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## ► To cite this version:

Mathilde Grandjacques, Alexandre Janon, Benoit Delinchant, Olivier Adrot. Pick-freeze estimation of Projection on the past sensitivity indices for models with dependent causal processes inputs. 2014. hal-00963649v1

**HAL Id: hal-00963649**

**<https://inria.hal.science/hal-00963649v1>**

Preprint submitted on 21 Mar 2014 (v1), last revised 11 Sep 2015 (v2)

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# Pick-freeze estimation of Projection on the past sensitivity indices for models with dependent causal processes inputs

Mathilde Grandjacques<sup>1</sup>, Alexandre Janon<sup>2</sup>, Benoît Delinchant<sup>1</sup>, Olivier Adrot<sup>3</sup>

## Abstract

This paper address sensibility theory for dynamic models, linking correlated inputs to observed outputs. Usual estimation methods of Sobol indices are based on the fact that the input variables are independent. We present in this paper a method to overpass this constraint for Gaussian processes of high dimension in a time related framework. A general method exists with very weak hypothesis but computations are quite impossible in high dimension. Our proposition leads to a natural generalization of Sobol indices for time dependent, causal and correlated inputs. The method of estimation is a modification of the pick-freeze scheme. After having detailed the scheme for the general Gaussian case we detailed the case of high dimensional autoregressive model, which can be also associated with state models. We then apply the results to the case of a building model.

## 1 Introduction

Many mathematical models encountered in applied sciences involve a large number of poorly-known parameters as inputs. It is important for the practitioner to assess the impact of this uncertainty on the model output. An aspect of this assessment is sensitivity analysis, which aims to identify the most sensitive variables, that is, variables having the largest influence on the output. In global stochastic sensitivity analysis (see for example [1] and references therein), the input variables are assumed to be independent random variables. Their probability distributions account for the practitioner's belief about the input uncertainty. This turns the model output into a random variable, whose total variance can be split down into different partial variances (this is the so-called Hoeffding decomposition, also known as functional ANOVA, see [2]). Each of these partial variances measures the uncertainty on the output induced by each input variable uncertainty. By considering the ratio of each partial variance to the total variance, we obtain a measure of importance for each input variable that is called the Sobol

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index or sensitivity index of the variable [3, 4]; the most sensitive variables can then be identified and ranked as the variables with the largest Sobol indices. Each partial variance can be written as the variance of the conditional expectation of the output with respect to each input variable. Even when the inputs are not independent, it seems reasonable to consider the same Sobol index but in a quite different approach.

Once the Sobol indices have been defined, the question of their effective computation or estimation remains open. In practice, those indices can be estimated by (in a statistical sense) using a finite sample (of size typically in the order of hundreds of thousands, if the input model is known and if it is easy to simulate) of evaluations of model outputs [5]. Indeed, many Monte Carlo or quasi Monte Carlo approaches have been developed by the experimental sciences and engineering communities. This includes the Sobol pick-freeze (SPF) scheme (see [4, 6]). In SPF a Sobol index is viewed as the regression coefficient between the output of the model and its pick-frozen replication. This replication is obtained by holding the value of the variable of interest (frozen variable) and by sampling the other variables (picked variables). The sampled replications are then combined to produce an estimator of the Sobol index. All these estimation methods crucially depend on the fact that the input variables are independent.

The first natural method when the dimension of the input is small is to applied a method an used to simulate multivariate random vectors. The method as been proposed by Paul Levy in 1937 and a clear exposition can be found and Rosenblatt [7].

When the inputs are given by there repartitions function  $F(x_1, \dots, x_p)$ , if  $F$  has a strictly positive density on his support, then it exists a transformation  $T$ ,  $U = T(x)$  from  $\mathbb{R}^p$  to  $\mathbb{R}^p$  such that the  $U$  coordinates  $(u_1, \dots, u_p)$  are independent and uniform distributed on  $(0, 1)$ . Moreover it is possible to compute  $T^{-1}$  using classical computations of conditional densities.

Thus from a pure theoretical view we can always use the following trick: simulate  $U$  (standard), compute  $X = T^{-1}(U)$  and then applied SPF method.

For more complicated input specifically when the input is a time depending model the previews trick can require to heavy computation. In this paper, we propose an alternative method, for Gaussian processes of high dimension and an other framework.

The main goal of this paper is to find an efficient method of estimation of the Sobol indices when the independence assumption on the input variables is relaxed. More precisely, we set ourselves in a time related framework and we study the following output:

$$Y : \mathbb{N} \rightarrow \mathbb{R}, t \mapsto Y_t = f(t, (X_s)_{s=0, \dots, t}, (Z_s)_{s=0, \dots, t}) \quad (1)$$

where, for all  $t \in \mathbb{N}$ ,  $f(t, \cdot, \cdot) : \mathbb{R}^{p(t+1)} \times \mathbb{R}^{q(t+1)} \rightarrow \mathbb{R}$ , and the input variables are two (not necessarily independent) vector values Gaussian processes  $(X_s)_{s \in \mathbb{N}} \subset \mathbb{R}^p$  and  $(Z_s)_{s \in \mathbb{N}} \subset \mathbb{R}^q$ . We suppose that all the processes that we consider are *causal inputs* models. In this context, we are interested in the sensitivity, for each  $t$ , of  $Y_t$  with respect to the process  $(X_s)_{s \in \mathbb{N}}$ .

Such outputs occur in various practical cases, for example for financial models, with stock prices as inputs, in electrical and thermal engineering, when modelling the temperature in a room (output) as a function of different adjacent temperatures (inputs).

