Variance-based global sensitivity analysis of numerical models using R

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Abstract

Sensitivity analysis plays an important role in the development of computer models/simulators through identifying the contribution of each (uncertain) input factor to the model output variability. This report investigates different aspects of the variance-based global sensitivity analysis in the context of complex black-box computer codes. The analysis is mainly conducted using two R packages, namely sensobol (Puy et al., 2021) and sensitivity (Iooss et al., 2021). While the package sensitivity is equipped with a rich set of methods to conduct sensitivity analysis, especially in the case of models with dependent inputs, the package sensobol offers a bunch of user-friendly tools for the visualisation purposes. Several illustrative examples are supplied that allow the user to learn both packages easily and benefit from their features.

Keywords: computer model, sensitivity analysis, Shapley value, Sobol’ indices, uncertainty

1 Introduction

In many situations it is impossible to implement physical experiments due to its huge cost (time and/or monetary). To overcome this issue, computer codes are developed in various scientific disciplines to reproduce a physical mechanism relying on complex mathematical equations, e.g., systems of nonlinear (partial) differential equations. Typically, a computer model takes a set of input parameters/factors and produces some output(s) quantity of interest. The inputs to the model are subject to uncertainty due to various reasons such as our lack of knowledge about the real system, missing physics, simplifying assumptions, measurement error, etc. The input uncertainty results in the response uncertainty which is a measure of model accuracy. Sensitivity analysis (SA) is a powerful technique whereby we can understand the impact of each input on the variability of model outputs.

In mathematical modelling, the main application of SA is to identify the relative importance of each input factor based on its contribution to the output variance. Such analysis is referred to as factor prioritization in the literature (Andrea Saltelli et al., 2004). Moreover, SA is an integral part of uncertainty quantification which is concerned with the estimation of uncertainty propagating through complex models. In this paradigm, SA can help to decrease the output variance by reducing the uncertainty in the inputs using techniques such as factor screening (Kleijnen, 2009) or factor fixing (Andrea Saltelli et al., 2004). Factor screening allows us to eliminate insignificant factors.

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especially when the model is data-driven and the number of inputs exceeds the number of model evaluations (Song et al., 2016). In factor fixing, uncertainty of noninfluential inputs is ignored by fixing them at their nominal values without a remarkable loss of information. Another approach is to consider noninfluential parameters as noise in the system. Factor fixing is more suitable for physics-based codes where excluding some of their input parameters is impractical.

There have been many methods to conduct SA, see e.g. (Borgonovo & Plischke, 2016; Da Veiga et al., 2021; Razavi et al., 2021) for a comprehensive review of them. Generally, they can be divided into two groups:

- **Local SA** where the impact of inputs’ variation on the output is assessed at a specific point in the parameter space. This is typically performed using partial derivatives (Gan et al., 2014). When computing the partial derivative with respect to a certain input, all other factors are held constant. As a result, the interaction among the inputs is neglected in local SA and the sensitivity measures are not comprehensive. However, local approaches are cheap in terms of computational cost.

- **Global SA (GSA)** where the output uncertainty is analysed over the entire variation range of the factors. Global methods provide more information about the model than local ones. For example, the interaction among the inputs can be captured in GSA since they are varied simultaneously. However, conducting GSA requires a large number of simulation runs which may not be affordable if the model is computationally intensive. A common way to combat this issue is to replace the simulator by a surrogate model (Marrel et al., 2012; Sudret, 2008). In Section 5, a Gaussian process emulator (Rasmussen & Williams, 2005) serves as a surrogate to alleviate computational burden of applying SA to stochastic simulators. The focus of this work is on variance-based GSA methods which are one of the most common way of measuring global sensitivity, even if the literature beyond variance-based SA is expanding very fast (see e.g., Chapter 6 in the book (Da Veiga et al., 2021)). From now on any reference to SA refers to GSA.

This report covers various aspects of variance-based SA in the context of complex black-box simulators from a practical point of view. The analysis is carried out using R packages, namely sensobol (Puy et al., 2021) and sensitivity (Iooss et al., 2021). These two libraries together offer a comprehensive set of tools for performing SA. Several examples are provided for each package that allow the user to learn them easily. A taxonomy of available software packages for SA in programming languages other than R can be found in (G. Qian & Mahdi, 2020). The rest of the paper is organised as follows. The statistical background of SA is reviewed in Section 2. Section 3 describes how to conduct SA with the packages sensobol and sensitivity. Section 4 deals with the problem of applying SA to simulators with dependent input variables. In Section 5, SA of stochastic model is discussed where different outputs are observed for an identical input. Finally, the conclusion is provided in Section 6.

