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# Test comparison for Sobol indices over nested sets of variables

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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. One crucial question is then to decide whether a given set of variables has a significant impact on the output. Sobol indices are often used to measure this impact but their estimation can be difficult as they usually require a particular design of experiment. In this work, we take advantage of the monotonicity of Sobol indices with respect to set inclusion to test the influence of some of the input variables. The method does not rely on a direct estimation of the Sobol indices and can be performed under classical iid sampling designs.

**Keywords:** Global sensitivity indices, Sobol indices, significance test, Donsker's Theorem

**AMS subject classification** 60F05, 62G05, 62G20, 62E20, 62F03, 62F05.

## 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. [1, 10]) while sensitivity analysis and meta-modelling are intensively used to optimize the airplanes designs [16]. Meta-models usually depend on many input variables and are computationally expensive. Thus, it is crucial to understand which of the input parameters have an influence on the output. One classical approach to deal with this kind of problem is to consider the inputs as random elements, a point of view generally called (global) sensitivity analysis. We refer to [2, 17, 18] for an overview of the practical aspects.

Sobol indices, based on the Hoeffding decomposition [9] of the output's variance, are one of the most used tools to perform global sensitivity analysis. They were first introduced in [15] and later revisited in [19]. In the general framework, a square integrable output variable  $Y$  is assumed to obey a non-parametric relation of the form

$$Y = f(Z_1, \dots, Z_q) \tag{1}$$

where the  $Z_j$ 's are input variables and  $f$  is an unknown function. In practice, an analytical expression for  $f$  is usually not available and the only access we have to  $f$  is through experimentation or computer code. The Sobol index of  $Y$  with respect to a subset  $u \subset \{1, \dots, p\}$  of input variables is then defined by

$$S^{(u)} := \frac{\text{var}(\mathbb{E}[Y|Z_j, j \in u])}{\text{var}(Y)}.$$

One of the main tasks the practitioner has to deal with is to decide whether a group of variables has any influence on the output  $Y$ . This objective can be pursued by noticing that the equality of Sobol indices for nested sets  $u \subset v$  reduces to the (almost sure) equality of the conditional expectations:

$$\forall u, v, u \subset v : S^{(u)} = S^{(v)} \iff \mathbb{E}[Y|Z_j, j \in u] \stackrel{a.s.}{=} \mathbb{E}[Y|Z_j, j \in v].$$

Thus, a non-parametric notion of significance can be established by comparing Sobol indices over nested sets of input variables.

Many different estimation procedures of the Sobol indices have been proposed in the literature. Some are based on Monte-Carlo or quasi Monte-Carlo designs of experiment, see [12, 14]. More recently, a method based on nested Monte-Carlo [8] has been developed. Other estimation procedures are based on different designs of experiment using for example polynomial chaos expansions [20]. An efficient estimation of the Sobol indices can be performed through the so-called ‘‘Pick-Freeze’’ method, whose theoretical properties (consistency, central limit theorem, concentration inequalities and Berry-Esseen bounds) have been studied in [6, 11]. In particular, the joint central limit theorem enables to build asymptotic comparison tests on Sobol indices. However, the Pick-Freeze method requires a specific design of experiment which makes it inapplicable in the classical iid framework and computationally expensive (for instance, the  $p$  order one Sobol indices estimators need  $n(p+1)$  computations of the function  $f$ ). This drawback was recently partially solved in [5], where the order one Sobol indices are estimated from rank statistics in the classical iid sample scheme. Nevertheless, the absence of a joint CLT in this case makes it impossible to test hypotheses involving more than one Sobol index at a time.

In this work, we present an alternative way to build non-parametric significance tests, used for the detection of non-influent variables. A main motivation of the proposed procedure is to perform non-parametric variable selection, in order for instance to reduce the cost of a computational code or simplify a meta-model. The originality of our approach stems from a reformulation of the null hypothesis in terms of the empirical process, thus bypassing the difficulty of having to estimate the Sobol indices. This allows to perform multiple significance tests using a single sample, thus potentially reducing the computational cost compared to alternative methods that rely on specific sampling designs. The framework and theoretical setting are presented in Section 2. Section 3 is dedicated to the construction of level  $\alpha$  statistical tests. In Section 4, we carry out a numerical study to compare the new statistical test procedure to the classical one introduced in [6, 11].

## 2 Theoretical framework

We consider the model

$$Y \stackrel{a.s.}{=} f(Z_1, \dots, Z_q) \tag{2}$$

and for any subsets  $u$  and  $v$  of  $\{1, \dots, q\}$  such that  $u \subset v$  we are interested in constructing a non-parametric significance test for either

- $H_0$  ;  $S^{(u)} = 0$  against  $H_1$  :  $S^{(u)} > 0$  or
- $H_0$  ;  $S^{(u)} = S^{(v)}$  against  $H_1$  :  $S^{(u)} < S^{(v)}$ .

Now if  $v = \{j_1, j_2, \dots, j_p\}$  then setting  $X_k = Z_{j_k}$ , the model (2) can always be rewritten as follows

$$Y \stackrel{a.s.}{=} f(X, W). \quad (3)$$

with  $X = (X_1, \dots, X_p)$  and  $W = (Z_j)_{j \notin v}$ .

