, on the other hand,
 9 allows to focus on different part of this correlation phase space. The proposed protocol here is to use the Archakov-
 10 Hansen approach with the central configuration shown in Figure 2(b)(A) and check that all conclusions hold with the
 11 non-symmetric cases displayed in Figures 2(a)(A) and 2(c)(A).

12 3.1.3 Generalising the interpretation: groundwork and vocabulary

13 The goal of this paper is to compare the various sensitivity methods introduced in § 2, starting from a simple intro-
 14 duction in § 3.2, to more refined investigations (looking at the impact of various parameters that can influence either
 15 the sensitivity indices behaviour, the resource consumption. . .). From now on, *configuration* will refer to as a given
 16 set of these parameters value, knowing that these can be split into two kinds:

- 17 • the size of the input space n_X , the size of the sample n_S , the nature of the input variable laws (choice of pdfs
 18 for instance). . .
- 19 • the approach chosen to generate the correlation matrix.

20 While the latter kind is solely specific to our chosen methodology, the former is the problem definition: every sensi-
 21 tivity analysis is defined by these parameters along with the chosen SA method.

22 For a given configuration, two metrics are considered in order to compare the results of the sensitivity methods:

- 23 • the value of the indices themselves. The comparison from one sensitivity method to another (for a given input
 24 variable) is rather straightforward.
- 25 • the rank of the indices. By ordering the index values, for a given method, in increasing order, the rank is a
 26 number that goes from 1 to n_X which organise into a hierarchy the input variables, the smallest rank value
 27 corresponding to the input variable with the lowest impact on our quantity of interest.

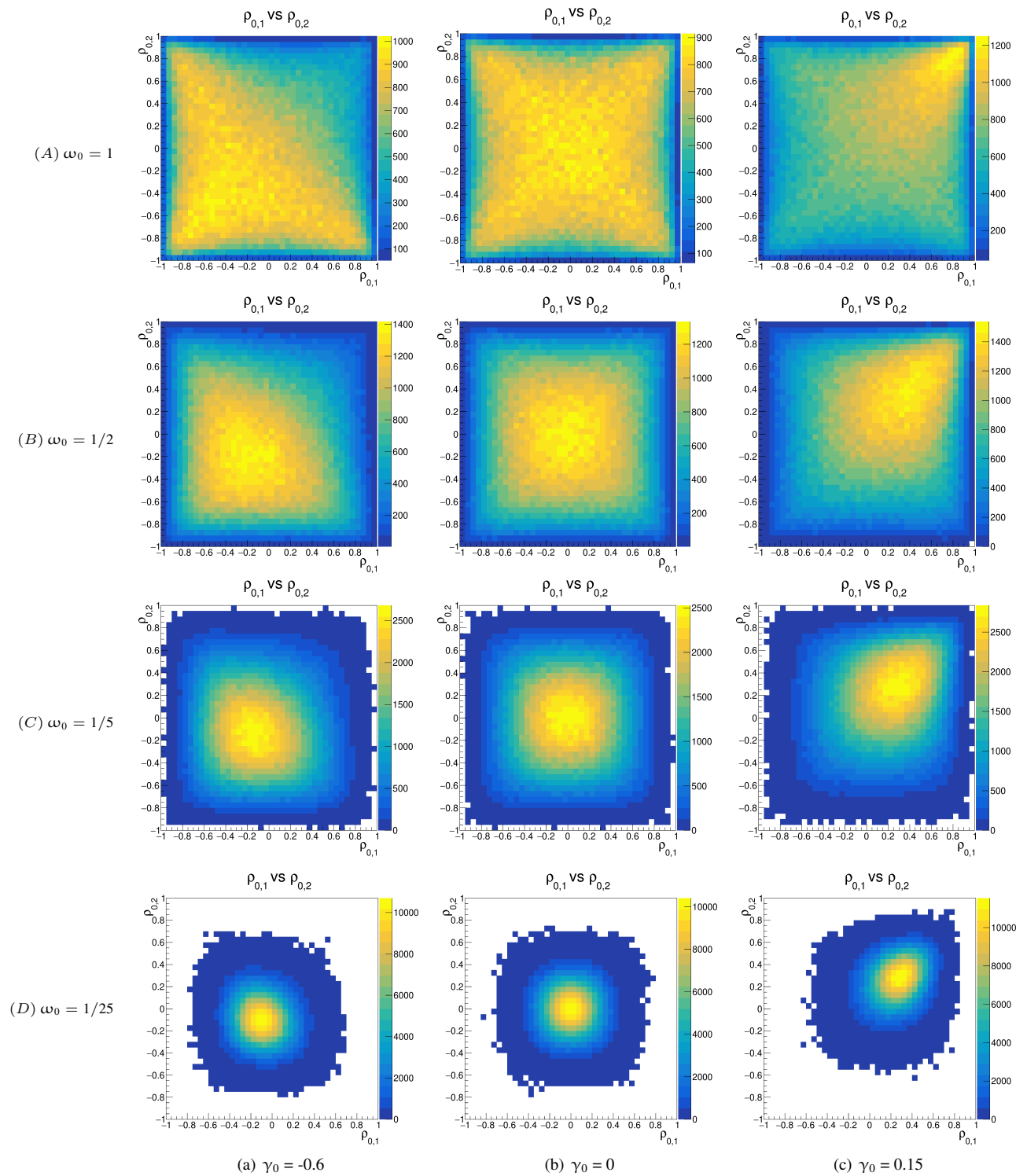


FIG. 2: Bivariate representation of $(\rho_{0,1}, \rho_{0,2})$ when drawn with the Archakov-Hansen procedure with $n_X = 12$, ω_0 set to 1 (line A), 1/2 (line B), 1/5 (line C) and 1/25 (line D) while γ_0 is set to -0.6 (a), 0 (b) and 0.15 (c).

1 For every configuration, there is a set of index and a set of rank for each and every sensitivity method. Since both
 2 the correlation matrix, whatever the chosen approach may be, and the sample, on which the indices estimation is
 3 performed, are randomly drawn, this procedure, latter referred to as an **estimation**, is repeated to overcome statistical
 4 fluctuations: few thousands of times in § 3.2 and from about 50 to about 150 times in § 4.

5 **3.2 Applying all methods: first observations**

6 In order to investigate the behaviour of all the indices, a given basis configuration is chosen to serve as a reference:

- 7 • the dimensions of the problem are set to $(n_X, n_S) = (12, 1000)$;
- 8 • all the inputs variables are set to have the same variance;
- 9 • the input variables are drawn as a multivariate normal distribution, $\mathbf{X} \sim \mathcal{N}(0, \mathbf{\Gamma}_{XX})$ where $\mathbf{\Gamma}_{XX}$ is taken
 10 either as the unitary matrix or drawn from the Gram or the Archakov-Hansen approach;

11 The last aforementioned item is let opened as starting with an already complicated correlated situation might compli-
 12 cate the interpretation due to a possible entanglement of various effects.

13 *3.2.1 Independent case with same variances*

14 In this section, large number of estimations have been done[§] in order to throw a first glance at the behaviour of the five
 15 indices introduced in § 2, along with the usual first-order coefficient[¶]. To check that our estimations are consistent
 16 with the expectations from the theory introduced in both Section 1 and 2, but also to look for any interesting trends,
 17 a first attempt is done setting $\mathbf{\Gamma}_{XX} = \mathbf{1}_{n_X}$.

18 Figure 3 shows all sensitivity indices distribution, for this peculiar configuration and few points can be raised
 19 from it:

- 20 • all the distributions, but weifila, are centred around 8.33 % which is expected as this correspond to a twelfth of
 21 the system output variance (since all variables are independent and have the same variance);
- 22 • the weifila index seems to provide very off-estimations. This instability (pointed out in the introduction of the
 23 method in § 2.5) is not particularly related to the size of the sample provided: it has been tested with $n_S = 10000$
 24 and in both cases, about 30 % of the events are in tails.

[§]unless otherwise specified, it exactly 8330 estimations, so that the total number of indices is roughly matching 100 000 entries.

[¶]The first-order coefficient results here used for illustration purposes will be computed throughout this paper using the *pick-and-freeze* method [21, 22]. This is out of the scope of this paper as the linear assumption has to be done (the sensitivity indices can not be estimated only with a provided sample) but the information drawn is interesting nonetheless.

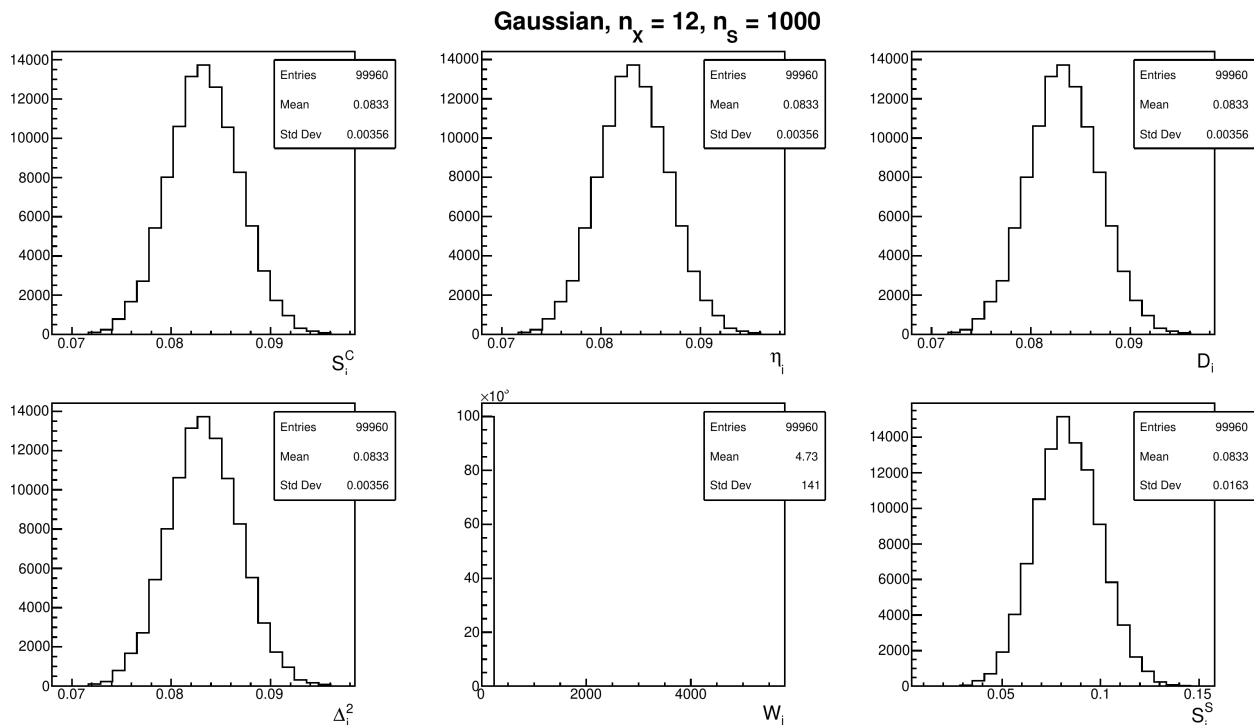


FIG. 3: Distribution of the sensitivity indices for several thousand estimations of the basis configuration in the independent case. From left to right and top to bottom, the indices are: covariance-based, Shapley value, LMG-GDI, relative weight, weifila and the first-order coefficient.

1 • the standard deviation from these distribution is directly linked to the size of the statistical sample (n_s). When
 2 a sample of size 10000 locations is used instead of $n_s = 1000$, all these values shrink. This is further illustrated
 3 in § 4.

4 • most of the distributions are very similar, at least from their statistical momentum point of view as they all
 5 derived from the same events and should lead (in this very simple case) to the same values (*c.f.* § 2).