### 2 Sensitivity indices

Let us start this section by introducing computer models rigorously. Suppose that the output of a deterministic numerical simulator is governed by an unknown function \( f : \mathbb{R}^d \rightarrow \mathbb{R} \) with inputs \( x = (x_1, \ldots, x_d)^\top \). Since the “true” value of the input parameters is unknown, each factor is considered as a random variable and the associated uncertainty is described in terms of probability distributions. This makes the model output a random variable even if \( f \) is deterministic because...
the input uncertainty induces the response uncertainty. As per convention that random variables are denoted by capital letters, the model output is written as

\[ Y = f(X), \quad X = (X_1, \ldots, X_d)\top, \]

where \( X \) consists of \( d \) statistically independent random variables with known distributions. A variance-based SA technique provides a framework whereby the variance of \( Y \) can be apportioned into different sources of uncertainty in the inputs (Andrea Saltelli et al., 2004). One of the most commonly used variance-based approaches is introduced by Sobol’ (Sobol’, 2001) relying on a functional decomposition of \( f \) as described below.

### 2.1 Sobol’ indices

The Sobol’ method (Sobol’, 2001) is a classical way of doing SA and has been successfully employed in various application areas; see e.g., (Harenberg et al., 2019; Pianosi et al., 2016; Zhang et al., 2013). The Sobol’ sensitivity indices benefit from several advantages including accuracy, clear interpretation and straightforward implementation (Burnaev et al., 2017). The Sobol’ method relies on the following functional ANOVA (FANOVA) decomposition scheme (Efron & Stein, 1981; Sobol’, 2001)

\[
Y = f(X) = f_0 + \sum_{i=1}^{d} f_i(X_i) + \sum_{i<j}^{d} f_{ij}(X_i, X_j) + \ldots + f_{1,2,\ldots,d}(X),
\]

wherein \( f_0 \) is a constant. The remaining \( 2^d - 1 \) elementary functions are centred (mean zero) and orthogonal (mutually uncorrelated) with each other:

\[
\mathbb{E}[f_I(X_I)] = 0, \\
\mathbb{E}[f_I(X_I)f_J(X_J)] = 0, \quad \forall I \neq J,
\]

in which \( I, J \subseteq \mathcal{D} = \{1, \ldots, d\} \). Applying the variance operator, \( \mathbb{V}(\cdot) \), to the both sides of (1) yields

\[
\mathbb{V}(Y) = \sum_{i=1}^{d} \mathbb{V}_i + \sum_{i<j}^{d} \mathbb{V}_{ij} + \ldots + \mathbb{V}_{1,2,\ldots,d},
\]

such that

\[
\mathbb{V}_i = \mathbb{V}(f_i(X_i)) = \mathbb{V}_{X_i}(\mathbb{E}_{X_{-i}}[Y \mid X_i]), \\
\mathbb{V}_{ij} = \mathbb{V}(f_{ij}(X_i, X_j)) = \mathbb{V}_{X_i,X_j}(\mathbb{E}_{X_{-i,j}}[Y \mid X_i, X_j]) - \mathbb{V}_i - \mathbb{V}_j,
\]

and the other terms are defined in a similar fashion. The notation \( X_{\sim i} (X_{\sim i,j}) \) is used to indicate all input factors except \( X_i (X_i \text{ and } X_j) \).