We assume that  $Y$  is square-integrable, in which case the conditional expectation  $\mathbb{E}[Y|X]$  can be defined as an orthogonal projection of  $Y$  in  $\mathbb{L}^2$  onto the linear space of square integrable measurable functions of  $X$ . In particular, the Hoeffding decomposition

$$\text{var}(Y) = \text{var}(\mathbb{E}[Y|X]) + \text{var}(Y - \mathbb{E}[Y|X])$$

follows from the Pythagorean theorem. The Sobol index of  $Y$  associated to  $X$  is defined by

$$S = \frac{\text{var}(\mathbb{E}[Y|X])}{\text{var}(Y)} \in [0; 1].$$

For any subset  $u$  of  $\{1, \dots, p\}$  and  $x = (x_1, \dots, x_p) \in \mathbb{R}^p$ , we denote  $x^{(u)} = (x_j)_{j \in u}$  with the convention  $x^{(u)} = 0$  if  $u = \emptyset$ , and by  $S^{(u)}$  the Sobol index associated to  $X^{(u)}$ :

$$S^{(u)} = \frac{\text{var}(\mathbb{E}[Y|X^{(u)}])}{\text{var}(Y)} \in [0, 1]. \quad (4)$$

Remark that, in view of the characterization of the conditional expectation as an orthogonal projection, Sobol indices are non-decreasing with respect to set inclusion:  $u \subseteq v \implies S^{(u)} \leq S^{(v)}$ . Letting  $\bar{u} = \{1, \dots, p\} \setminus u$ , we say that the variables  $X^{(\bar{u})}$  are not significant to explain  $Y$  in the presence of  $X^{(u)}$  if

$$\mathbb{E}[Y|X^{(u)}] = \mathbb{E}[Y|X]$$

or equivalently, if  $S^{(u)} = S$ . Remark that since the conditional expectation is only defined in an almost sure sense, the equality here, and throughout, is meant almost surely. The aim of this paper is to construct a non-parametric significance test based on the hypotheses

$$H_0 : S^{(u)} = S \quad \text{against} \quad H_1 : S^{(u)} < S.$$

The global Sobol index  $S$  is allowed to be smaller than one so that any nested non-parametric significance test can be performed using an appropriate choice for  $X$  and  $u$ , leaving the remaining unused variables as part of  $W$ . For instance, the significance of a single variable  $X_1$  via the null hypothesis  $H_0 : \mathbb{E}[Y|X_1] = \mathbb{E}[Y]$  is achieved by setting  $X = X_1$  and  $u = \emptyset$ .

**Paragraph de justification avec computer code** When rewriting the model (2) in the framework of Equation (3) the variable  $W$  can be interpreted in two ways

1. You discard in  $W$  all the variables you are not interested in (which is the approach we use in this work)

2. Or  $W$  is seen as an extra hidden random input which is naturally present for classical modelization of stochastic codes, we refer to [13, 4] for more details. Hence all our methodology applies when working with stochastic codes. Nevertheless, we decide to focuss our work on the classical framework of deterministic black box.

A natural test for  $H_0$  exists whenever one can construct estimators of the Sobol indices with known (or estimable) joint limit distribution. However, typical estimation methods such as Pick-Freeze usually requires a specific design of experiment. The test procedure proposed in this paper does not rely on a direct estimation of the Sobol indices and applies in the typical iid sampling design. The method makes use of an equivalent formulation of  $H_0$  described in Lemma 2.1 below.

For two vectors  $a = (a_1, \dots, a_k), b = (b_1, \dots, b_k), a \wedge b := (a_1 \wedge b_1, \dots, a_k \wedge b_k)$  denotes the component-wise minimum, while the inequality  $a \leq b$  is meant as  $a \wedge b = a$ . The indicator function is denoted by  $\mathbb{1}\{\cdot\}$ .

**Lemma 2.1.** *If  $X_1, \dots, X_p, W$  are independent, then for all  $u \subseteq \{1, \dots, p\}$ , the following assertions are equivalent:*

- i)  $S^{(u)} = S$ .
- ii)  $\mathbb{E}[Y|X^{(u)}] = \mathbb{E}[Y|X]$ .
- iii) For all  $x \in \mathbb{R}^p$  such that  $\mathbb{P}(X \leq x) > 0$ ,  $\mathbb{E}[Y|X^{(u)} \leq x^{(u)}] = \mathbb{E}[Y|X \leq x]$ .
- iv) For all  $x \in \mathbb{R}^p$ ,  $\mathbb{E}[Y\mathbb{1}\{X \leq x\}] = \mathbb{E}[Y\mathbb{1}\{X^{(u)} \leq x^{(u)}\}]\mathbb{P}(X^{(\bar{u})} \leq x^{(\bar{u})})$ .

*Proof.* Let  $Z = \mathbb{E}[Y|X]$  and remark that  $\mathbb{E}[Y|X^{(u)}] = \mathbb{E}[Z|X^{(u)}]$ . The equivalence between i) and ii) follows from the well known decomposition

$$\text{var}(Z) = \text{var}(\mathbb{E}[Z|X^{(u)}]) + \mathbb{E}[\text{var}(Z|X^{(u)})],$$

where the non-negative term  $\mathbb{E}[\text{var}(Z|X^{(u)})]$  is zero if, and only if,  $\mathbb{E}[Z|X^{(u)}] = Z$ . By definition of the conditional expectation

$$\mathbb{E}[Y|X] = \mathbb{E}[Y|X^{(u)}] \iff \forall x \in \mathbb{R}^p, \mathbb{E}[Y\mathbb{1}\{X \leq x\}] = \mathbb{E}[\mathbb{E}[Y|X^{(u)}]\mathbb{1}\{X \leq x\}].$$

The independence of the  $X_j$ 's and the fact that  $\mathbb{1}\{X \leq x\} = \mathbb{1}\{X^{(u)} \leq x^{(u)}\}\mathbb{1}\{X^{(\bar{u})} \leq x^{(\bar{u})}\}$  give

$$\mathbb{E}[\mathbb{E}[Y|X^{(u)}]\mathbb{1}\{X \leq x\}] = \mathbb{E}[Y\mathbb{1}\{X^{(u)} \leq x^{(u)}\}]\mathbb{P}(X^{(\bar{u})} \leq x^{(\bar{u})})$$

which shows ii)  $\iff$  iv). The equivalence iii)  $\iff$  iv) follows by dividing both sides of the equality iii) by  $\mathbb{P}(X \leq x)$ .  $\square$

Assume we observe an iid sample  $(Y_1, X_1), \dots, (Y_n, X_n)$  drawn from the same distribution as  $(Y, X)$ . For all  $k \in \{0, 1, 2\}$  and  $u \subseteq \{1, \dots, p\}$ , let  $m_k^{(u)} : x \mapsto \mathbb{E}[Y^k\mathbb{1}\{X^{(u)} \leq x^{(u)}\}]$  and denote by  $\hat{m}_k^{(u)}(\cdot)$  its empirical counterpart:

$$\hat{m}_k^{(u)}(x) = \frac{1}{n} \sum_{i=1}^n Y_i^k \mathbb{1}\{X_i^{(u)} \leq x^{(u)}\}, \quad x \in \mathbb{R}^p.$$

For ease of notation, we shall simply write  $m_k$  and  $\hat{m}_k$  for the case  $u = \{1, \dots, p\}$ . By Lemma 2.1, we know that the null hypothesis  $H_0 : S^{(u)} = S$  can be stated as  $\xi := m_1 - m_1^{(u)}m_0^{(\bar{u})}$  being identically zero.