For a non-time dependent setting, several approaches have been proposed in the literature. In his introduction, Mara et al. [8] cites some of them, which are claimed to be relevant

only in the case of a linear system. In this last paper, the authors introduce an estimation method for the Sobol index but this method seems computationally intricate. On the other hand, Kucherenko et al. [9] rewrites, as we will do, the Sobol index as a covariance between the output and a dependent copy of the output. This allows to propose an efficient and justified estimation method. Another method ([10]) modify the Sobol index definition, which leads indices that are hard to estimate, as well as results that may seem counterintuitive (for instance, the indices may not be between 0 and 1).

For times dependent models it should be possible to use the Karhunen-Loeve method [11]. It is based on the covariance  $\mathbf{Cov}(t_1, t_2)$  of the input random vectors. If the inputs coordinates are not independent the computation is very heavy. Moreover if we want to use the SPF method with Karhunen-Loeve representation all the distributions have to be known and thus practically it is necessary to assume Gaussianity of the model. In many practical situations the main weakness of Karhunen-Loeve representation is that is not a sequential method and so it is unable to use the causality properties. The principal advantage of Karhunen-Loeve method is that it offers a natural way for model reduction.

Our proposition of indices, which we call *Projection on the past sensitivity indices* (POPSI) is a natural generalization of Sobol indices for causal and dependent inputs. Besides, the method of estimation that we propose is a specific modification of the pick-freeze scheme. This feature is shared with the proposition of [9], the difference being in the simulation algorithm for the inputs. Our method shares a lot of desirable features with this scheme. For instance, theoretical studies already performed in the independent case can be straightforwardly used in the dependent case. Indeed, the POPSIs can be seen as Sobol indices of a particular model whose inputs are independent, leading to a natural extension of properties and estimation methods that are relevant to Sobol indices.

## 2 Sobol indices: definition in a time dependent framework

### 2.1 Context and definition

We consider the model:

$$\chi = g(\xi, \eta) \tag{2}$$

with

$$g : \mathbb{R}^p \times \mathbb{R}^q \rightarrow \mathbb{R},$$

and  $\xi \in \mathbb{R}^p$  and  $\eta \in \mathbb{R}^q$  are random vectors with known distributions. We assume that all coordinates of  $\xi$  and  $\eta$ , and  $\chi$  have a finite non zero variance.

We define the Sobol index with respect to  $\xi$  by:

$$S^\xi = \frac{\mathbf{VarE}(\chi|\xi)}{\mathbf{Var}_\chi}. \tag{3}$$

**Remark:** One traditionally writes the model as:

$$\chi = g(\xi_1, \dots, \xi_p),$$

where  $\xi_1, \dots, \xi_p$  are random real variables. It is easy to see that the Sobol index with respect to  $\xi_i$  ( $i = 1, \dots, p$ ) is  $S^\xi$  where, in (2), we take  $\xi = \xi_i$  and  $\eta = (\xi_1, \dots, \xi_{i-1}, \xi_{i+1}, \dots, \xi_p)$ . More generally,  $S^\xi$  is the closed Sobol index with respect to the group of variables in  $\xi$ . Total indices and higher-order Sobol indices can also be written by taking sums or differences of closed indices. Hence, we can restrict ourselves to the case of two (possibly vector) inputs in the model.

We now introduce time dimension and the input-output relation:

$$Y_t = f(t, (X_s)_{s \leq t}, (Z_s)_{s \leq t}) \quad (4)$$

where for all  $t \in \mathbb{N}$  or  $\mathbb{Z}$ ,  $f(t, \cdot, \cdot) : \mathbb{R}^{p(t+1)} \times \mathbb{R}^{q(t+1)} \rightarrow \mathbb{R}$  and  $(X_s)_{s \in \mathbb{N}} \subset \mathbb{R}^p$ ,  $(Z_s)_{s \in \mathbb{N}} \subset \mathbb{R}^q$  are two (not necessarily independent) vector-valued stochastic process. We assume that they are causal processes.

For each  $t \in \mathbb{N}$ , we define a measure of the sensitivity of  $Y_t$  with respect to  $(X_s)_{s \leq t}$  by:

$$S_t^X = \frac{\text{VarE}(Y_t | (X_s)_{s \leq t})}{\text{Var}Y} \quad (5)$$

The index  $S_t^X$  is called the *projection on the past sensitivity index (POPSI) with respect to X*. We notice that, at a given time  $t$ , we consider the sensitivity of  $Y_t$  with respect to all the past of the  $X$  process, not just its present value  $X_t$ . Conditioning with respect to all the past of  $X$  is relevant in such a causal context.

Of course, the conditionnal expectation with respect to  $(X_s)_{s \leq t}$  takes into account the dependence of  $(Z_s)_{s \leq t}$  with respect to  $(X_s)_{s \leq t}$ .

Suppose that we are able to get an other expression of the output  $Y_t$  of the form:

$$Y_t = g(t, (\bar{X}_s)_{s \leq t}, (W_s)_{s \leq t}).$$

where  $(\bar{X}_s)_{s \leq t}$  is  $(X_s)_{s \leq t}$  measurable,  $(W_s)_{s \leq t}$  is a stochastic process independent of  $(X_s)_{s \leq t}$ ,  $(W_s)_{s \leq t}$  being  $(X_s, Z_s)_{s \leq t}$  measurable.