6 In order to investigate further the fourth observation, the difference of all indices value is computed for all
 7 selected pairs of methods, some of which are represented in Figure 4 for example. The two left-handed plots show
 8 that whatever the configuration considered, the covariance-based, relative weight and Shapley values are fairly close
 9 but not exactly the same. The comparison of the classical first-order coefficients with all other measurements is also
 10 consistent, as shown by the third plot of Figure 4 once compared to covariance-based values, but limited by the size
 11 of the sample (as discussed later in § 4). Finally, the latest plot (the right one) focus on the fact that Shapley values
 12 and LMG-GDI ones seem to be exactly equivalent. This is confirmed throughout all cases in this paper and is proven
 13 analytically in § 5.1.

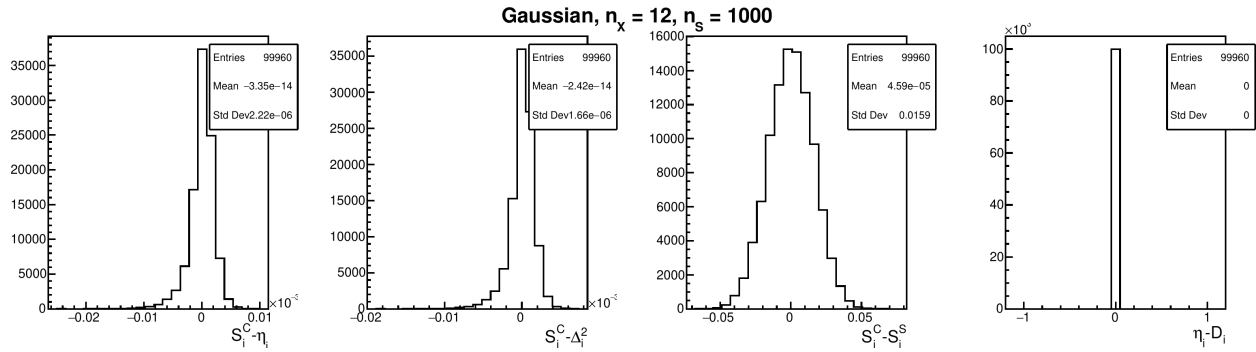


FIG. 4: Distribution of the difference of sensitivity indices measured for several thousand estimations of the basis configuration in the independent case. These differences are taken from the covariance-based with other methods such as relative weight (left), Shapley values (middle-left) and LMG-GDI ones (middle-right). The right plot shows the difference of sensitivity indices measured from the Shapley values and the LMG-GDI ones.

1 To further investigate this, it is possible to look at the rank distributions. By construction, in this case where n_X is
 2 set to 12, the rank distribution is the exact same one from one method to another: it is a Dirac comb with integer value
 3 going from 1 to 12, each of the corresponding bins having exactly the same number of entries. All the observations
 4 above are confirmed by looking at the other metric, the indices rank: when the indices value computations are mainly
 5 tainted with statistical fluctuations, the difference in indices rank should reflect this with a wide standard deviation and
 6 a regular distribution of difference as shown in the middle-right part of Figure 5. This is mainly because all variables
 7 should account for a twelfth of the output system variance. Apart from the absolute equality between Shapley values
 8 and LMG-GDI ones, confirmed by the right part of Figure 5, the observations done between the other pairs of indices,
 9 setting aside weifila for the moment, are confirmed respectively by the left and middle-left part of Figure 5: the
 10 methods, in this particular configuration, provide almost the same results.

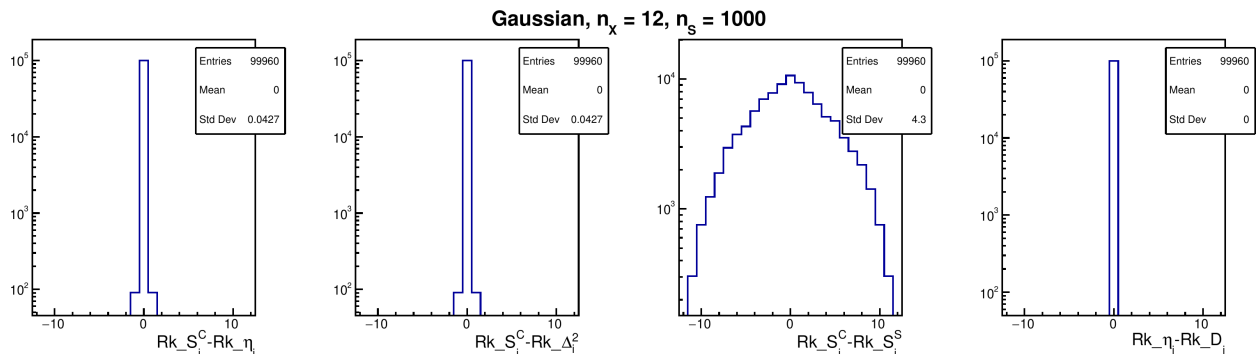


FIG. 5: Distribution of the difference in ranking of sensitivity indices measured for several thousand estimations of the basis configuration in the independent case. These differences are taken from the covariance-based with other methods such as relative weight (left), Shapley values (middle-left) and LMG-GDI ones (middle-right). The right plot shows the difference of sensitivity indices measured from the Shapley values and the LMG-GDI ones.

1 3.2.2 Independent case with different variances

2 Another important hypothesis, from the basis configuration defined at the beginning of § 3.2, is the fact that all input
 3 variables have the same variance which leads to the equal contribution of each of them to the system output (a twelfth
 4 when $n_X = 12$). In this part, the variance distribution is split into two groups: in the first one, half the input variables
 5 still have a variance of 1, while in the second group it is set to $\sigma = 5$. Looking at Figure 6, that shows that all
 6 sensitivity indices distribution are very similar:

- 7 • all the distributions have an average value around 8.33 % (still the twelfth of the system output variance) but
 8 this time split into two regions, as expected;
- 9 • the weifila index seems to provide more stable results, in agreement with the rest of the methods;
- 10 • the standard deviation from these distribution is now driven by the fact that the indices are split into two regions.
 11 The spread of both peaks, on the other side, are still directly linked to the size of the statistical sample (n_S).

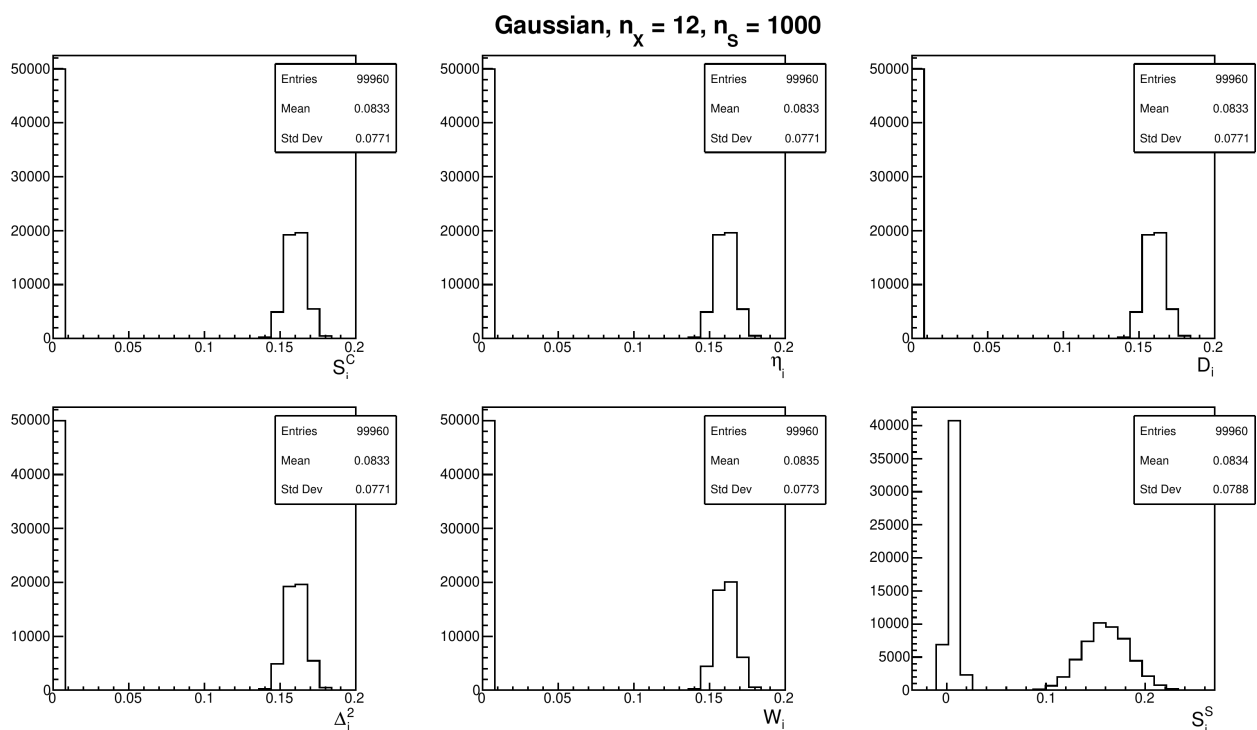


FIG. 6: Distribution of the sensitivity indices for several thousand estimations of the basis configuration in the independent case with two variance values for the input variables. From left to right and top to bottom, the indices are: covariance-based, Shapley value, LMG-GDI, relative weight, weifila and the first-order coefficient.

12 As for the independent case where all input variables bring the same contributions, the first observation mentioned

1 previously can be tested by looking at the difference of of all indices with both metrics: their values in Figure 7 or their
 2 ranks in Figure 8. The conclusions drawn from § 3.2.1 remain: there is a very good agreement between all indices
 3 with very low variations between covariance-based, LMG-GDI, relative weight and Shapley values, as shown by the
 4 left and middle-left parts of both Figures 7 and 8. The first-order coefficient results are still very limited by the sample
 5 size while the weifila results, even though stable now for every configurations, show tails with respect to every other
 6 indices, as shown respectively by the middle-right and right parts of both Figures 7 and 8.

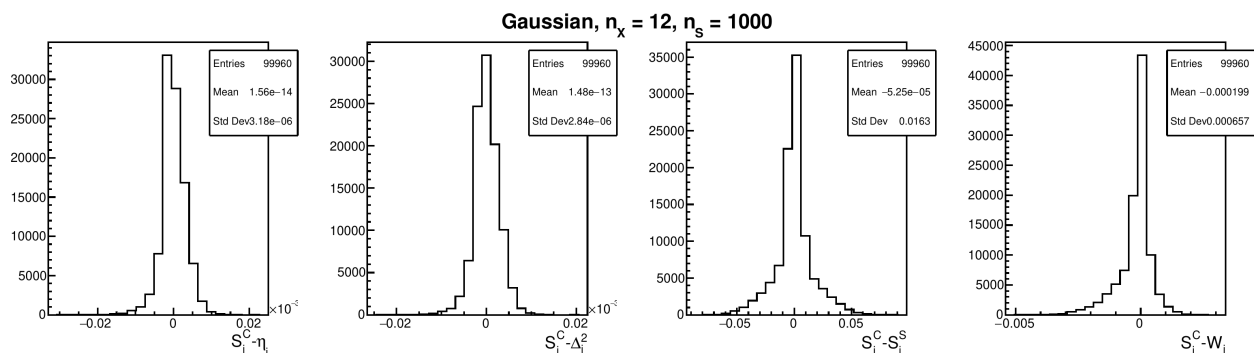


FIG. 7: Distribution of the difference of sensitivity indices measured for several thousand estimations of the basis configuration in the independent case with two variance values for the input variables. These differences are taken from the covariance-based with other methods such as relative weight (left), Shapley values (middle-left), LMG-GDI ones (middle-right) and weifila (right).