The Sobol’ indices are defined as

\[
S_i = \frac{\mathbb{V}_i}{\mathbb{V}(Y)}, \quad S_{ij} = \frac{\mathbb{V}_{ij}}{\mathbb{V}(Y)}, \ldots,
\]

where \( S_i \) is the first order (or main) effect of \( X_i \), \( S_{ij} \) is the second order effect of \( (X_i, X_j) \) (which represents the contribution of interaction between \( X_i \) and \( X_j \) on the model output uncertainty without their individual effects), and so on. Note that the sum of all the sensitivity indices is equal to one:

\[
\sum_{i=1}^{d} S_i + \sum_{i<j}^{d} S_{ij} + \ldots + S_{1,2,\ldots,d} = 1.
\]
Among the terms defined in (7), $S_i$ is of great significance; it reflects the direct contribution of $X_i$ on the total variance $\mathbb{V}(Y)$, and is used as a measure of importance of $X_i$. The first order index can be interpreted as the expected reduction in the total variance $\mathbb{V}(Y)$ when $X_i$ is fixed to a constant (Andrea Saltelli et al., 2004). This is shown below using the law of total variance

$$S_i = \frac{\mathbb{V}_{X_i}(\mathbb{E}_{X_{\sim i}}[Y | X_i])}{\mathbb{V}(Y)} = \frac{\mathbb{V}(Y) - \mathbb{E}_{X_i}[\mathbb{V}_{X_{\sim i}}(Y | X_i)]}{\mathbb{V}(Y)}. \quad (9)$$

Another consequential sensitivity metric which complements the first order effect is the total order index denoted by $S_{T_i}$. It measures the main effect of $X_i$ together with its higher order effects (interactions) with all the other factors. For example, in a model with three input parameters, the total effect of $X_1$ obeys:

$$S_{T_1} = S_1 + S_{1,2} + S_{1,3} + S_{1,2,3}. \quad (10)$$

Notice that the total order index can be computed directly

$$S_{T_i} = \frac{\mathbb{V}(Y) - \mathbb{V}_{X_{\sim i}}(\mathbb{E}_{X_i}[Y | X_{\sim i}])}{\mathbb{V}(Y)} = \frac{\mathbb{E}_{X_i}[\mathbb{V}_{X_{\sim i}}(Y | X_{\sim i})]}{\mathbb{V}(Y)}, \quad (11)$$

in which $\mathbb{V}_{X_{\sim i}}(\mathbb{E}_{X_i}[Y | X_{\sim i}])$ stands for the first order effect of $X_{\sim i}$, i.e., all factors but $X_i$. Therefore, $\mathbb{V}(Y)$ minus $\mathbb{V}_{X_{\sim i}}(\mathbb{E}_{X_i}[Y | X_{\sim i}])$ incorporates the contribution of all the terms that include $X_i$ to the output uncertainty.

In practice, only the first and total indices are considered for sensitivity studies. The main effects are typically used for factor prioritization, i.e., ranking the input parameters according to their contribution to the total response variance. Also, the main effects can be employed to identify additive models where there is no interaction between the factors. In this situation, we have $\sum_{i=1}^{d} S_i = 1$. We note that the interaction of $X_i$ with the other factors is simply the difference between its main and total indices: $S_{T_i} - S_i$. The total effects are suit for factor fixing where insignificant inputs are set to a given value over their range of uncertainty (Andrea Saltelli et al., 2004). A factor $X_i$ is said to be noninfluential if its total order index is close to zero. Finally, the following relation holds between the first and total effect indices given that the input parameters are independent:

$$\sum_{i=1}^{d} S_i \leq 1 \leq \sum_{i=1}^{d} S_{T_i}, \quad (12)$$

which holds with equalities if the model is perfectly additive (Song et al., 2016).

### 2.2 Estimation of Sobol’ indices

To calculate the sensitivity indices, the expectation and variance operators (see e.g., Equation (11)) need to be expressed in their integral forms. On the one hand, solving such integrals numerically requires a huge number of model evaluations which can be computationally expensive. On the other hand, it may not be possible to find closed-form expressions for the decomposition components in Equation (1). To overcome these issues, several sampling-based estimators (specially for the main and total effects) are developed which are computationally “efficient”. For example, Jansen (Jansen, 1999) proposed the following estimators for the first and total order indices

$$\hat{S}_i = 1 - \frac{1}{N} \sum_{i=1}^{d} \left[ f(B) - f(A_B^{(i)}) \right]^{2} \mathbb{V}(Y), \quad (13)$$

$$\hat{S}_{T_i} = \frac{1}{N} \sum_{i=1}^{d} \left[ f(A) - f(A_B^{(i)}) \right]^{2} \mathbb{V}(Y). \quad (14)$$
Here, $N$ is the number of samples and $A$ and $B$ are two random matrices of size $N \times d$. The matrix $A_B^{(i)}$ is the same as $A$ except that its $i$-th column comes from $B$; see below.