Then:

$$\bar{S}_t^X = \frac{\text{VarE}(Y_t | (\bar{X}_s)_{s \leq t})}{\text{Var}Y} \quad (6)$$

is defined in the classical case of independence.

The estimation of  $S_t^X$  by a Monte-Carlo method is a challenging task, as one can not take  $\xi = ((X_s)_{s \leq t})$  and  $\eta = ((Z_s)_{s \leq t})$  in (22) since  $\xi$  and  $\eta$  are not independent. However, we will see, in the next Section, that, in an important particular case of dependency structure between  $(X_s)$  and  $(Z_s)$ , an efficient pick-freeze scheme may be built.

## 2.2 Properties of the sensitivity POPSI as $t \rightarrow \infty$ for stationary inputs and outputs

Suppose that  $(U_t)_{t \in \mathbb{Z}} = (X_t, Z_t)_{t \in \mathbb{Z}}$  is a stationary process thus define for  $t \in \mathbb{Z}$  that

$$Y_t = f((X_s)_{s \leq t}, (Z_s)_{s \leq t}).$$

is also stationary ( $f$  depends on  $t$  only through  $(U_s)_{s \leq t}$ ).

Then

$$V_t = E(Y_t | (X_s)_{s \leq t}) \quad (7)$$

is also a stationary process (by shift invariance) and thus  $E(V_t^2) < \infty$ , which is  $S^X$  the global sensitivity of  $Y$  with respect to  $X$  is a constant.

In applications  $t \in \mathbb{N}$  (we consider  $X_t = Z_t = 0$  for  $t < 0$ ), thus we have to take as a definition of the sensitivity  $E(V_t^{*2})$  where:

$$V_t^* = E(Y_t | (X_s)_{0 \leq s \leq t}) \quad (8)$$

which is a truncation of the previous  $S^X$ .

We don't study here, in a quite general situation the effect of the truncation which depends of course of the contraction properties of  $f$  and the form of the memory of  $U$ .

Suppose the inputs are Gaussian and

$$Y_t = \alpha Y_{t-1} + BX_t + CW_t + \eta_t$$

with  $X_t$  and  $W_t$  is independent (we show later that we can always have this property starting from any Gaussian  $U$ ) and  $\eta_t$  is a white noise, stationary independent of  $X_t$  and  $W_t$ .

$$E(Y_t | (X_s)_{s \leq t}) = \alpha E(Y_{t-1} | (X_s)_{s \leq t-1}) + BX_t$$

from independence and causality.

Thus:

$$(1 - \alpha d)V_t = BX_t$$

where  $d$  is the shift backward operator of time translation.

$$\begin{aligned} V_t &= \sum_{k=0}^{\infty} \alpha^k d^k BX_t \\ &= \sum_{k=0}^{\infty} \alpha^k BX_{t-k} \end{aligned} \quad (9)$$

and:

$$V_t^* = \sum_{k=0}^t \alpha^k BX_{t-k} \quad (10)$$

$$E|V_t - V_t^*|^2 = E|\sum_{k=t+1}^{\infty} \alpha^k BX_{t-k}|^2 \quad (11)$$

From the stationarity of  $Y$ ,  $|\alpha| < 1$  and thus:

$$E|V_t - V_t^*|^2 \leq \text{constant} * \alpha^{2t} \quad (12)$$

**Lemma 1.** *For a stationary gaussian multivariate process  $(Y_t, U_t)$  satisfying (10), with  $|\alpha| < 1$  then the global sensitivity  $S_t^X$  is independent of  $t$ , and the truncated sensitivity  $(S_t^X)^* \rightarrow S^X$  with an exponential speed  $|\alpha|^t$*

## 2.3 The Gaussian case: reduction to independent $X$ and $Z$

We make the following assumption:

$((X_s, Z_s))_{s \in \mathbb{N}}$  is a Gaussian process.

There exists

$$g : \mathbb{N} \times \mathbb{R}^{p(t+1)} \times \mathbb{R}^{q(t+1)} \times \mathbb{R}^{q(t+1)} \rightarrow \mathbb{R},$$

and two  $\mathbb{R}^q$ -valued processes  $(\tilde{X}_t)_t$  and  $(W_t)_t$  so that:

$$\forall t \in \mathbb{N}, Y_t = g(t, (X_s)_{s \leq t}, (\tilde{X}_s)_{s \leq t}, (W_s)_{s \leq t}), \quad (13)$$

$$\forall t \in \mathbb{N}, \tilde{X}_t \text{ is } (X_s)_{s \leq t} \text{ measurable}, \quad (14)$$

$$(W_s)_{s \in \mathbb{N}} \text{ and } (X_s)_{s \in \mathbb{N}} \text{ are independent.} \quad (15)$$

*Proof.* It is easy to check that taking, for all  $(t, x, v, w) \in \mathbb{N} \times \mathbb{R}^{p(t+1)} \times \mathbb{R}^{q(t+1)} \times \mathbb{R}^{q(t+1)}$ ,

$$\begin{aligned} g(t, x, v, w) &= f(t, x, v + w), \\ \tilde{X}_t &= \mathbf{E}(Z_t | (X_s)_{s \leq t}), \\ W_t &= Z_t - \mathbf{E}(Z_t | (X_s)_{s \leq t}) \end{aligned}$$

is an admissible choice. Note that (15) holds thanks to the gaussianity assumption.  $\square$

Now the problem is how to compute  $W_t$  in order to simulate using a simple algorithm. We give a sequential algorithm in a specific situation which is the most popular in applications. Other gaussian model can be considered with more complicated sequential algorithm.