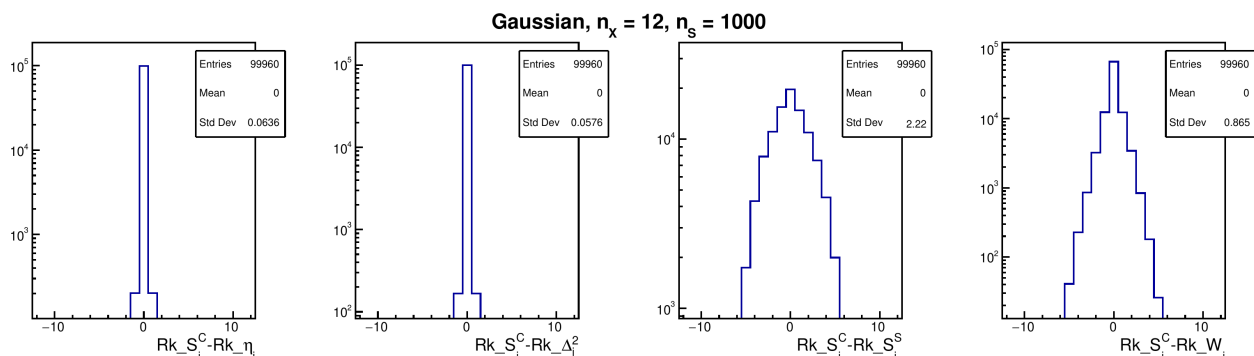


FIG. 8: Distribution of the difference of sensitivity indices measured for several thousand estimations of the basis configuration in the independent case with two variance values for the input variables. These differences are taken from the covariance-based with other methods such as relative weight (left), Shapley values (middle-left), LMG-GDI ones (middle-right) and weifila (right).

7 3.2.3 Gram and Archakov-Hansen random matrix cases

8 In this section, another large number of estimations have been done and the distributions of all the methods intro-
 9 duced in § 2, along with the usual first-order coefficient, using now random correlation matrices, either drawn from

1 the Gram or the Archakov-Hansen approach, are shown respectively in Figures 9 and 10. As a remainder, the corre-
2 sponding distribution of correlation coefficients can be seen respectively in Figure 1(c) and in Figure 2(b)(A), as in
3 the Archakov-Hansen approach, the chosen setup is $(\gamma_0, \omega_0) = (0, 1)$. Few observations can be drawn from these
4 two sets of distribution:

- 5 • the weifila results using the Gram approach is still suffering from instabilities which would suggest that one
6 might be tempted to discard them;
- 7 • once again, all the distributions, but the aforementioned one, have an average value around 8.33 % (the
8 twelfth of the system output variance) but this time the methods can be split into two kinds: the positive-only
9 ones (Shapley value, LMG-GDI, relative weight and weifila) and the others with possibly negative results
10 (covariance-based, first-order coefficient);
- 11 • bearing in mind the split in methods introduced in previous item, the variances of the distribution, going from
12 the Gram to the Archakov-Hansen approach, are fairly stable for the positive-only methods while they are
13 increasing significantly for the others.

14 The first and third observations above are completing the analysis done when looking at the distributions of
15 the correlation coefficient taken out of either the Gram or the Archakov-Hansen approach: the former is providing
16 correlation coefficients closer and closer to 0 as the input dimension is increasing (*c.f.* Figure 1 and the expected PDF
17 of these coefficients introduced in equation (44)) while the latter is more representative of the full possible variability.

18 The second observation is of utmost importance: as already discussed in § 2.4 when introducing the covariance-
19 based method, some total indices might be negative or null. The former case implies that the relative contribution
20 is weakening so much its structural counterpart that it flips the global index sign but the amplitude helps pointing out
21 that the variable under study should not be dropped. Interpreting the latter case might be a bit more tricky as a close
22 to 0 value might arise either when both the structural and relative contributions are negligible, meaning that the
23 impact of the variable is indeed negligible, but also when both contributions have equivalent amplitude but cancel out
24 one another.

25 Combining these two aspects explains why going from the Gram to the Archakov-Hansen approach means having
26 a significant increase in the standard deviation of the indices distributions for the non-positive-only methods: the
27 covariance are allowed to be larger in the latter case (given our chosen parameter values γ_0 and ω_0) so there might be
28 more widely spread resulting indices. Since the covariance can significantly impact the influence of a given variable,

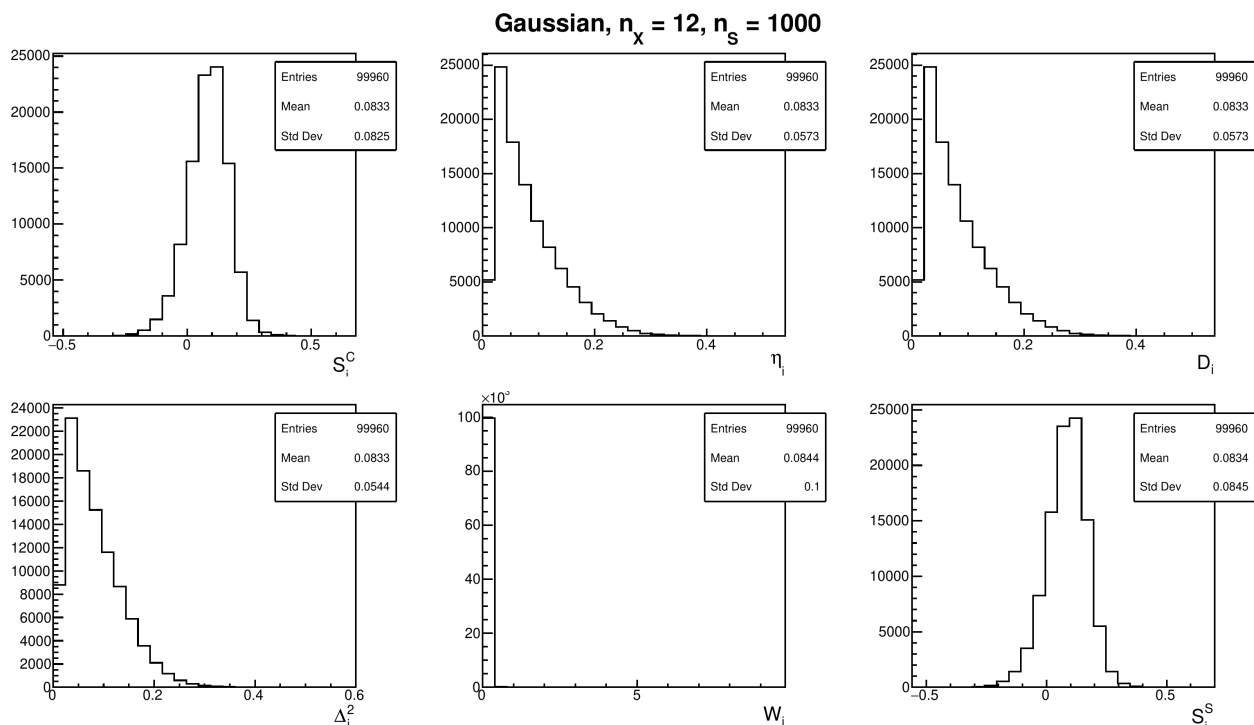


FIG. 9: Distribution of the sensitivity indices for several thousand estimations of the basis configuration using the Gram approach. From left to right and top to bottom, the indices are: covariance-based, Shapley value, LMG-GDI, relative weight, weifila and the first-order coefficient.

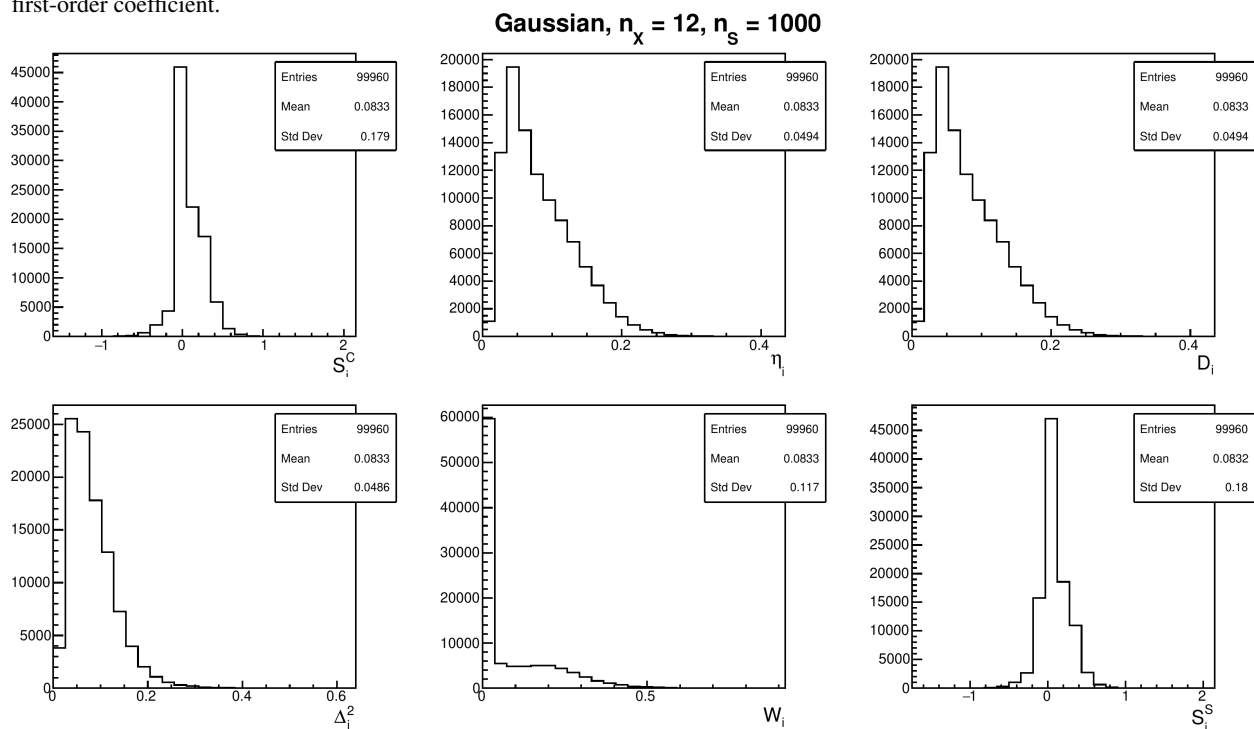


FIG. 10: Distribution of the sensitivity indices for several thousand estimations of the basis configuration using the Archakov-Hansen approach with $(\gamma_0, \omega_0) = (0, 1)$. From left to right and top to bottom, the indices are: covariance-based, Shapley value, LMG-GDI, relative weight, weifila and the first-order coefficient.

1 in order to be as exhaustive as possible, the Gram approach is discarded in the rest of this paper and the Archakov-
 2 Hansen one is kept as a baseline, with $(\gamma_0, \omega_0) = (0, 1)$, changing this couple of parameter from time to time to
 3 check the consistency of the following conclusions.

4 Finally, in order to be able to compare indices numerically, all indices have been normalised in a similar fashion,
 5 in order to circumvent the difference in behaviour between positive-only and non-positive-only methods, following
 6 this principle:

$$|\kappa_i| = \frac{|\kappa_i|}{\sum_{j=1}^{n_X} |\kappa_j|}. \quad (45)$$

7 Figure 11 shows the distributions of the indices in their normalised form which can be compared to their original
 8 form already shown in Figure 10.