In this logic, we use the empirical version  $\widehat{\xi}$  to build a test statistics for  $H_0$ .

For the next proposition, we denote by  $\eta = (m_1, m_1^{(u)}, m_0^{(\bar{u})})^\top$  and  $\widehat{\eta} := (\widehat{m}_1, \widehat{m}_1^{(u)}, \widehat{m}_0^{(\bar{u})})^\top$  its empirical counterpart. Moreover, let us write  $x^{(u)} \oplus x'^{(\bar{u})}$  for the vector of  $\mathbb{R}^p$  with components  $x_i$  if  $i \in u$  and  $x'_i$  if  $i \notin u$ .

**Proposition 2.2.** *The normalized process  $\sqrt{n}(\widehat{\eta} - \eta)$  converges in finite-dimensional distribution towards a 3-dimensional centered Gaussian field indexed by  $\mathbb{R}^p$  with auto-covariance function*

$$\Omega(x, x') := \begin{bmatrix} m_2(x \wedge x') & m_2((x \wedge x')^{(u)} \oplus x^{(\bar{u})}) & m_1(x^{(u)} \oplus (x \wedge x')^{(\bar{u})}) \\ m_2((x \wedge x')^{(u)} \oplus x'^{(\bar{u})}) & m_2^{(u)}(x \wedge x') & m_1(x^{(u)} \oplus x'^{(\bar{u})}) \\ m_1(x'^{(u)} \oplus (x \wedge x')^{(\bar{u})}) & m_1(x'^{(u)} \oplus x^{(\bar{u})}) & m_0^{(\bar{u})}(x \wedge x') \end{bmatrix} - \eta(x)\eta(x')^\top$$

for all  $x, x' \in \mathbb{R}^p$ .

The proof is a straightforward consequence of the central-limit theorem. The convergence in distribution can be shown without any particular obstacle using Vapnik-Chervonenkis' theory although this result is not needed for the theoretical validity of the test.

### 3 The test procedure

Consider the process  $\widehat{\xi} = \widehat{m}_1 - \widehat{m}_1^{(u)}\widehat{m}_0^{(\bar{u})}$ , whose asymptotic distribution can be derived from the delta method applied to the smooth function  $\phi : (s, t, u) \mapsto s - tu$  from  $\mathbb{R}^3$  to  $\mathbb{R}$ , using Proposition 2.2. Given a fixed collection  $\mathbf{x} = (x_1, \dots, x_K)$  of points in  $\mathbb{R}^p$  chosen independently from the sample, the random vector  $\widehat{\xi}(\mathbf{x}) = (\widehat{\xi}(x_1), \dots, \widehat{\xi}(x_K))^\top$  is asymptotically Gaussian

$$\sqrt{n}(\widehat{\xi}(\mathbf{x}) - \xi(\mathbf{x})) \xrightarrow[n \rightarrow \infty]{d} \mathcal{N}(0, \Sigma(\mathbf{x}))$$

with covariance matrix

$$\Sigma(\mathbf{x}) := \left( \nabla \phi(x_k)^\top \Omega(x_k, x_{k'}) \nabla \phi(x_{k'}) \right)_{k, k'=1, \dots, K}.$$

The empirical version  $\widehat{\Sigma}(\mathbf{x})$  obtained by replacing the functions  $m_k^{(u)}$  by their empirical counterparts  $\widehat{m}_k^{(u)}$ , is clearly a consistent estimator of  $\Sigma(\mathbf{x})$  in virtue of the law of large numbers. Since the hypothesis  $H_0 : S^{(u)} = S$  can be stated equivalently as  $H_0 : \xi = 0$ , a test can be performed by comparing the observed value of  $\|\widehat{\xi}(\mathbf{x})\|$  (for a well chosen norm  $\|\cdot\|$  on  $\mathbb{R}^K$ ) to the appropriate quantile of the asymptotic distribution under  $H_0$ . Two natural approaches are then possible:

1. If  $\|\cdot\|$  is the natural Euclidean norm on  $\mathbb{R}^K$ , then under  $H_0$ ,

$$T := n\|\widehat{\xi}(\mathbf{x})\|^2 = n \sum_{k=1}^K \widehat{\xi}(x_k)^2 \tag{5}$$

converges in distribution towards a weighted  $\chi^2$  distribution with weights given by the eigenvalues  $\lambda_1, \dots, \lambda_K \geq 0$  of  $\Sigma(\mathbf{x})$ . In other words,  $n\|\widehat{\xi}(\mathbf{x})\|^2$  has the same distribution asymptotically (under  $H_0$ ) as  $\epsilon^\top \Sigma(\mathbf{x}) \epsilon$  where  $\epsilon$  is a standard Gaussian vector in  $\mathbb{R}^K$ . This distribution can be approximated

by Monte-Carlo using the empirical version  $\widehat{\Sigma}(\mathbf{x})$  instead of the unknown  $\Sigma(\mathbf{x})$ , in order to determine the threshold  $\tau_\alpha$  over which the hypothesis is rejected, at any given significance level  $\alpha \in (0, 1)$ . The Monte-Carlo part can be time consuming as a large number of replications may be needed to approximate the asymptotic distribution and corresponding quantile sufficiently well.