## 2.4 Sequential algorithm

Let  $(U_t)_{t \in \mathbb{N}}$  a gaussian causal process with  $U_0$  given. Under some weak hypothesis as stationarity, we have the representation ([12])  $U_t = \sum \alpha_k w_{t-k}$  where  $(w_{t,k})$  is a white noise, the innovation process and  $\sum \alpha_k^2 < \infty$

When  $U_t$  is stationary, we have

$$U_t = \sum_{k=0}^{\infty} \alpha_k w_{t-k}$$

but this representation uses  $w_s$  for  $s$  from  $-\infty$  to  $t$  and thus we need a truncation, this can be done if  $U_t$  has a short memory process as shown previously.

Here we give consider the following model

$$U_t = A_t U_{t-1} + w_t$$

where  $A_t$  can change with  $t$  (see the application to cyclo-stationary process) with  $\sup \|A_t\| < \infty$  and detailed for simplicity the proof for  $A$  constant that is an AR(1) stationary process.

**Remark 1.** *This is a classical model if  $U$  is got through a state space representation*

We write the  $AR(1)$  model as:

$$\begin{pmatrix} X_t \\ Z_t \end{pmatrix} = A \begin{pmatrix} X_{t-1} \\ Z_{t-1} \end{pmatrix} + \omega_t \quad (16)$$

where  $X_{-1} = Z_{-1} = 0$ ,  $A$  is a  $(p+q) \times (p+q)$  matrix, and  $(\omega_t)_{t \in \mathbb{N}} = (\omega_t^j)_{t \in \mathbb{N}, j=1, \dots, p+q}$  are  $(p+q)$ -dimensional iid standard Gaussian variables with identity as covariance.

We have of course:

$$\begin{pmatrix} X_t \\ Z_t \end{pmatrix} = \sum_{k=0}^t A^k \omega_{t-k} \quad (17)$$

For  $k \in \{0, \dots, t\}$ , let  $T_k$  be the  $p \times (p+q)$  matrix formed by the first  $p$  lines of  $A^k$ . Similarly, let  $B_k$  be the  $q \times (p+q)$  matrix formed by the last  $q$  lines of  $A^k$ .

For  $t \geq 0$ , we can write  $X_t$  and  $Z_t$  as sums of  $t+1$  independent random variables:

$$X_t = \sum_{k=0}^t T_k \omega_{t-k} \quad \text{and} \quad Z_t = \sum_{k=0}^t B_k \omega_{t-k}.$$

#### 2.4.1 Projection point-of-view

We endow  $L^2(\Omega, \mathcal{F}, P)$  with the usual scalar product:

$$\langle T, V \rangle = \mathbf{E}(TV) \quad T, V \in L^2(\Omega, \mathcal{F}, P).$$

For  $t \geq 0$ , we denote by  $\Omega_t$  the innovation space:

$$\Omega_t = \text{Span}\{\omega_t^j, 1 \leq j \leq p+q\}$$

so that (17) is a decomposition of  $(X_t, Z_t)$  on natural bases of the spaces  $\Omega_s$  for  $0 \leq s \leq t$ .

We also define:

$$\Omega_t^X = \text{Span}\{\omega_t^j, 1 \leq j \leq p\}, \quad \Omega_t^Z = \text{Span}\{\omega_t^j, p+1 \leq j \leq p+q\},$$

and notice that, thanks to the iid. assumption on  $(\omega_t^j)_{t \in \mathbb{N}, j \in \mathbb{N}}$ :

$$\Omega_t = \Omega_t^X \oplus \Omega_t^Z,$$

where the  $\oplus$  symbol designates orthogonal sum of subspaces.

We consider:

$$H_t^X = \text{Span}\{X_s^j, 0 \leq s \leq t, 1 \leq j \leq p\},$$

and:

$$H_t^{X,Z} = \text{Span}\{X_s^j, 0 \leq s \leq t, 1 \leq j \leq p\} + \text{Span}\{Z_s^j, 0 \leq s \leq t, 1 \leq j \leq q\}.$$



We have the following orthogonal decomposition:

$$H_t^{X,Z} = H_{t-1}^{X,Z} \oplus \Omega_t.$$

We denote by  $K_t^X$  the orthogonal complement of  $H_t^X$  in  $H_t^{X,Z}$ , and, by  $\Pi_F$  the orthogonal projection onto a subspace  $F \subset L^2(\mathbb{R})$ . We now want to express the  $(W_t)_{t \in \mathbb{N}}$  process (15). First, thanks to the Gaussian assumption,

$$W_t = Z_t - \mathbf{E}(Z_t|X_t) = \Pi_{K_t^X} Z_t, \quad (18)$$

Further we have the following lemma:

**Lemma 2.** *We have, for all  $t \geq 1$ :*

$$K_t^X = K_{t-1}^X \oplus \Omega_t^Z, \quad (19)$$

$$\Pi_{K_t^X} = \Pi_{K_{t-1}^X} \oplus \Pi_{\Omega_t^Z}. \quad (20)$$

*Proof.* We have, on the one hand:

$$\begin{aligned} H_t^{X,Z} &= H_{t-1}^{X,Z} \oplus \Omega_t \\ &= H_{t-1}^{X,Z} \oplus \Omega_t^X \oplus \Omega_t^Z \\ &= H_{t-1}^X \oplus K_{t-1}^X \oplus \Omega_t^X \oplus \Omega_t^Z \\ &= H_t^X \oplus K_{t-1}^X \oplus \Omega_t^Z, \end{aligned}$$

and, on the other hand:

$$H_t^{X,Z} = H_t^X \oplus K_t^X.$$

Equation (19) follows by identifying the orthogonal complements of  $\Omega_t^Z$  in  $H_t^{X,Z}$ ; (20) is a consequence of (19).  $\square$