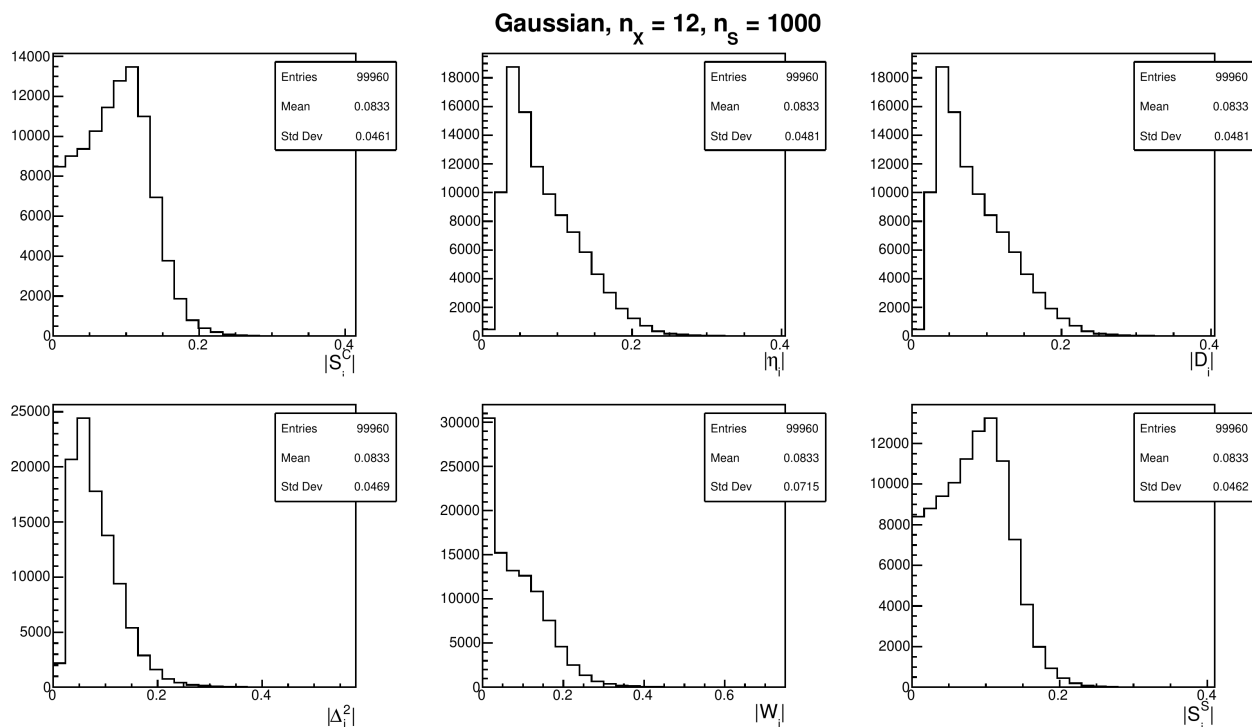


FIG. 11: Distribution of the sensitivity indices for several thousand estimations of the basis configuration using the Archakov-Hansen approach with $(\gamma_0, \omega_0) = (0, 1)$. From left to right and top to bottom, the indices are shown in their normalised version as defined in equation (45): covariance-based, Shapley value, LMG-GDI, relative weight, weifila and the first-order coefficient.

9 This step allows to get all sets of indices evolving in a common range, helping sorting out the non-positive-only
 10 in a very common way to the rest of the positive-only methods. Indeed, for a given estimation, a negative value of a
 11 covariance-based index for instance, reflect that the correlative part is larger than its structural counterpart for the input
 12 under consideration. By considering only its value, its ranking will be smaller than every other input variables with

1 a positive index, even those whose index is lower than the absolute value of the one under consideration, hence this
 2 normalisation proposition. This provides, when computing the difference between all the methods and the covariance-
 3 based values, fairly coherent results from one method to another as shown by the distributions in value in Figure 12
 4 and in rank in Figure 13. With our basis configuration, using the $(\gamma_0, \omega_0) = (0, 1)$ configuration which results in
 5 widely distributed correlation coefficients, all the differences are unbiased (from a statistical point of view), with a
 6 reasonable standard deviation. The conclusions seen above are completed with new ones:

- 7 • as expected, the impact of the normalisation on the positive-only results is nonexistent: all the n_X results were
 8 already positive for each and every estimations and their sum is set to 1 by construction;
- 9 • the covariance-based results and first-order coefficients are very likely before and after normalisation. This can
 10 be seen both from the values and the rankings distributions.
- 11 • all the positive-only measurements are in a nice agreement with the normalised covariance-based results, which
 12 can be seen from both the values and rankings distributions
- 13 • even though there are more tails in the comparison of covariance-based results and weifila ones (probably due
 14 to the stability of the weifila method), the rankings are more coherent for covariance-based and weifila than
 15 for covariance-based and the rest of originally positive-only methods (LMG-GDI, Shapley values and relative
 16 weight).

17 The agreement seen and discussed here is getting better once choosing a stronger correlation in between the
 18 variable: the exact same procedure has been redone with random correlation matrices drawn with the Archakov-
 19 Hansen procedure, setting now the parameters to the following values $(\gamma_0, \omega_0) = (0.15, 1)$, as already introduced
 20 in Figure 2(c)(A). Using this peculiar configuration leads to higher correlation coefficient values and an even better
 21 agreement between all the methods, as can be seen in Figures A.20 and A.21

22 Now that all these methods have been shown to have their differences but to converge to common conclusion,
 23 the dependence to all the parameters used to define the basis configuration will be studied in more details in § 4.

24 4. TESTING DEPENDENCIES

25 In this part, the conclusions drawn from § 3.2 are set aside in order to focus on the way the considered methods
 26 might be depending on some of the basis configuration parameters considered fixed (those detailed in the preamble
 27 of § 3.2). The idea is to investigate a possible impact on several interesting features such as the average difference

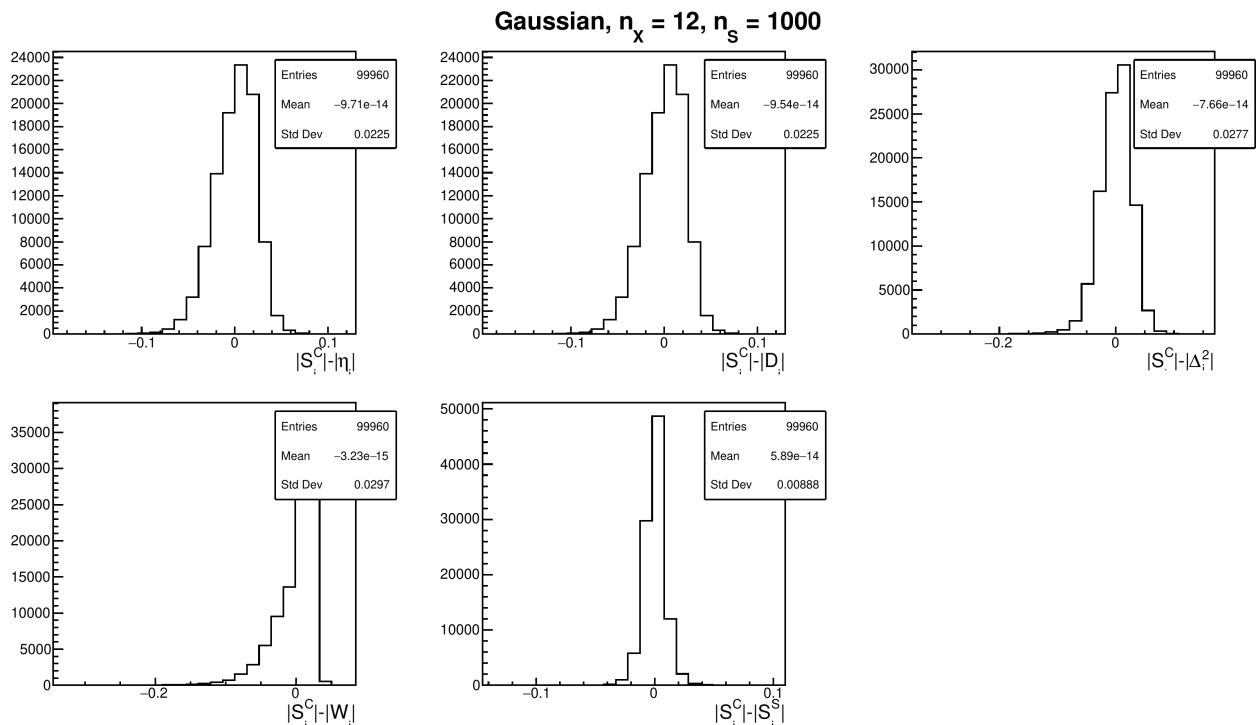


FIG. 12: Differences of the normalised sensitivity indices with the normalised covariance-based results, for several thousand estimations using the Archakov-Hansen with $(\gamma_0, \omega_0) = (0, 1)$. The methods used are the Shapley values (top-left), the LMG-GDI (top-middle), the relative weight (top-right), the weifila (bottom-left) and the first-order coefficient (bottom-right).

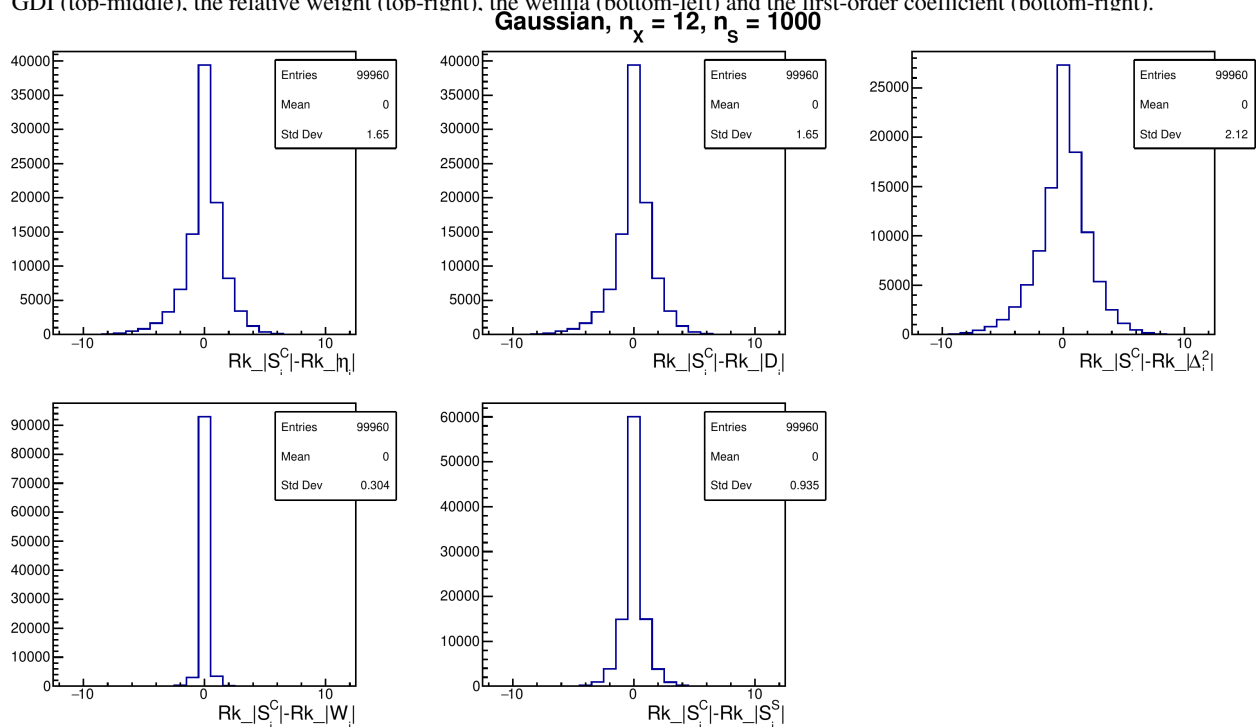


FIG. 13: Differences of the ranking of normalised sensitivity indices with the one of the normalised covariance-based results, for several thousand estimations using the Archakov-Hansen $(\gamma_0, \omega_0) = (0, 1)$. The methods used are the Shapley values (top-left), the LMG-GDI (top-middle), the relative weights (top-right), the weifila (bottom-left) and the first-order coefficients (bottom-right).