2. A different approach consists in normalizing the vector  $\widehat{\xi}(\mathbf{x})$  in order to achieve a true (non-weighted)  $\chi^2$  asymptotic distribution under  $H_0$ . If  $\Sigma(\mathbf{x})$  is invertible, with inverse  $\Gamma(\mathbf{x})$ , a test statistics

$$T := n\widehat{\xi}(\mathbf{x})^\top \widehat{\Gamma}(\mathbf{x})\widehat{\xi}(\mathbf{x}) \quad (6)$$

for  $\widehat{\Gamma}(\mathbf{x})$  a consistent estimator of  $\Gamma(\mathbf{x})$ , has the asymptotic distribution  $\chi^2(K)$  under  $H_0$ , as  $n \rightarrow \infty$ . In practice, the naive estimator

$$\widehat{\Gamma}(\mathbf{x}) = \widehat{\Sigma}(\mathbf{x})^{-1}$$

is rarely a good choice, especially if  $\widehat{\Sigma}(\mathbf{x})$  is close to singular. In this case, a regularized version of the inverse leads to a better approximation of the asymptotic distribution. Typically,  $\widehat{\Gamma}(\mathbf{x})$  can be obtained by truncated singular value decomposition where the eigenvalues of  $\widehat{\Sigma}(\mathbf{x})$  below a certain threshold  $t$  are ignored (see for instance [3] for further details on inverse matrix regularization). The observed value of the test statistics is then compared to the quantile of the  $\chi^2$  distribution with  $r = \text{rank}(\widehat{\Gamma}(\mathbf{x}))$  degrees of freedom. In the numerical study, we use the regularization threshold  $t = 0.1n^{-1/3}\rho(\widehat{\Sigma}(\mathbf{x}))\lambda_1$  where  $\lambda_1$  is the largest eigenvalue of  $\widehat{\Sigma}(\mathbf{x})$ , which ensures in particular that  $r \geq 1$ . Further details are discussed in Section 4.

For both these approaches, the number  $K$  of points over which the empirical process  $\widehat{\xi}$  is evaluated is only constrained by the computation time. A larger experimental design  $\mathbf{x}$  may improve the power of the test with no negative impact on the significance level, as we discuss in Section 4.

In practice, the  $x_k$ 's may be drawn uniformly on the domain of  $X$  if it is bounded, or from an arbitrary distribution  $\mu$  on  $\mathbb{R}^p$ . In this case, the normalized test statistics can be viewed as a Monte-Carlo approximation of the integral  $\int n\widehat{\xi}^2 d\mu$ . Although possible in practice, we do not recommend using the available sample  $(X_1, \dots, X_n)$  as the design due to the poor resulting performance of the test. If the distribution of the  $X_i$ 's is known to the practitioner, we may use the same distribution to draw the  $x_k$ 's. Under the alternative  $H_1$ , the power of the test highly depends on the design  $\mathbf{x}$  (or the underlying distribution  $\mu$ ) which should ideally favor regions of the space for which  $\xi$  is far from zero, enabling the test statistics to grow more rapidly to infinity.

## 4 Numerical application

Let  $(Y_1, X_1), \dots, (Y_n, X_n)$  be an iid sample on  $\mathbb{R} \times \mathbb{R}^3$  obeying the relation

$$Y_i = f(X_i) , \quad i = 1, \dots, n$$

where

$$f(x) = (2 + x_3^4) \sin(x_1) + 7 \sin^2(x_2) , \quad x = (x_1, x_2, x_3) \in \mathbb{R}^3.$$

The  $X_i$ 's are assumed independent with the uniform distribution on  $[-\pi, \pi]^3$ . This function is commonly used in sensitivity analysis as a test case and is classically referred to as the Ishigami function.

From the two possible approaches discussed in the previous section, we choose the second one due to its faster computation time. Thus, the test statistics is given by

$$T = n\widehat{\xi}(\mathbf{x})^\top \widehat{\Gamma}(\mathbf{x})\widehat{\xi}(\mathbf{x})$$

where  $\widehat{\Gamma}(\mathbf{x})$  is a regularized inverse of the empirical estimator  $\widehat{\Sigma}(\mathbf{x})$ , whose precise construction will be detailed below.

The experimental design  $\mathbf{x} = (x_1, \dots, x_K)$  is drawn from the same distribution as the original sample, namely a uniform distribution on  $[-\pi, \pi]^3$ . We draw  $K = 10$  points to build the test. This seemingly small value ended up providing satisfactory results while keeping the computation time reasonable. The power of the test can be slightly improved by taking a larger experimental design  $\mathbf{x}$  but the additional time is too much amplified in our framework where numerous replications were made to evaluate the performances of the test. For an actual application of the method where the algorithm is run only once, the computation takes at most a few minutes and the size of  $\mathbf{x}$  is not much of a limiting factor.

The matrix  $\widehat{\Gamma}(\mathbf{x})$  is obtained from a truncated singular value decomposition of  $\widehat{\Sigma}(\mathbf{x})$ . Precisely, let  $\lambda_1 \geq \dots \geq \lambda_K$  be the ordered eigenvalues of  $\widehat{\Sigma}(\mathbf{x})$  and consider the singular value decomposition

$$\widehat{\Sigma}(\mathbf{x}) = P \text{Diag}(\lambda_1, \dots, \lambda_K) P^\top$$

where  $P$  is orthogonal (i.e.  $PP^\top = P^\top P = I$ ). We define

$$\widehat{\Gamma}(\mathbf{x}) = P \text{Diag}(g_t(\lambda_1), \dots, g_t(\lambda_K)) P^\top$$

where  $g_t$  is the so-called truncated SVD filter function  $g_t(x) = 1/x$  if  $x > t$  and  $g_t(x) = 0$  otherwise. The test statistics  $T$  is then compared to the quantile of the  $\chi^2$  distribution with  $r$  degrees of freedom, where  $r = \text{rank}(\widehat{\Gamma}(\mathbf{x}))$  is the number of eigenvalues of  $\widehat{\Sigma}(\mathbf{x})$  larger than  $t$ . The hypothesis is rejected if the observed value of  $T$  exceeds the  $(1 - \alpha)$ -quantile of the  $\chi^2(r)$  distribution. To ensure that  $r > 0$ , we choose  $t$  equal to a vanishing proportion  $\tau_n \in (0, 1)$  of the spectral radius  $\lambda_1$  of  $\widehat{\Sigma}(\mathbf{x})$ :

$$t = \tau_n \lambda_1. \tag{7}$$

The rule of thumb  $\tau_n = 0.1n^{-1/3}$  is used in the simulations.