$$
A = \begin{bmatrix}
a_{11} & \ldots & a_{1d} \\
\vdots & \ddots & \vdots \\
a_{N1} & \ldots & a_{Nd}
\end{bmatrix},
B = \begin{bmatrix}
b_{11} & \ldots & b_{1d} \\
\vdots & \ddots & \vdots \\
b_{N1} & \ldots & b_{Nd}
\end{bmatrix}
\Rightarrow A_B^{(i)} = \begin{bmatrix}
a_{11} & \ldots & b_{1i} & \ldots & a_{1d} \\
\vdots & \ddots & \vdots & \ddots & \vdots \\
a_{N1} & \ldots & b_{Ni} & \ldots & a_{Nd}
\end{bmatrix}.
$$

Note that the matrices $A$, $B$ and $A_B^{(i)}$, $i = 1, \ldots, d$, together provide a total number of $N \times (d + 2)$ samples to be evaluated by the simulator. This way of generating samples is referred to as the pick-freeze scheme first introduced by Sobol’ (Sobol’, 2001). The pick-freeze scheme is used in different estimators which can be found in e.g., (Homma & Saltelli, 1996; Janon et al., 2014; Andrea Saltelli, 2002; Sobol’, 2001). An alternative to sampling-based methods for the estimation of Sobol’ indices is spectral approaches (Cukier et al., 1978; A. Saltelli et al., 1999). They are based on a spectral decomposition of $f$ with some regularity assumptions in terms of decay conditions on the coefficients. Such spectral approaches are beyond the scope of this work.

The matrices $A$ and $B$ used in the pick-freeze scheme can be built using a Monte Carlo (MC) approach. It is found, however, that the MC methods are not efficient for the estimation of the Sobol’ indices specially when $N$ is small (Da Veiga et al., 2021). Besides, a clustering of points can happen in some regions of the space since the MC approach does not record the history of previous points. Quasi-MC (QMC) methods such as Halton (Halton, 1960) or Sobol’ (Sobol’, 1967) sequences yield a more uniform spread of points than MC ones. A QMC method uses a low discrepancy sequence to produce samples where the discrepancy criterion is a measure of deviation from a perfectly uniform distribution of points (Niederreiter, 1992). The $L^2$-discrepancy of the set $A \subset [0,1]^d$ is defined as

$$
D_2(A) = \left[ \int_{[0,1]^d} \left| \frac{\text{Num}(A,h_x)}{N} - \text{Vol}(h_x) \right|^2 \, dx \right]^{1/2},
$$

where $h_x$ denotes the interval $[0, x) = [0, x_1) \times [0, x_2) \times \ldots \times [0, x_d)$, $\text{Num}(A, h_x)$ is the number of points of $A$ falling in $h_x$, and $\text{Vol}(h_x)$ denotes the volume of $h_x$. In this work, the samples are generated via the Sobol’ QMC method (Sobol’, 1967).

A Latin hypercube sampling (LHS) design (McKay et al., 1979; Stein, 1987) is another strategy to place the sample points in a uniform manner across the input space. The iterative construction of LHS is discussed in (Gilquin et al., 2017; P. Z. G. Qian, 2009). (Gilquin et al., 2019; Tissot & Prieur, 2015) proposed a replicated LHS for the estimation of Sobol’ indices. Figure 1 illustrates the samples based on MC (left), LHS (middle) and QMC (right). The two random variables follow a uniform distribution in $[0,1]^2$, and $N = 100$. The QMC and LHS samples are obtained by the packages randtoolbox (Chalabi et al., 2020) and DiceDesign (Dupuy et al., 2015), respectively.

```r
library(randtoolbox)
library(DiceDesign)
set.seed(123)
d <- 2
N <- 100
A_MC <- data.frame(matrix(runif(N*d), ncol = d))
A_LHS <- data.frame(lhsDesign(N, d)$design)
A_QMC <- data.frame(sobol(N, d))
plot(A_MC); grid(nx = 5, ny = 5, lty = 2, lwd = 2.5)
```
plot(A_LHS); grid(nx = 5, ny = 5, lty = 2, lwd = 2.5)
plot(A_QMC); grid(nx = 5, ny = 5, lty = 2, lwd = 2.5)

Figure 1: Sample points generated by MC (left), LHS (middle) and QMC (right) in \([0, 1]^2\). The LHS and QMC samples are produced using the functions \texttt{lhsDesign()} and \texttt{sobol()} implemented in the packages \texttt{DiceDesign} and \texttt{randtoolbox}, respectively. The number of samples is: \(N = 100\).