1 between normalised method results, the spread of the difference between normalised method results and the running
 2 time for every methods, when varying

- 3 • the sample size n_S ;
- 4 • the input space size n_X ;
- 5 • the nature of the input law;
- 6 • the variability of the input laws;

7 As for the preliminary analysis done in § 3.2, estimations have been generated to test several steps in the all the
 8 aforementioned parameters, the number of estimation going from 50 to 166, so that the estimators used to the average
 9 and standard deviation estimation might be accurate enough while the total number of estimated indices is as close to
 10 a thousand as possible. Every following sections will deal with on the item defined above.

11 In each case, disregarding the parameter under investigation, tests are done in order, on the one hand, to check
 12 the consistency of the sensitivity indices measurements from one method to the other, but also, on the other hand, to
 13 investigate the self consistency of every methods (average and spread evolution) when the parameter is changing.

14 For the rest of this section, the time measurement is done with the *chrono* C++-package for every estimation of
 15 each method separately, using a regular i9-9880H processor with 8 cores (16 threads) on a laptop. In order not to
 16 affect too much the measured time, the number of parallelised processes have been limited to 6 at the same time.

17 **4.1 Impact of the sample size**

18 In this section, the sample size is tested, going from a hundred locations to four thousand ones. The most interesting
 19 results are gathered in Figure 14.

20 Figure 14(a) shows both the average and spread of the differences in the values of all sensitivity indices with the
 21 covariance-based results. The first observation is that no bias is seen through all the n_S steps tested, as the average bias
 22 is well below 10^{-10} . However, the spread is evolving as displayed in Figure 14(b), which shows that all the methods
 23 but the first-order coefficients have a very stable spread with respect to the number of locations. For the latter, on
 24 the other hand the spread is decreasing fast with the number of locations which is expected from the *pick-and-freeze*
 25 method used with the provided sample.

26 As for the resource, the time consumption is displayed in Figure 14(c) in logarithmic scale with respect to the
 27 sample size, and shows that all the methods but the first-order coefficients are fairly stable. For the latter, the evolution
 28 is the one expected from the *pick-and-freeze* method.

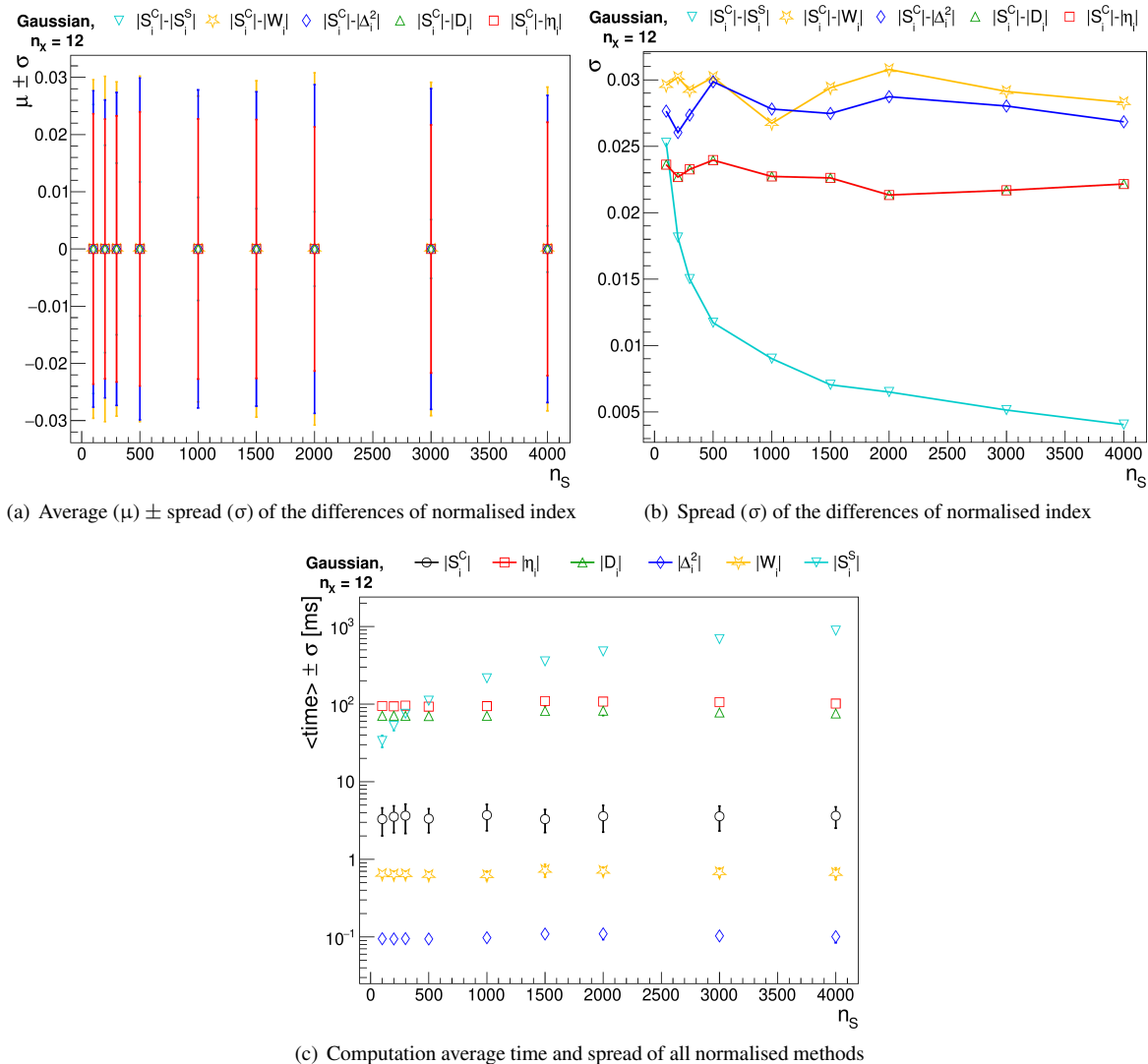


FIG. 14: Evolution, as a function of the sample size, of the average differences and spreads in normalised value (14(a)), of the spread of these differences (14(b)), and the average time consumption for every methods (14(c)).

1 From all these observations, the sample size does not seem to be of utmost importance with respect to the chosen
2 protocol in this paper.

3 4.2 Impact of the input space size

4 In this section, the input space size is tested, going from 4 to 20 input variables. The most interesting results are
5 gathered in Figure 15.

6 Figure 15(a) shows both the average and spread of the differences in the value of all sensitivity indices with

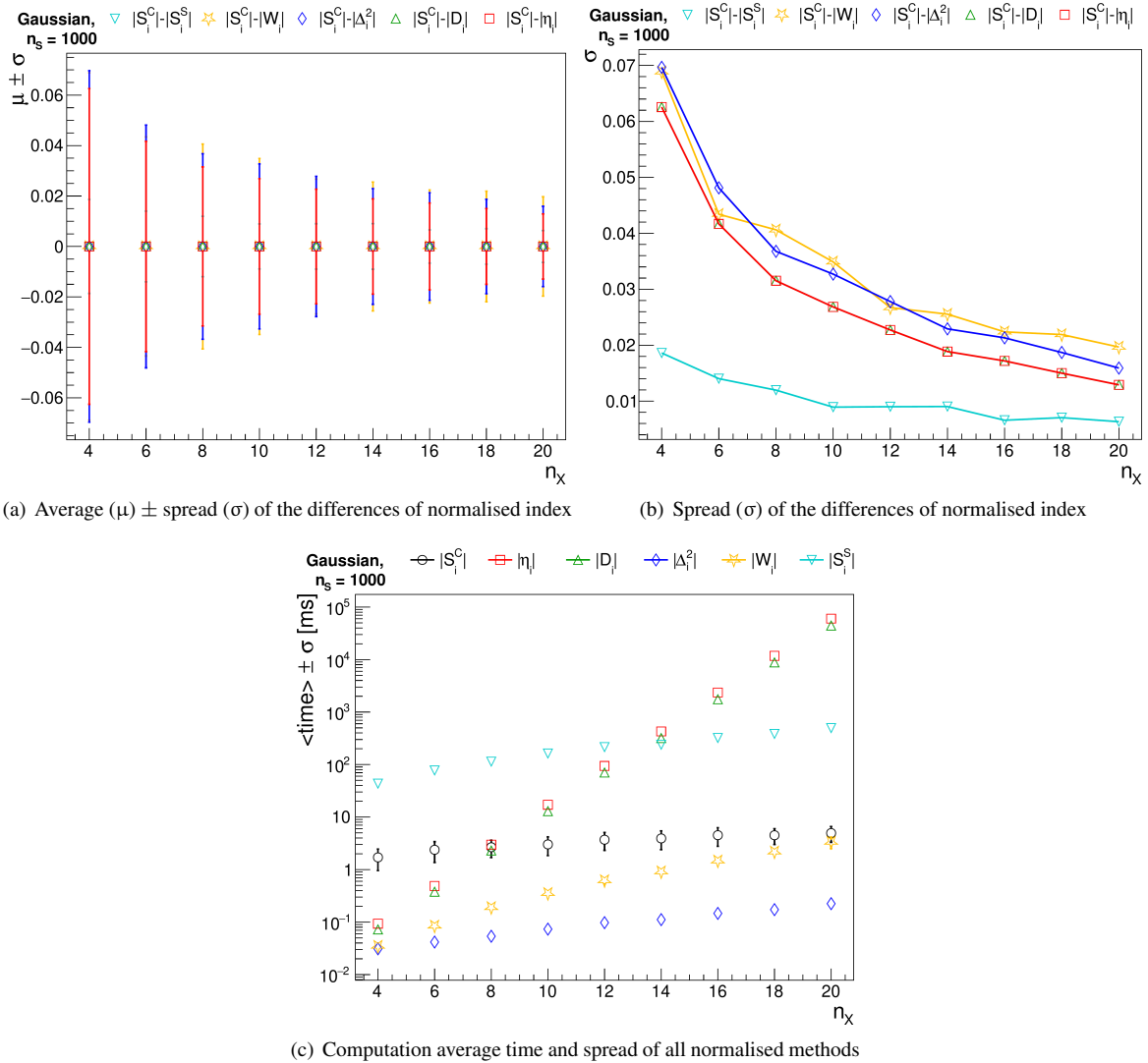


FIG. 15: Evolution, as a function of the input space size, of the average differences and spreads in normalised value (15(a)), of the spread of these differences (15(b)), and the average time consumption for every methods (15(c)).

1 the covariance-based results. The first observation is that no bias is seen through all the n_x steps tested, as the
 2 average bias is again well below 10^{-10} . However, the spread is evolving significantly for all methods as displayed in
 3 Figure 15(b), but two groups can be seen: the first-order coefficients on one side and the rest of the indices on the
 4 other. For the former it has already been stated that the first-order coefficients and the covariance-based results are in
 5 a very good agreement while for the latter all the other methods share the same pattern with a quick reduction of the
 6 spread with the input space size.

7 As for the resource, the time consumption is displayed in Figure 15(c) in logarithmic scale with respect to the

1 input space size, and shows that all the methods are sensitive to the input space size but with very different impact:
2 relative weights, covariance-based and first-order coefficients time consumption is increasing slightly, with less than
3 an order of magnitude when going from 4 to 20 inputs even though their respective starting point is different. The
4 computation time evolution for the weifila method is not so far from the three previously discussed ones, it changes
5 by a bit less than two orders of magnitude. The two remaining methods suffers from severe time dependencies has,
6 the evolution of their average computation time seems linear in logarithmic scale with respect to the input space size,
7 increasing by more than 5 orders of magnitudes in our current testing conditions.