The test statistics and resulting p-values are calculated over  $N = 10000$  replications of the experiments. Four different hypotheses are considered:

1.  $H_0 : S^{(3)} = 0 \iff \mathbb{E}[Y|X_3] = \mathbb{E}[Y]$
2.  $H_0 : S^{(2,3)} = S^{(2)} \iff \mathbb{E}[Y|X_2, X_3] = \mathbb{E}[Y|X_2]$
3.  $H_0 : S^{(1)} = 0 \iff \mathbb{E}[Y|X_1] = \mathbb{E}[Y]$
4.  $H_0 : S^{(1,3)} = S^{(1)} \iff \mathbb{E}[Y|X_1, X_3] = \mathbb{E}[Y|X_1]$

As discussed previously, these hypotheses boil down to testing the non-parametric significance of some input variables, e.g. the first one reduces to testing the influence of  $X_3$  on  $Y$  while the second one corresponds to testing the influence of  $X_3$  in presence of  $X_2$ . The null hypothesis is true in the first two cases

where the simulations aim to evaluate the actual significance level as a function of the nominal value  $\alpha$  the test is supposed to achieve. For the last two cases, the null hypothesis is false with actual values of the Sobol indices being and  $S^{(1)} \approx 0.402$  and  $S^{(1,3)} \approx 0.989$ . The simulations thus aim to evaluate the power of the test in these last two cases.

The results are compared with the test built from the Pick-Freeze estimators of the Sobol indices presented in [7]. For each scenario, the expression in Equation (3) is used, and the p-value for the unilateral test is calculated. To easily differentiate the results of the two methods in what follows, the Pick-Freeze based test will be abbreviated to PF, while the method introduced in this paper will be referred to as the Empirical Process (EP) test.

We represent the probability of rejecting the null hypothesis for all  $\alpha \in [0, 1]$  to give a global view of the distribution of the p-value, although, only the discrepancies between the actual and nominal values for  $\alpha$  smaller than say 0.1 (the range of values typically used in practice) are relevant to measure the reliability of the test procedure for practical purposes. The results are computed for three sample sizes  $n$  which designate the number of calls to the function  $f$ . We emphasize that a specific sampling design is needed for the Pick-Freeze method, which is not the case for the EP test. In particular, all four hypotheses can be tested from a unique sample by the EP approach while individual samples need to be generated for each hypothesis for the PF test. In this aspect, the EP test provides a clear advantage to reduce the number of calls to  $f$  if multiple hypotheses are to be tested.

Probability of rejecting  $H_0 : S^{(3)} = 0$

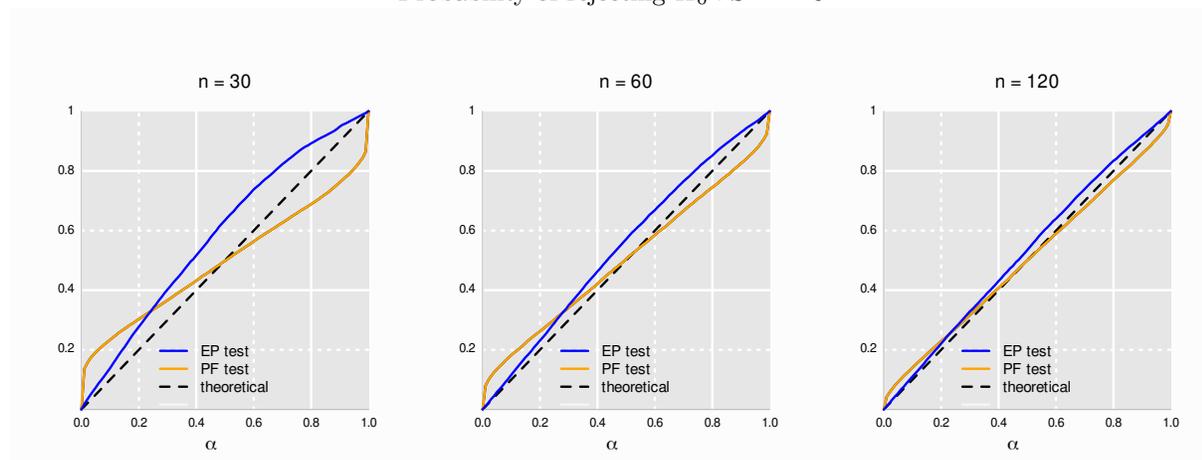


Figure 1: Estimated probability of rejecting the null hypothesis  $H_0 : S^{(3)} = 0$  for the Empirical Process (EP) and Pick-Freeze (PF) tests. The empirical cdf of the tests' p-values are calculated on  $N = 10000$  iterations and return the (estimated) actual significance level of the test as a function of the nominal level  $\alpha$ .

Probability of rejecting  $H_0 : S^{(2,3)} = S^{(2)}$

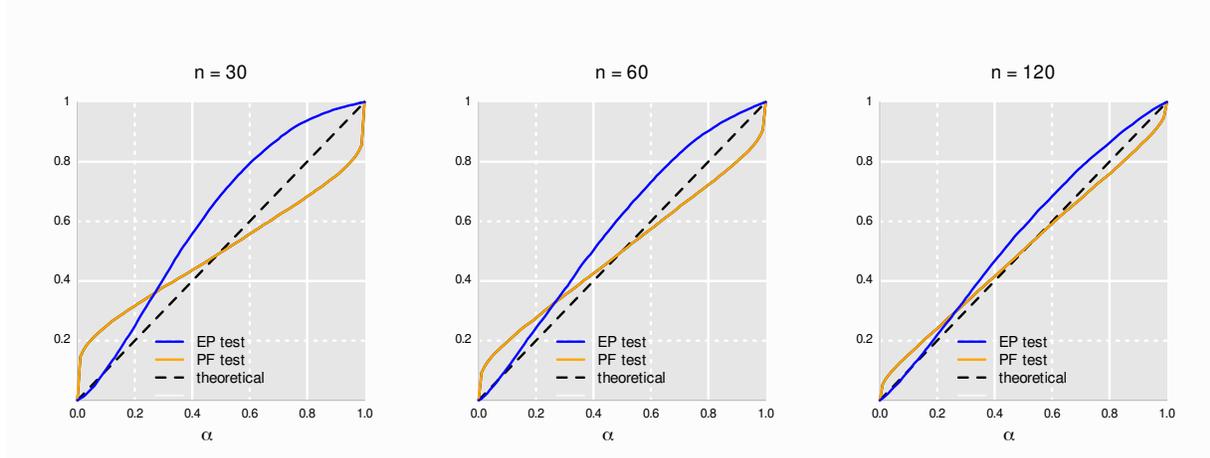


Figure 2: Estimated probability of rejecting the null hypothesis  $H_0 : S^{(2,3)} = S^{(2)}$  for the EP and PF tests, as a function of the nominal significance level  $\alpha$ .