**Remark 2.** : *When the covariance  $\Sigma$  of  $w_t$  is not the identity matrix*

$$\begin{pmatrix} X_t \\ Z_t \end{pmatrix} = A \begin{pmatrix} X_{t-1} \\ Z_{t-1} \end{pmatrix} + \begin{pmatrix} \theta_t \\ \eta_t \end{pmatrix}$$

$\eta_t = \alpha\theta_t^X + \beta\theta_t^W$  with  $\theta_t^X \in H_t^X$  and  $\theta_t^W \in H_t^W$ . It is obvious to compute  $\alpha$  and  $\beta$  and then to extend the previous results. Starting from

$$\eta_t = \Pi_{H_t^X} w_t \oplus \Pi_{K_t^X} w_t$$

We can now give the wanted expression of  $(W_t)_{t \in \mathbb{N}}$ .

**Lemma 3.**  *$(W_t)_{t \in \mathbb{N}}$  is an AR(1) process :*

$$\forall t \geq 0, \quad W_t = QW_{t-1} + \theta_t, \quad W_{-1} = 0. \quad (21)$$

with  $Q = (A_{j,k}, \quad p+1 \leq j, k \leq p+q)$  and  $\theta_t = (\omega_t^j, \quad p+1 \leq j \leq p+q)$ .

*Proof.* We use the following relations, which are consequences of Lemma 2: for all  $t \geq 0$  and  $1 \leq j \leq p + q$ ,

$$\begin{aligned} Z_t^j &= \sum_{k=1}^p A_{p+j,k} X_{t-1}^k + \sum_{k=1}^q A_{p+j,p+k} Z_{t-1}^k + \omega_t^{j+p} \\ \Pi_{K_t^X} X_{t-1}^k &= 0 \\ \Pi_{K_t^X} Z_{t-1}^k &= \Pi_{K_{t-1}^X} Z_{t-1}^k + \Pi_{\Omega_t^Z} Z_{t-1}^k = W_{t-1}^k \\ \Pi_{K_t^X} \omega_t^{p+j} &= \Pi_{K_{t-1}^X} \omega_t^{p+j} + \Pi_{\Omega_t^Z} \omega_t^{p+j} = \omega_t^{p+j} \end{aligned}$$

This leads to:

$$W_t^j = \Pi_{K_t^X} Z_t^j = \sum_{k=1}^q A_{p+j,p+k} W_{t-1}^k + \omega_t^{p+j}.$$

□

### 3 Estimation of $S^X$

There exist many methods for estimating  $S_\xi$ . One of them is the so-called pick-freeze scheme [4, 3], which uses the following expression of  $S^\xi$  when  $\xi$  and  $\eta$  are independent:

$$S^\xi = \frac{\mathbf{Cov}(\chi, \chi^\xi)}{\mathbf{Var}_\chi}, \quad (22)$$

where

$$\chi^\xi = g(\xi, \eta'),$$

where  $\eta'$  is an independent copy of  $\eta$ .

Now we take an independent  $N$ -sample  $\{(\chi_1, \chi_1^\xi), \dots, (\chi_N, \chi_N^\xi)\}$  and consider the following natural estimator of  $S^\xi$ .

$$\widehat{S}^\xi = \frac{\frac{1}{N} \sum_{i=1}^N \chi_i \chi_i^\xi - (\frac{1}{N} \sum_{i=1}^N \chi_i)(\frac{1}{N} \sum_{i=1}^N \chi_i^\xi)}{\frac{1}{N} \sum_{i=1}^N \chi_i^2 - (\frac{1}{N} \sum_{i=1}^N \chi_i)^2} \quad (23)$$

If  $\xi$  and  $\eta$  are finite dimensional random vector this formula can be justified by asymptotic properties as  $N \rightarrow \infty$

In the case of  $((X_s, Z_s))_{s \in \mathbb{N}}$  are two Gaussian dependent processes, we have thanks to (14), POPSI (5) can be rewrite:

$$S_t^X = \frac{\mathbf{VarE} \left( Y | (X_s)_{s \leq t}, (\tilde{X}_s)_{s \leq t} \right)}{\mathbf{Var} Y}.$$

This is an immediate consequence of (13) and (22) with  $\xi = ((X_s)_{s \leq t}, (\tilde{X}_s)_{s \leq t})$  and  $\eta = (W_s)_{s \leq t}$ , which are independent thanks to (15).

Let  $g$ ,  $(\tilde{X}_s)_s$  and  $(W_s)_s$  and  $(W'_s)_s$  be an independent process distributed as  $(W_s)_s$ .

We have, for all  $t \in \mathbb{N}$ :

$$S_t^X = \frac{\mathbf{Cov}(Y_t, Y_t^X)}{\mathbf{Var}Y_t},$$

where  $Y_t^X = g\left(t, (X_s)_{s \leq t}, (\tilde{X}_s)_{s \leq t}, (W'_s)_{s \leq t}\right)$ . where  $(X_s)_{s \leq t}$  and  $(\tilde{X}_s)_{s \leq t}$  are frozen.

Note that  $\mathbf{Cov}(Y_t, Y_t^X)$  does not depend on the particular choice of  $g$ ,  $(\tilde{X}_s)$  and  $(W_s)$ .