8 From all these observations, the input space size does not seem to be of utmost importance when only considering
9 the precision and consistency of one method with respect to the others. On the other hand, it remains crucial in the
10 limitation of resources and might become a stopping points once this parameters is set to be too high to be properly
11 handled with the current proposed implementation for at least the Shapley value and LMG-GDI approaches.

12 **4.3 Impact of the input law**

13 Even though no effect is expected from the input law hypothesis stated in the basis configuration definition in § 3.2,
14 it might be fair to test this by changing the input law, keeping the rest of the covariance structure. Figure 16 shows
15 that changing the input law from the Gaussian hypothesis to seven other probability density functions with well
16 chosen parameters so that their statistical momentum are equivalent, does not affect the three important metric under
17 investigation. The averages and the spreads of the differences in value of all sensitivity indices with respect to the
18 covariance-based results are indeed completely consistent from one law to the other, as shown in Figure 16(a), as the
19 computation time requested by each and every algorithm to get a single estimation (*c.f.* Figure 16(b)).

20 **4.4 Impact of the variance of the input variables**

21 As discussed, at least in the independent case in § 3.2.2, one of the basis configuration hypothesis is the fact that all
22 input variables have the same variance which leads to the equal contribution of each of them to the system output
23 variance. In the correlated case, this sentence can be rephrased as “this leads to the equal structural contribution”
24 meaning that the differences in importance between all input variables come as the by-product of the correlation
25 structure injected.

26 In this part it is interesting to vary the input variables variance, exactly as done in § 3.2.2. The variance division is
27 indeed split into two groups: in the first one, half the input variables still have a variance of 1, while in the second group
28 the standard deviation of the rest of the inputs is set to one of the seven pre-selected values $\{0.01, 0.1, 1, 2, 3, 4, 5\}$. The

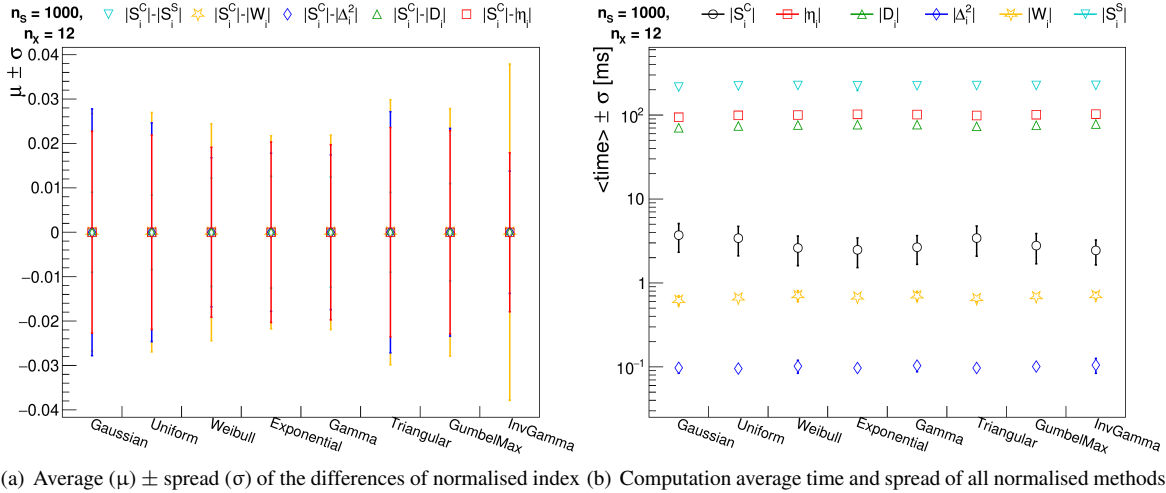


FIG. 16: Evolution, as a function of the input law, of the average differences and spreads in normalized value (16(a)) and the average time consumption for every methods (16(b)).

1 meaningful impact of these modifications is shown in Figure 17 and further explained, for instance, by distributions
 2 like those displayed in Figure 18.

3 The overall impact of the variation of the standard deviation of half the input variables, meaning when consid-
 4 ering all these variables at once, seem negligible on the average bias, *c.f.* Figure 17(a), which only shows wide (and
 5 significant) variations of the spread (increasing as soon as $\sigma_{\text{half var}} \neq 1$). This can be explained once one focuses on
 6 the two groups of input variables, the same plot being done only for the variable with unchanged standard deviation,
 7 *c.f.* Figure 17(b). In this case, a significant bias seems to arise as soon as $\sigma_{\text{half var}} \neq 1$, for three methods at least:
 8 Shapley values, relative weightand LMG-GDI. This is further illustrated by Figures 17(c) and 17(d) which display
 9 only the average bias of input variables respectively for unchanged and varied standard deviation.

10 Bearing in mind that the bias under consideration is with respect to the covariance-based method, all these plots
 11 show that there are, if considered with a coarse approximation, two kind of methods:

- 12 1. methods that share evenly the full contribution between correlated variables, later referred to as “Type-I”;
- 13 2. methods that disentangle the structural and correlated parts, later referred to as “Type-II”.

14 With this, it appears that the non-positive-only methods are “Type-II” methods, while most of the positive-only
 15 methods are “Type-I” ones. This interpretation is in agreement with the definition itself of some of these methods: the
 16 Shapley values are constructed to be a “fair” distribution of the “gain” when all players are collaborating (*c.f.* § 2.1.1);
 17 On the other hand, the covariance-based results are constructed from the dichotomic separation of the structural

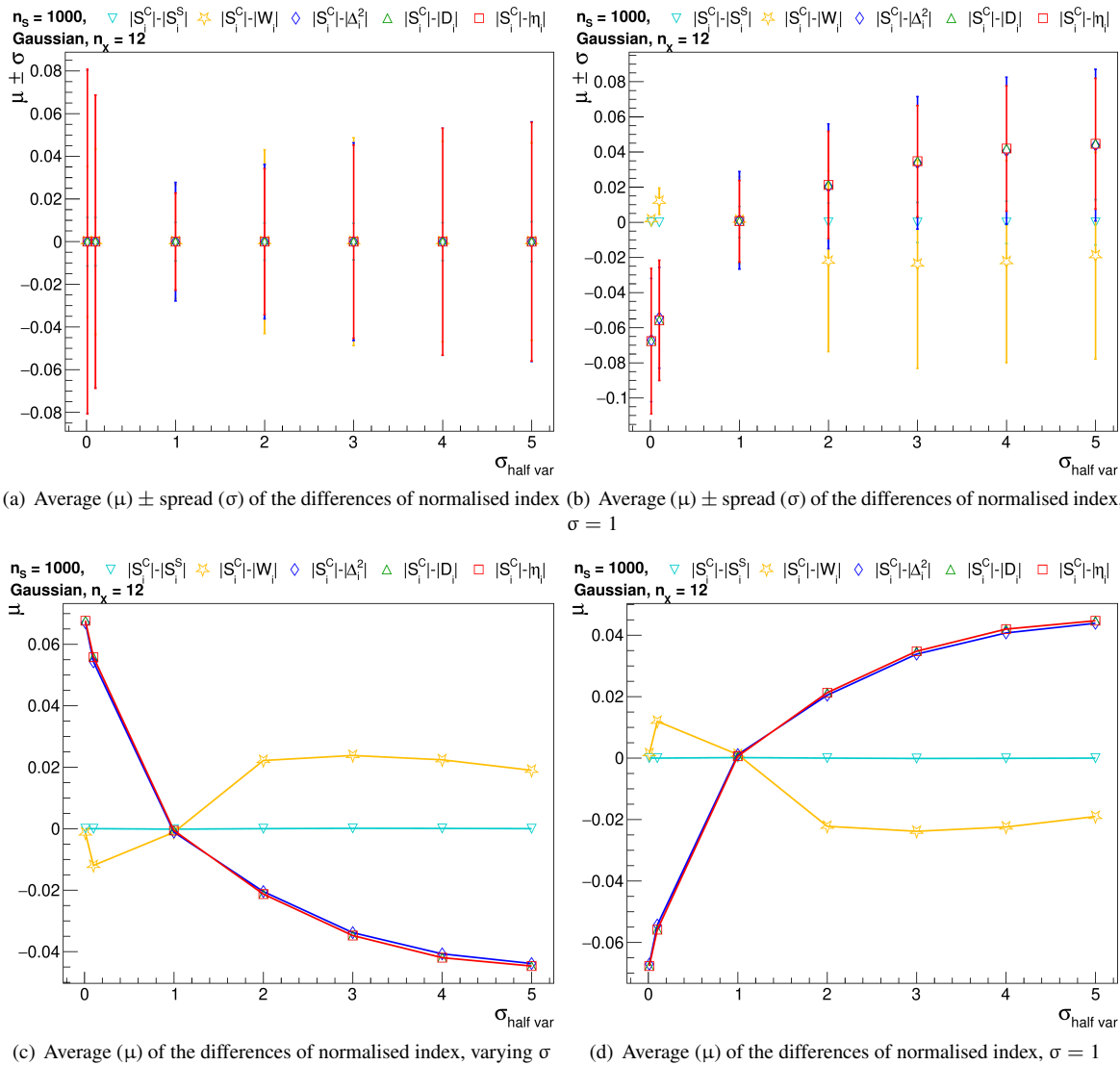


FIG. 17: Evolution, as a function of the standard deviation of half the input variables, of the average differences and spreads in normalised value for all variables (17(a)), for those whose variance has not changed (17(b)). A focus is done specifically on the averages, for variables with changing σ (17(c)) and for variables with $\sigma = 1$ (17(d)).

1 and correlated contributions. The LMG-GDI results being equivalent to the Shapley values (see § 5.1), the only
 2 other “Type-I” behaviour methods, the relative weight, was also expected from its definition. The second step indeed
 3 regresses \mathbf{X} onto \mathbf{Z} in order, in the case where the original variables are highly correlated, to take into account the
 4 fact that the Z variables are not a close representation of the X , hence producing a set of weights that redistribute
 5 the variance in between correlated variable. This is why the relative weight, from the author point of view [39], and
 6 confirmed by all the results discussed so far, are a very good approximation of the Shapley values.