As seen in Figures 1, and 2, the EP method appears more reliable than the PF approach for the null hypotheses  $H_0 : S^{(3)} = 0$  and  $H_0 : S^{(2,3)} = S^{(2)}$ , as the (estimated) actual significance level is closer to the nominal value. Here, the rule of thumb with  $\tau_n = 0.1n^{-1/3}$  used for the TSVD regularization of  $\hat{\Sigma}(\mathbf{x})$  seems to yield a well calibrated test for a nominal significance level  $\alpha$  below 10%. Unsurprisingly, the discrepancy is more pronounced for small sample sizes. The PF test seems unreliable in these cases as shown by the highly underestimated significance level for small values of  $\alpha$ . This could be due to a too slow convergence of the Sobol index estimator to a Gaussian distribution, on which the calculations of the critical regions of the PF test are based on.

Probability of rejecting  $H_0 : S^{(1)} = 0$

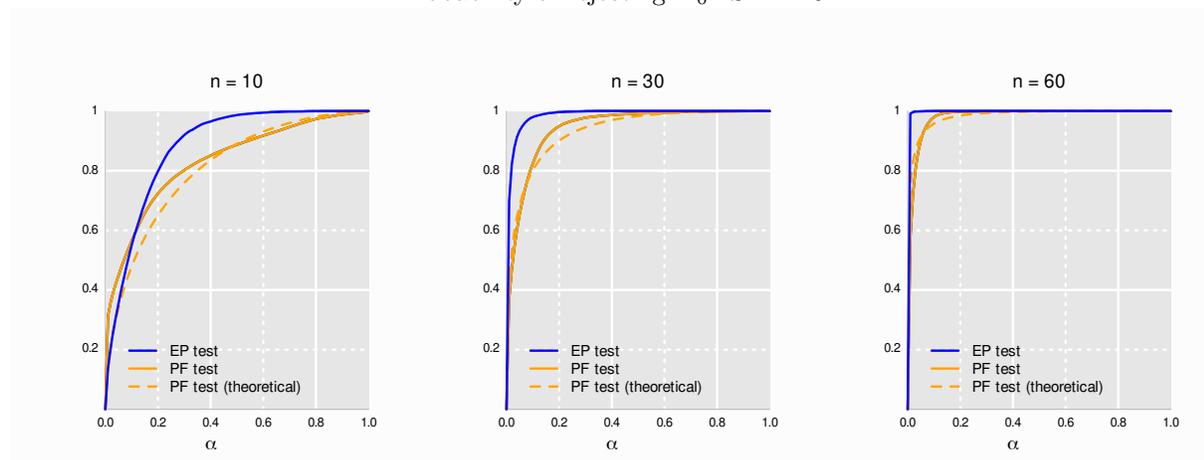


Figure 3: Estimated probability of rejecting the null hypothesis  $H_0 : S^{(1)} = 0$  for the EP and PF tests. The orange dashed line gives the asymptotic theoretical power of the PF test obtained under the limit Gaussian distribution of the Pick-Freeze estimator of  $S^{(1)}$ . In this case where the null hypothesis is not verified ( $S^{(1)} \approx 0.402$ ), the empirical cdf of the tests' p-values returns the estimated power of the test as a function of the nominal significance level  $\alpha$ .

Probability of rejecting  $H_0 : S^{(1,3)} = S^{(1)}$

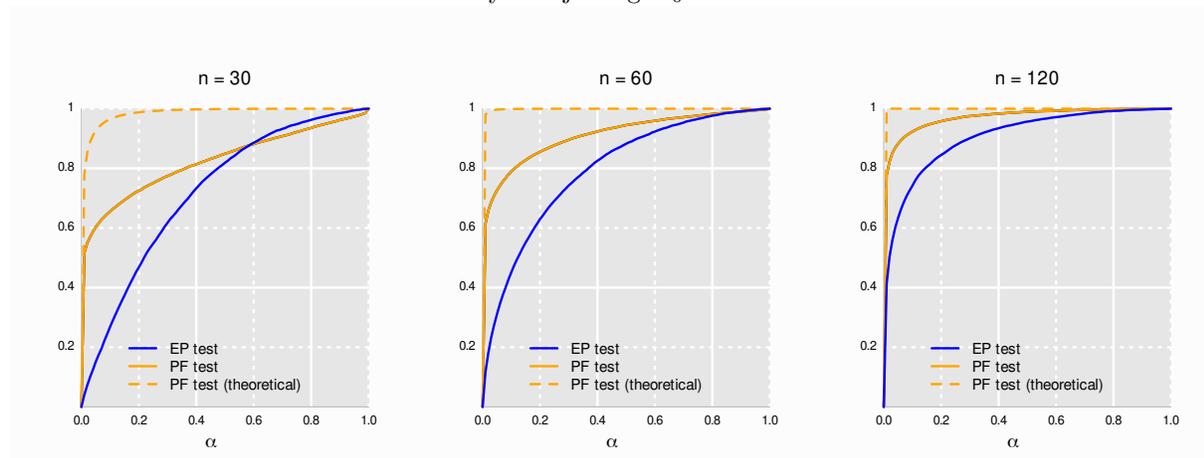


Figure 4: Power of the EP and PF tests for the null hypothesis  $H_0 : S^{(1,3)} = S^{(1)}$  as a function of the significance level  $\alpha$ . The null hypothesis is false in this case where the true values of the Sobol indices actually differ from  $S^{(1,3)} - S^{(1)} \approx 0.587$ .