Now let, for  $N \in \mathbb{N}^*$ , an iid sample  $\left\{ \left( Y_t^i, Y_t^{X,i} \right) \right\}_{i=1, \dots, N}$  of  $(Y_t, Y_t^X)$  where we set, for all  $t \in \mathbb{N}$ :

$$Y_t = f(t, (X_s)_{s \leq t}, (Z_s)_{s \leq t}), \quad Y_t^X = f(f, (X_s)_{s \leq t}, (Z''_s)_{s \leq t}),$$

where  $Z''_s = Z_s - W_s + W'_s = \tilde{X}_s + W'_s$ .

Then,  $\hat{S}_t^X$  defined by:

$$\hat{S}_t^X = \frac{\frac{1}{N} \sum_{i=1}^N Y_t^i Y_t^{X,i} - \left( \frac{1}{N} \sum_{i=1}^N Y_t^i \right) \left( \frac{1}{N} \sum_{i=1}^N Y_t^{X,i} \right)}{\frac{1}{N} \sum_{i=1}^N (Y_t^i)^2 - \left( \frac{1}{N} \sum_{i=1}^N Y_t^i \right)^2}. \quad (24)$$

is a consistent estimator of  $S_t^X$ .

## 4 Application

### 4.1 Toy model

We first simulate a toy model given by:

$$Y_t = \alpha Y_t + X_t + Z_t$$

where  $Z_t$  and  $X_t$  are independent  $|\alpha| = 0.6 < 1$ , in order to illustrate the speed of convergence of the estimator  $\hat{S}_t^X$  we choose first  $N = 500$  and then  $N = 25000$ .

$X_t$  and  $Z_t$  are an AR(1) process given by:

$$\begin{pmatrix} X_t \\ Z_t \end{pmatrix} = \begin{pmatrix} 0.1 & 0 \\ 0 & 0.5 \end{pmatrix} \begin{pmatrix} X_{t-1} \\ Z_{t-1} \end{pmatrix} + \omega_t \quad (25)$$

with  $\omega_t$  a white noise.

The sensitivity index converges to its limit in gradually as time evolves, but the limit is not reached. It's due to convergence speed of this estimator, this one converges slowly. If we change the number of simulations we see that the maximum size of oscillations is divided by 2.5 .

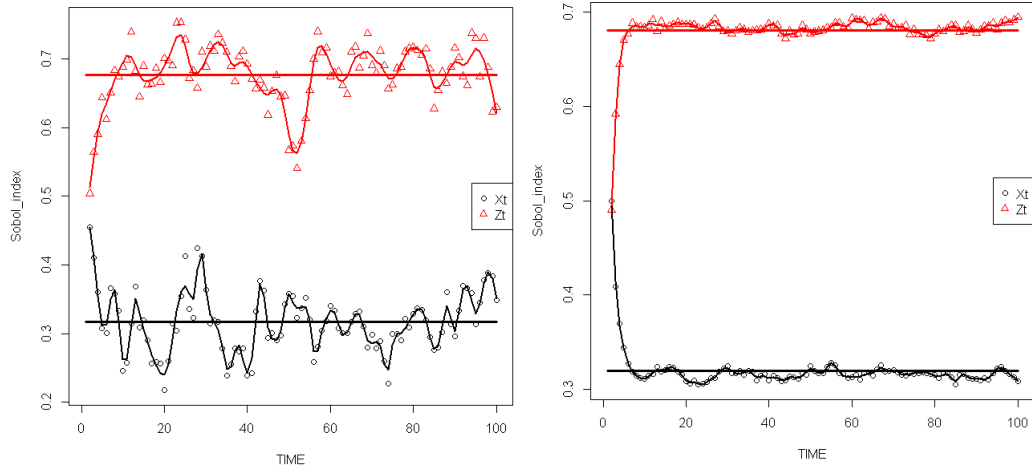


Figure 1: Toy model: Sobol index estimation in function of time. Left one used 500 points and right one 25000 points.

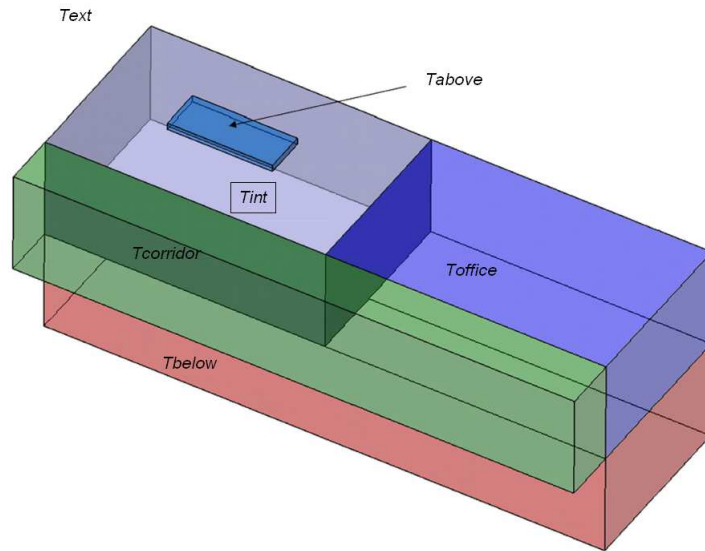


Figure 2: Locations of the different temperatures of interest in the building.

## 4.2 A thermal model

We then consider a building model quite simple, with observed data.