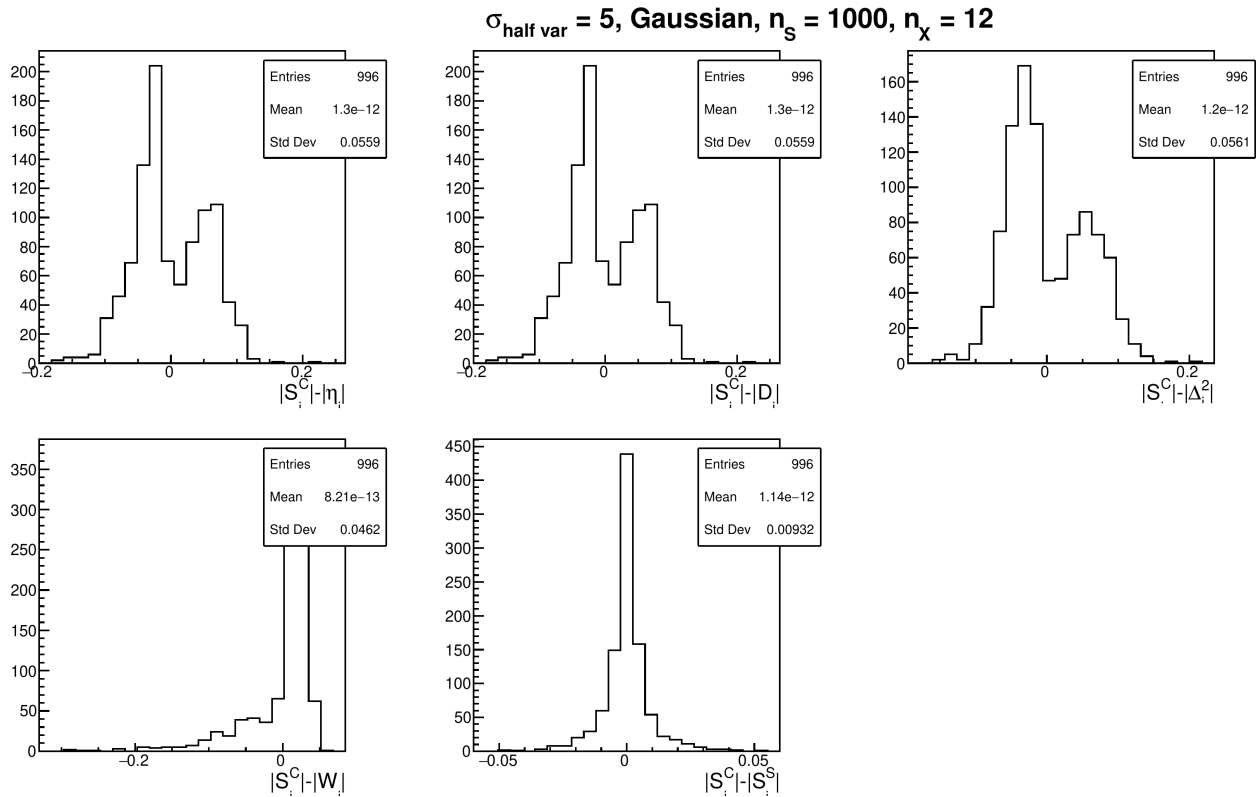


FIG. 18: Distribution of the difference of normalised sensitivity indices measured in the Archakov-Hansen $(\gamma_0, \omega_0) = (0, 1)$ configuration when half the input variables have $\sigma = 5$. These differences are taken from the covariance-based with other methods such as Shapley values (top-left), LMG-GDI ones (top-middle), relative weights (top-right), weifila results (bottom-left) and first-order coefficients (bottom-middle).

1 The only positive-only method which is not really a “Type-I” kind is the weifila one. For this one, even though
 2 the average bias is changing with respect to $\sigma_{\text{half var}}$, it remains consistent with a null bias when considering the
 3 spread (*c.f.* Figure 17(b)), which has been confirmed with a very large statistic sample, as those used in § 3.2, with
 4 $\sigma_{\text{half var}}$ was set to 5: no significant bias was seen with respect to the spread. A last attempt was done with $\sigma_{\text{half var}}$
 5 case, choosing the $(\gamma_0, \omega_0) = (0.15, 0.04)$ configuration, shown in Figure 2(c)(D) which generates high values of
 6 correlation coefficient with a narrow standard deviation: all these conclusions hold, the weifila average bias being
 7 consistent with 0, even though on the very edge, once considering one standard deviation of the bias distribution.

8 5. DISCUSSION AND CONCLUSIONS

9 This final section provides a mathematical demonstration of the equality of the LG-Shapley method and the LMG-
 10 GDI one in the linear-Gaussian case before further summarise all the conclusions drawn at every steps of this paper.

1 5.1 Comparing LG-Shapley and LMG-GDI

In the linear model assumption, the β coefficients can be estimated from the minimisation of $\|\mathbf{Y} - \mathbf{X}\beta\|^2$ which leads to the usual $\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$ (when $n > n_X$ and if $(\mathbf{X}^T\mathbf{X})$ is invertible). With the hypothesis that our input variables \mathbf{X} have been centred and reduced, it is possible to express the estimation of the β coefficients using correlation matrix, as done below:

$$\begin{aligned}\hat{\beta} &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} \\ &= (n\hat{\Gamma}_{\mathbf{X}\mathbf{X}})^{-1}(n\sigma_Y\hat{\Gamma}_{\mathbf{X}\mathbf{Y}}) \\ &= \sigma_Y\hat{\Gamma}_{\mathbf{X}\mathbf{X}}^{-1}\hat{\Gamma}_{\mathbf{X}\mathbf{Y}}.\end{aligned}\tag{46}$$

The variance of the linear model can be written, using this notation, as:

$$\begin{aligned}\text{Var}(\mathbf{Y}) &= \frac{1}{n}\mathbf{Y}^T\mathbf{Y} = \frac{1}{n}\hat{\beta}^T\mathbf{X}^T\mathbf{X}\hat{\beta} = \hat{\beta}^T\hat{\Gamma}_{\mathbf{X}\mathbf{X}}\hat{\beta} \\ &= (\sigma_Y\hat{\Gamma}_{\mathbf{Y}\mathbf{X}}\hat{\Gamma}_{\mathbf{X}\mathbf{X}}^{-1})\hat{\Gamma}_{\mathbf{X}\mathbf{X}}(\sigma_Y\hat{\Gamma}_{\mathbf{X}\mathbf{X}}^{-1}\hat{\Gamma}_{\mathbf{X}\mathbf{Y}}) \\ &= \sigma_Y^2\hat{\Gamma}_{\mathbf{Y}\mathbf{X}}\hat{\Gamma}_{\mathbf{X}\mathbf{X}}^{-1}\hat{\Gamma}_{\mathbf{X}\mathbf{Y}} = \sigma_Y^2R^2.\end{aligned}\tag{47}$$

2 This simple exercise emphasise the already known relationship between the coefficient of determination and the
3 variance of the considered variable: the linear regression being a projection on the subspace spanned by the regressors,
4 the variance of the projected variable is decomposed into a part explained by the linear model and its complementary
5 part. If the variable under study follows a pure linear relation, then its variance is fully explained by the regressors
6 and the coefficient of determination is therefore equal to 1.

Comparing both equations (27) and (30) shows interesting similarities, and one could try to express the coefficient of determination when dealing only with a subset u of input variables, as a function of the input variables properties and the β coefficients. Given the linear hypothesis, not focusing on a specific sample anymore, one can indeed write:

$$\begin{aligned}\Gamma_{uy} &= \mathbb{E}(X_u^T Y) = \mathbb{E}(X_u^T X \beta) = \begin{pmatrix} \Gamma_{uu} & \Gamma_{u-u} \end{pmatrix} \begin{pmatrix} \beta_u \\ \beta_{-u} \end{pmatrix} \\ &= \Gamma_{uu}\beta_u + \Gamma_{u-u}\beta_{-u}.\end{aligned}\tag{48}$$

Injecting this into equation (32) leads to:

$$\begin{aligned}
R_u^2 &= (\beta_u^T \Gamma_{uu} + \beta_{-u}^T \Gamma_{-uu}) \Gamma_{uu}^{-1} (\Gamma_{uu} \beta_u + \Gamma_{u-u} \beta_{-u}) \\
&= (\beta_u^T + \beta_{-u}^T \Gamma_{-uu} \Gamma_{uu}^{-1}) (\Gamma_{uu} \beta_u + \Gamma_{u-u} \beta_{-u}) \\
&= \beta_u^T \Gamma_{uu} \beta_u + \beta_{-u}^T \Gamma_{-uu} \beta_u + \beta_u^T \Gamma_{u-u} \beta_{-u} + \beta_{-u}^T \Gamma_{-uu} \Gamma_{uu}^{-1} \Gamma_{u-u} \beta_{-u} \\
&= \beta^T \Gamma_{XX} \beta - \beta_{-u}^T \Gamma_{-u-u} \beta_{-u} + \beta_{-u}^T \Gamma_{-uu} \Gamma_{uu}^{-1} \Gamma_{u-u} \beta_{-u} \\
&= \beta^T \Gamma_{XX} \beta - \beta_{-u}^T (\Gamma_{-u-u} - \Gamma_{-uu} \Gamma_{uu}^{-1} \Gamma_{u-u}) \beta_{-u}.
\end{aligned} \tag{49}$$

By looking at equations (27) and (30), the two interesting quantities that should be linked are: the difference between the coefficient of determination and the difference between the conditional variance, both when using the subset v (defined as $v = u \cup i$) and the subset u of input variables. Writing the difference between the coefficient of determination using equation (49) is done below:

$$R_v^2 - R_u^2 = \beta_{-u}^T (\Gamma_{-u-u} - \Gamma_{-uu} \Gamma_{uu}^{-1} \Gamma_{u-u}) \beta_{-u} - \beta_{-v}^T (\Gamma_{-v-v} - \Gamma_{-vv} \Gamma_{vv}^{-1} \Gamma_{v-v}) \beta_{-v} \tag{50}$$

$$= \frac{1}{\text{Var}(Y)} (V_u - V_v). \tag{51}$$

1 The equality in equation (51) is straightforward once the equation (50) is compared to the difference between the
2 conditional variance, expressed thanks to the equation (28), established in the Gaussian framework. It shows indeed
3 that both methods, disregarding the fact that they have been developed at different moments, from different paradigms
4 and applied in different fields of research, lead rigorously to the same estimation. The main difference arise from the
5 genericity of the LMG-GDI one: the only strong hypothesis is the linear assumption, and even if the global coefficient
6 of determination were to be different from 1 but close (let's say 0.95), this would mean that the GD indices provide
7 the hierarchy of the input variables for 95% of the variance. On the other hand, the equation (27) has been derived
8 using the Gaussian conditioning theorem meaning that the paradigm was to only consider problem were the linear
9 assumption is correct and $X \sim \mathcal{N}(\mu, \Gamma_{XX})$.

10 5.2 Conclusions

11 This paper is a review that aims in comparing some ways to perform global sensitivity analysis for highly correlated
12 model (meaning when the input variable are not independent) and when no information are known on either the join
13 or the conditional probability density functions. To limit the scope and the complexity of this issue, only an output

1 system of the form of a linear combination of inputs is considered which remains useful as stated in the § 1 where
2 various field of research and engineering facing this problem are introduced. There have been many developments to
3 circumvent this, arising from various fields of research. This is the starting point of this paper: using methods that
4 allow estimation of sensitivity indices from a provided sample (disregarding whether it might arise from simulation or
5 experimental data) without any specific information on the inputs correlation assuming only that our system response
6 is well described by a linear combination of all the inputs.

7 An introduction is setting the historical approach, from the decomposition of a function in § 1.2 with independent
8 input variables to a more generalised description without any hypothesis on the probability density functions and the
9 covariance structure. The textbook techniques, in the independent case, have been recalled in § 1.3 before introducing
10 all the methods of interest used throughout this paper in § 2: the covariance-based measurement, the Shapley values,
11 the first-order coefficients, the LMG-GDI, the relative weights and the weifila method. As this paper focuses on the
12 linear dependent case, the simple covariance-based estimation proposed in [43] is used as reference when comparisons
13 are done.

14 A protocol to compare all methods is defined in § 3.1 by generating a very large number of non-singular cor-
15 relation matrix with a non-trivial intrinsic correlation structure. Two approaches have been tested, the classical one,
16 referred to as the Gram method, and a new one, referred to as the Archakov-Hansen one in this paper, which allows
17 to handle with a great precision the way the correlation coefficients are distributed. The latter has been shown to be
18 more compelling as it can represent a large variety of possible correlation configuration which cannot be achieved
19 by the former, the historical Gram one, which only provides very small correlation coefficients as soon as the input
20 space dimension grows. Using this historical approach is not representative of the full available spectrum and the
21 conclusions that might be drawn out of this procedure might be biased.