Figures 3 and 4 display the estimated probability of rightfully rejecting  $H_0 : S^{(1)} = 0$  and  $H_0 : S^{(1,3)} = S^{(1)}$  respectively, as a function of the nominal significance level  $\alpha$  for the EP and PF tests. The EP test seems to perform better overall for the simple hypothesis  $H_0 : S^{(1)} = 0$ . The power rapidly converges

towards 1 for both tests, which conveys the high (non-parametric) influence of  $X_1$  in this situation. The Gaussian approximation used to calibrate the PF test is satisfactory in this case as shown by the theoretical asymptotic power being close to its actual value. On the contrary, the PF test rightfully rejects the null hypothesis  $H_0 : S^{(1,3)} = S^{(1)}$  more often than the EP test. Despite the relatively high difference  $S^{(1,3)} - S^{(1)} \approx 0.587$ , the EP test is less powerful than for the previous simple hypothesis  $H_0 : S^{(1)} = 0$ . Nevertheless, while the PF test is more powerful in this case, the convergence to the Gaussian limit appears to be slow as indicated by the high difference between the theoretical asymptotic power and its actual value.

Probability of rejecting  $H_0$

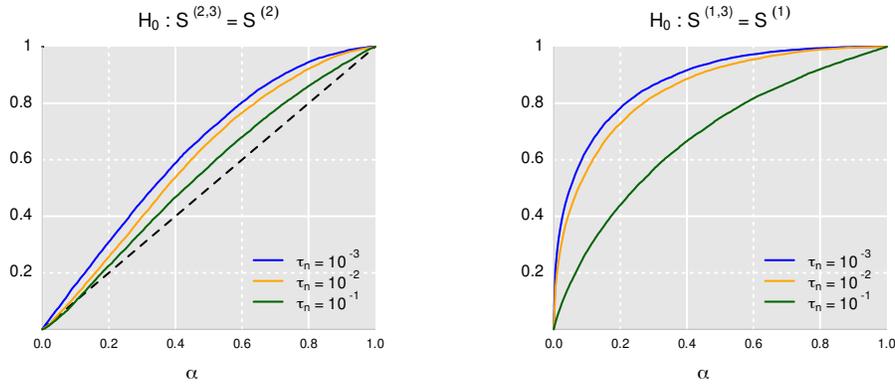


Figure 5: Estimated significance level for  $H_0 : S^{(2,3)} = S^{(2)}$  (left) and power for  $H_0 : S^{(1,3)} = S^{(1)}$  (right) for a TSVD threshold obtained with  $\tau_n = 10^{-3}, 10^{-2}$  and  $10^{-1}$  (see Eq. (7)). The sample size is  $n = 60$  and design size  $K = 10$ .

Finally, the calibration of the regularization threshold used in the estimation of  $\Gamma(\mathbf{x})$  has a non negligible impact on the quality of the test. In Figure 5, we show the difference in both power and significance level for three different values of  $\tau_n$ . In this case, the rule of thumb gives the somewhat conservative  $\tau_n = 0.1n^{-1/3} \approx 0.026$ , which ensures a reliable test in term of significance level. Remark that although both thresholds  $\tau_n = 10^{-2}$  and  $\tau_n = 10^{-1}$  lead to similar and somewhat accurate levels, we observe a significant improvement in term of power. This suggests that the EP test procedure has room for improvement, at least through optimizing the choice of the regularization threshold.

#### 4.1 Fuel consumption for aeronautical missions (Nicolas)

the aeronautical and aerospace sector. Fuel consumption in aeronautics is  
Description des données:

- Liste des variables d'entrée (inputs)  $X_1, \dots, X_p$
- Variable de sortie (sur-consommation)  $Y$
- D'où proviennent les données

- Motivation: comprendre et limiter la sur-consommation

The behavior of the excess fuel consumption  $Y$  with respect to each of the nine inputs is shown in Figure 6. Since in this model, the input variables are real valued, we use the estimators based on rank statistics (see [5] for the definition of this estimator and its theoretical properties) to estimate all the order one Sobol indices using the unique sample we have at our disposal.