The variables are  $T^{\text{ext}}$ , the air temperature outside and  $T^{\text{above}}, T^{\text{below}}, T^{\text{cor}}, T^{\text{off}}$  the temperatures in immediate proximity of the room of interest:  $T^{\text{int}}$  (see 2).

These are random processes seasonal, that we write:

$$\bar{T}_t^e = S(t) + V(t) * T_t^e \quad \forall e \in \mathcal{E}$$

where  $\mathcal{E} = \{\text{int}, \text{ext}, \text{above}, \text{below}, \text{cor}, \text{off}\}$ ,  $S(t)$  is the mean with period 24 hours and  $V(t)$  the variance periodic function.

All these temperatures are measured.

We model the process  $T_t^{\text{ext}}$  by an  $AR(p)$  process with a gaussian white noise. Using Akaike criteria we find  $p = 6$ . In fact it remains some periodicity into the covariance of  $T_t^{\text{ext}}$ , that is the process is cyclo-stationary instant of stationary.

$$T_t^{\text{ext}} = \sum_{j=1}^6 \beta T_{t-j}^{\text{ext}} + \omega_t^{\text{ext}}$$

The temperature of four rooms ( $T^{\text{above}}, T^{\text{below}}, T^{\text{cor}}, T^{\text{off}}$ ) are modelled by a multivariate autoregressive stochastic process with an exogenous variable  $T^{\text{ext}}$  of order 6.

$$\forall t \geq 6, \forall e' \in \mathcal{E}' = \mathcal{E} \setminus \{T^{\text{int}}, T^{\text{ext}}\}, \quad T_t^{e'} = \sum_{f \in \mathcal{E}'} \sum_{j=1}^6 \gamma_f^j T_{t-j}^f + \sum_{j=1}^6 \psi^j T_{t-j}^{\text{ext}} + \omega_t^{e'},$$

where  $(\omega_t^{e'})_{t \in \mathbb{N}, e' \in \mathcal{E}'}$  are Gaussian variables

The coefficients are estimates by maximum of likelihood method.

Indeed, the equivalent model of the previous one is to consider  $U_t = (T^{\text{above}}, T^{\text{below}}, T^{\text{cor}}, T^{\text{off}}, T^{\text{ext}})$

$$Q_t = \sum_{j=0}^p D_j Q_{t-j} + \eta_t$$

We compute for every  $p$  the maximum of likelihood taken on all the parameter  $(D_l, l = 1, \dots, p, \Gamma)$  where  $\Gamma$  is the matrix of covariance of  $\eta$  and  $D_l$  is a set of matrix constraints by the stationarity of the autoregressive process of order  $p$ .

By Akaike criteria, we choose  $p = 6$ .

**Remark 3.** All  $AR(p)$  model can be rewrite obviously like an  $AR(1)$  (equation (16)).

Here for all

$$Z_t = \left( T_t^f, T_{t-1}^f, \dots, T_{t-5}^f, f \in \mathcal{E}' \right)^T = A Z_{t-1}$$

and  $A$  matrix  $(6 \times 6)$  such as:

$$A = \begin{pmatrix} \gamma_e^1 & \gamma_e^2 & \gamma_e^3 & \cdots & \gamma_e^6 \\ 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 1 & 0 \end{pmatrix} \quad (26)$$

Using this representation, we obtain :

$$U_t = FU_{t-1} + \rho_t$$

where  $F$  is a matrix  $30 \times 30$  deduced by straightforward computations from  $((D_l)_{l=1, \dots, 6}, (\beta)_{l=1, \dots, 6}, \Gamma)$

We consider the internal temperature<sup>1</sup>  $T^{\text{int}} = T^{\text{int}}(t)$  of a room, which is modelled by an autoregressive stochastic process on  $T^{\text{int}}$  with exogenous variables  $T^{\text{above}}, T^{\text{below}}, T^{\text{cor}}, T^{\text{off}}$  of order 6. It's the input-output model.

$$T^{\text{int}}(0) = T^{\text{int}}(1) = \cdots = T^{\text{int}}(6) = 0, \quad (27)$$

$$\forall t \geq 6, \quad T^{\text{int}}(t) = T^{\text{int}}(t, T^{\text{above}}, T^{\text{below}}, T^{\text{cor}}, T^{\text{off}}) = \sum_{v \in \mathcal{V}} \sum_{j=1}^6 \phi_{j,v} T_{v,t-j} \quad (28)$$

where  $\mathcal{V} = \{\text{int}, \text{above}, \text{below}, \text{cor}, \text{off}\}$ ,  $\phi_{j,v}$ ,  $j = 1, \dots, 6$ ,  $e \in \mathcal{V}$  are coefficients estimates by the same method described before for the inputs.

**Remark 4.**  $T^{\text{int}}$  (28) can be rewrite like a function of  $\mathcal{E}' = \{\text{above}, \text{below}, \text{cor}, \text{off}\}$ .

We note that:

$$\begin{aligned} T^{\text{int}}(t) &= AT^{\text{int}}(t-1) + BT_{e',t-1} \text{ with } e' \in \mathcal{E}' \\ T^{\text{int}}(t) &= \sum_{k=0}^t A^k BT_{e',t-1-k} \end{aligned} \quad (29)$$

Then we apply to  $U_t$  the sequential algorithm describe in the previous part to write  $U_t$  as  $(\tilde{U}_t^1, W_t)$   $\tilde{U}_t^1$  and  $W_t$  independent. Then we compute the sensitivity index with respect to the temperature  $\tilde{U}^1$  using part 3 of the paper.