22 From there, a first set of tests have been performed using dedicated high-statistics samples, once a basis con-
23 figuration has been defined in § 3.2. The first conclusion drawn from this configuration is the complete equivalence
24 between the Shapley values and the LMG-GDI results in the linear case, which is mathematically established in § 5.1.
25 The second one is the stability problem that arises from the weifila definition itself, as stated as soon as the equations
26 are provided in § 2.5, which is problematic as soon as the correlation structure is not too strong and which diminish
27 considerably the trust in a singled-out measurement.

28 Finally all these methods are tested, still in a statistical approach, to test the dependencies and the consistency of
29 their results (with themselves or the rest of the methods) once the size of the sample, the size of the input space or the
30 nature of the input laws are varied. The main conclusions are that, once all methods are normalised, their results are

1 fairly consistent but some might suffer from instability (the weifila method as already stated), severe time limitation
 2 when the input space size increase (Shapley values and the LMG-GDI method) leading to the interesting trade-off of
 3 the relative weight approach, when focusing on the “Type-I” methods. Finally the study of the impact of changing
 4 the variance of some input variables shows that more investigations should be done to develop methods which can
 5 provide a dichotomy between the structural and correlative nature of the importance: this might be of a greater help
 6 in the purpose of ranking the variables.

7 APPENDIX A. APPENDIX

8 APPENDIX A.1 Normalised distributions and differences with higher correlation coefficients

9 In this section the distributions of the sensitivity indices and their differences in value and ranking are shown in
 10 Figure A.19, in Figure A.20 and in Figure A.21 respectively. As a remainder, the correlation coefficient original
 11 distribution is shown in Figure 2(c)(A) and these plots introduced below should be compared to the reference config-
 12 uration value exposed in § 3.2, knowing respectively Figure 11, Figure 12 and Figure 13.

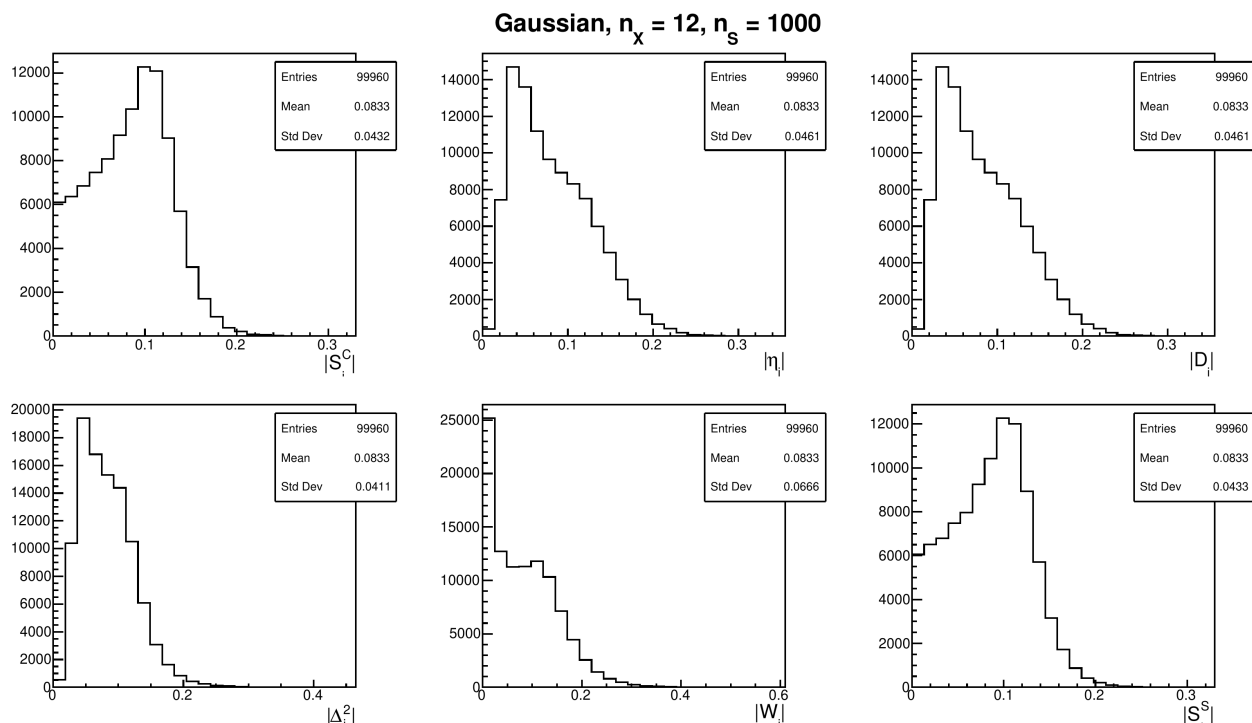


FIG. A.19: Distribution of the sensitivity indices for several thousand estimations of the basis configuration using the Archakov-Hansen approach with $(\gamma_0, \omega_0) = (0.15, 1)$. From left to right and top to bottom, the indices are shown in their normalised version as defined in equation (45): covariance-based, Shapley value, LMG-GDI, relative weight, weifila and the first-order coefficient.

1 As for the distributions in Figure 11, those in Figure A.19 have an average value of 8.33 % so about a twelfth of
2 the system output variance, but their standard deviations are consistently smaller, which is expected as the spread of
3 the correlation is more constrained in this configuration of the Archakov-Hansen approach.

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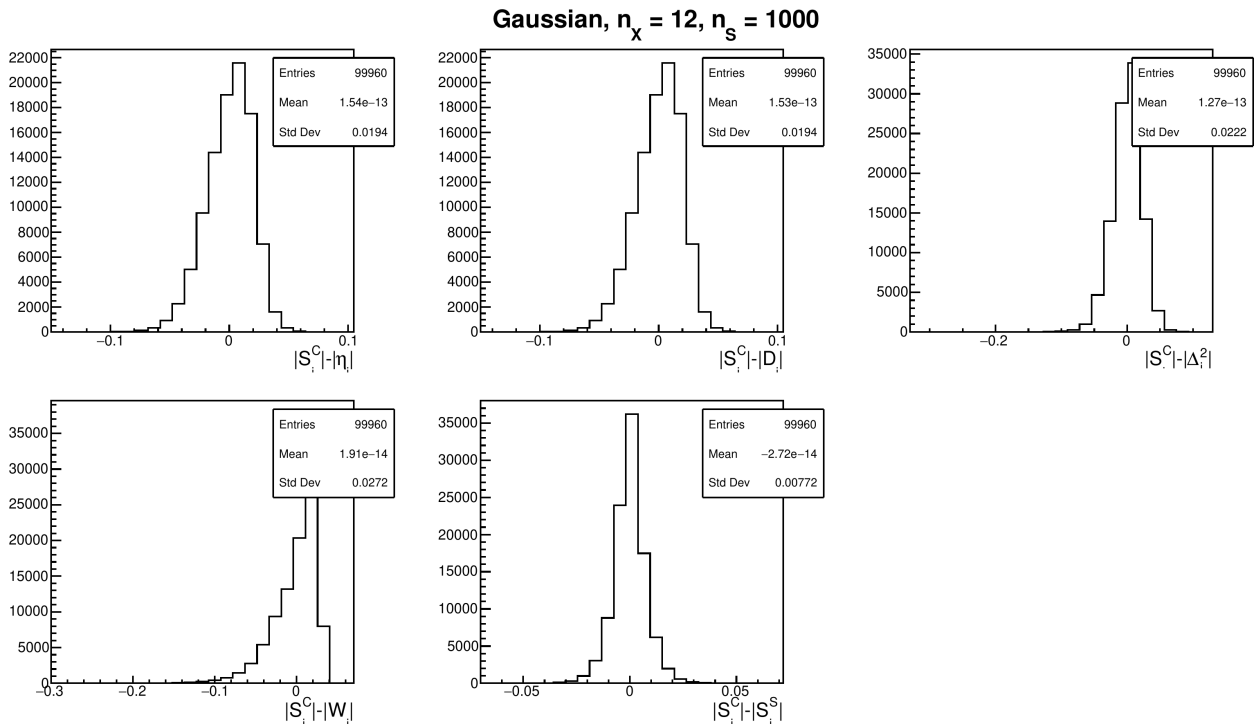


FIG. A.20: Differences of the normalised sensitivity indices with the normalised covariance-based results, for several thousand estimations using the Archakov-Hansen with $(\gamma_0, \omega_0) = (0.15, 1)$. The methods used are the Shapley values (top-left), the LMG-GDI (top-middle), the relative weight (top-right), the weifila (bottom-left) and the first-order coefficient (bottom-right).

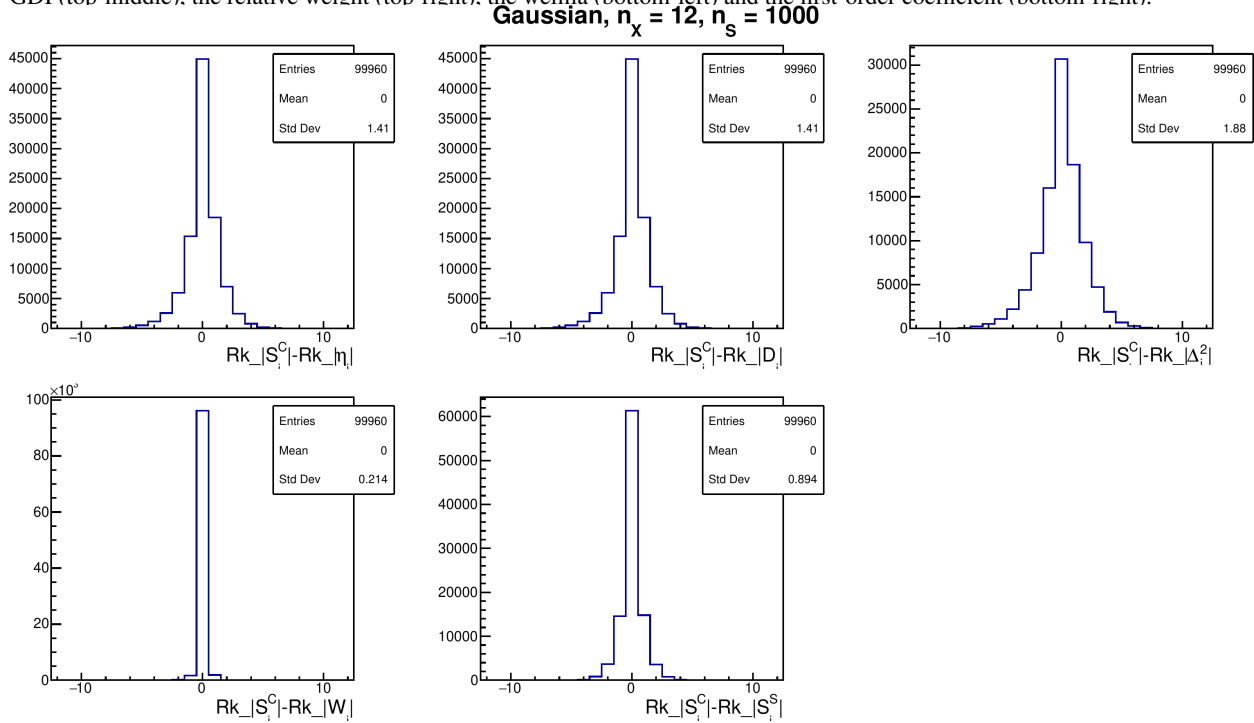


FIG. A.21: Differences of the rank of normalised sensitivity indices with respect to the normalised covariance-based ones, for several thousand estimations using the Archakov-Hansen $(\gamma_0, \omega_0) = (0.15, 1)$. The methods used are the Shapley values (top-left), the LMG-GDI (top-middle), the relative weights (top-right), the weifila (bottom-left) and the first-order coefficients (bottom-right).

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