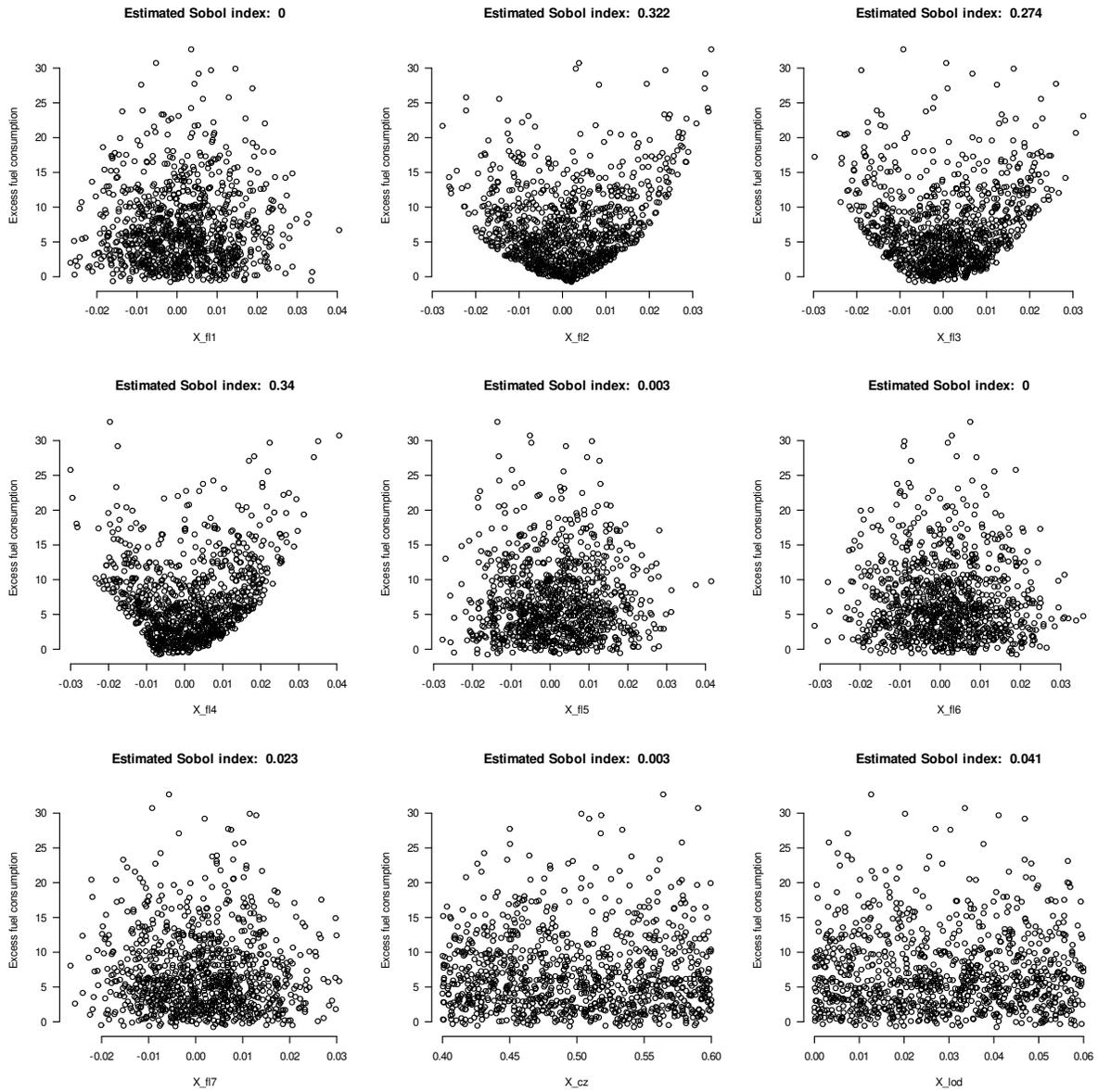


Figure 6: Bi-variate representation of the excess fuel consumption with respect to each of the inputs  $X_{f11}, \dots, X_{f17}, X_{cz}, X_{lod}$ , with the associated estimated simple Sobol index.

	$X_{\text{fl1}}$	$X_{\text{fl2}}$	$X_{\text{fl3}}$	$X_{\text{fl4}}$	$X_{\text{fl5}}$	$X_{\text{fl6}}$	$X_{\text{fl7}}$	$X_{\text{cz}}$	$X_{\text{lod}}$
p-value (Test 1)	0.5367	0	0	0	0.896	0.387	0.394	0.704	0.867
p-value (Test 2)	0.778	0	0	0	0.938	0.283	0.502	0.615	0.571

Table 1: p-values of the tests for the simple hypothesis  $H_0 : S^X = 0$  calculated for the nine inputs  $X = X_{\text{fl1}}, \dots, X_{\text{fl7}}, X_{\text{cz}}, X_{\text{lod}}$  individually. Both approaches for the computation of the p-values, namely that of Eq.(5) (Test 1) and the less time consuming Eq.(6) (Test 2), are considered.

As we can see, only the inputs  $X_{\text{fl2}}, X_{\text{fl3}}, X_{\text{fl4}}$  are judged relevant individually to explain the excess fuel consumption. Moreover, denoting by  $S$  the global Sobol index associated to all nine inputs, the tests for the null hypothesis

$$H_0 : S^{X_{\text{fl2}}, X_{\text{fl3}}, X_{\text{fl4}}} = S$$

returns p-values of around 0.48 and 0.73 respectively. This indicates that the inputs  $X_{\text{fl2}}, X_{\text{fl3}}, X_{\text{fl4}}$  are sufficient to explain the excess fuel consumption, and no effect of possible interactions with other inputs is detected. Based on these results, it is tempting to assume a non-parametric relation of the form

$$\mathbb{E}(Y|X_{\text{fl1}}, \dots, X_{\text{fl7}}, X_{\text{cz}}, X_{\text{lod}}) = f(X_{\text{fl2}}, X_{\text{fl3}}, X_{\text{fl4}}).$$

The test can then be used as a tool for non-parametric variable selection, where the influence of each input, either added to or removed from the model, can be tested individually. For instance, the significance of  $X_{\text{fl2}}$  in the model is calculated by considering the null hypothesis

$$H_0 : S^{X_{\text{fl2}}, X_{\text{fl3}}, X_{\text{fl4}}} = S^{X_{\text{fl3}}, X_{\text{fl4}}}.$$

The test returns a p-value of zero for all three inputs  $X_{\text{fl2}}, X_{\text{fl3}}, X_{\text{fl4}}$  confirming their high individual significance in this model. Conversely, the significance of an input excluded from the model, say  $X_{\text{fl1}}$  for instance, is assessed by considering the null hypothesis

$$H_0 : S^{X_{\text{fl2}}, X_{\text{fl3}}, X_{\text{fl4}}} = S^{X_{\text{fl1}}, X_{\text{fl2}}, X_{\text{fl3}}, X_{\text{fl4}}}.$$

The results, summarized in the next table, conclude unambiguously that none of the input excluded from the model carry any additional information on the excess fuel consumption.

	$X_{\text{fl1}}$	$X_{\text{fl5}}$	$X_{\text{fl6}}$	$X_{\text{fl7}}$	$X_{\text{cz}}$	$X_{\text{lod}}$
p-value (Test 1)	0.776	0.229	0.822	0.365	0.734	0.998
p-value (Test 2)	0.715	0.294	0.375	0.422	0.413	0.815

Table 2: p-values of the EP test to assess the significance of the inputs  $X_{\text{fl1}}, X_{\text{fl5}}, X_{\text{fl6}}, X_{\text{fl7}}, X_{\text{cz}}, X_{\text{lod}}$  in presence of  $X_{\text{fl2}}, X_{\text{fl3}}, X_{\text{fl4}}$ . Both test statistics described in Equations (5) and (6) are given for sake of completeness.

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