We now fix an input process of interest  $(X_t)_{t \in \mathbb{N}} = (T_t^{e'}, T_{t-1}^{e'}, \dots, T_{t-6}^{e'})_t$ , for  $e' \in \mathcal{E}'$ .

### 4.3 Numerical results

We then compute the different estimators  $\hat{S}_t^X = \hat{S}_t^e$ , for  $t = 2, \dots, 336$  and  $e \in \mathcal{E}'$ . The results are gathered in Figure 3.

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<sup>1</sup>Note that  $T^{\text{int}}$  is actually the difference of the temperature with a (deterministic) reference temperature, which is irrelevant to consider for sensitivity analyses.

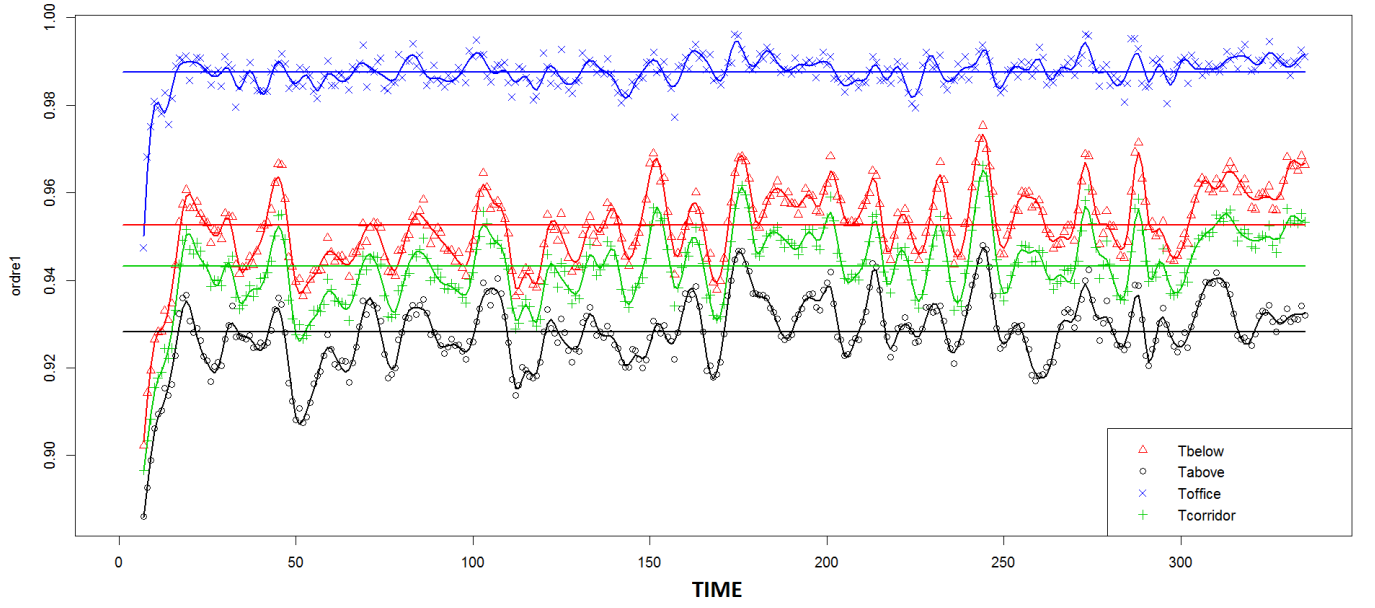


Figure 3: Plots of POPSIs applied to model (28) .

We can observe that the most influent input processes are the temperature in the office which is next to the room of interest ( $T^{\text{off}}$ ) and the temperature of the room below  $T^{\text{below}}$ . Note that, due to the dependency in the input variables, there is no reason that the POPSIs add up to unity.

Like in the toy model the index converge quickly to its limit but don't reach it.

Another remark is about the use of  $T^{\text{off}}$  to predict  $T^{\text{int}}$ : without considering sensitivity indices, one may have a look at different realizations of scatterplots of  $T^{\text{off}}$  vs.  $T^{\text{int}}$ , see Figure 4. As these plots are close to a straight  $45^\circ$  line, one may be tempted to use a common model for  $T^{\text{off}}$  and  $T^{\text{int}}$ . The computation of the sensitivity indices indicate that almost 99% of the variance of  $T^{\text{int}}$  is capture by  $T^{\text{off}}$ . It's what we can expect like the both temperature are similar.

Finally, the ranking of the variables by order of influence is in conformity with the expectations of the practitioners.

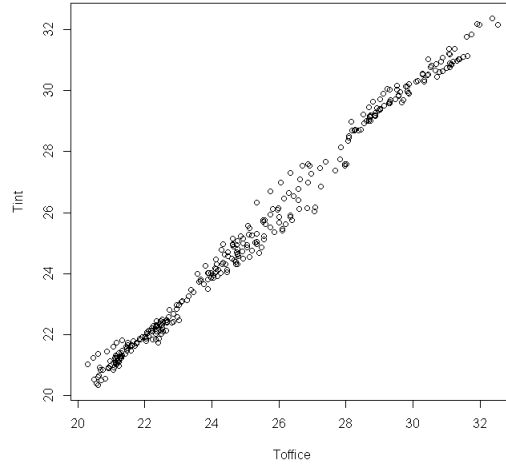


Figure 4: Scatterplots of  $T^{\text{off}}$  vs.  $T^{\text{int}}$ . Different point styles indicate different random outcomes for the  $T^{\text{off}}$  process and the  $T^{\text{int}}$  output.

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