3 Sensitivity analysis with R

In this section, the packages \texttt{sensobol} (v1.0.1) (Puy et al., 2021) and \texttt{sensitivity} (v1.25.0) (Iooss et al., 2021) are employed to conduct SA on two test functions serve as “true” models. The functions are selected such that their sensitivity indices (first and total) can be computed analytically. This allows us to compare the estimated indices with their actual values. The number of sample points and bootstrap replicates to get confidence intervals for the estimates is \(N = 5000\) and \(R = 1000\), respectively.

3.1 Polynomial function

The first test example is a polynomial function with four independent input variables distributed uniformly

\[
Y = 3X_1^2 + X_2X_3 - 2X_4, \quad X_1, \ldots, X_4 \sim \mathcal{U}(0, 1).
\]

To compute the sensitivity indices analytically we need the variance of each component in the function. The variance of the first, the second and the last term on the right hand side of (16) is

\[
V(3X_1^2) = 9 \left( \mathbb{E}[X_1^4] - \mathbb{E}[X_1^2]^2 \right) = 9 \left( \frac{1}{5} - \frac{1}{3} \right)^2 = 0.8,
\]

(17)

\[
V(X_2X_3) = \mathbb{E}[X_2^2]\mathbb{E}[X_3^2] - \mathbb{E}[X_2]^2\mathbb{E}[X_3]^2 = \frac{1}{9} - \frac{1}{16} \approx 0.049,
\]

(18)

\[
V(-2X_4) \approx 0.333,
\]

(19)

given that the \(q\)-th moment of \(X \sim \mathcal{U}(a, b)\) has the following form

\[
\mathbb{E}[X^q] = \frac{b^{q+1} - a^{q+1}}{(q + 1)(b - a)}.
\]

The total output variance is simply the sum of all the variances in Equations (17)-(19) since the input variables are independent: \(V(Y) = 0.8 + 0.049 + 0.333 = 1.182\). Now, we can easily calculate the theoretical sensitivity indices as described in Section 2. The results are summarised in Table 1.
The sensitivity indices of the polynomial function are estimated with the functions `sobol_indices()` (sensobol package) and `sobolSalt()` (sensitivity package) using their default settings. This is shown in the code chunk below. To create the random matrices $A$ and $B$ we use the function `sobol_matrices()` implemented in the package sensobol. The outcome of this function (stored in the object `mat`) consists of $A$, $B$ and $A_{ii}^j$, $i = 1, \ldots, d$. By default, the function `sobol_matrices()` generates samples based on the Sobol’ QMC method via a call to the function `sobol()` of the randtoolbox package. The results are rounded to the third significant digit. We observe that the results of the two packages are very similar and the estimated indices are close to their actual values (Table 1).

$$$
\begin{array}{l|ll}
\text{First order} & \text{Total order} \\
\hline
X_1 & 0.677 & 0.677 \\
X_2 & 0 & 0.041 \\
X_3 & 0 & 0.041 \\
X_4 & 0.282 & 0.282 \\
\end{array}
$$$

The sensitivity indices of the polynomial function are estimated with the functions `sobol_indices()` (sensobol package) and `sobolSalt()` (sensitivity package) using their default settings. This is shown in the code chunk below. To create the random matrices $A$ and $B$ we use the function `sobol_matrices()` implemented in the package sensobol. The outcome of this function (stored in the object `mat`) consists of $A$, $B$ and $A_{ii}^j$, $i = 1, \ldots, d$. By default, the function `sobol_matrices()` generates samples based on the Sobol’ QMC method via a call to the function `sobol()` of the randtoolbox package. The results are rounded to the third significant digit. We observe that the results of the two packages are very similar and the estimated indices are close to their actual values (Table 1).

```r
library(sensobol)
library(sensitivity)
library(data.table)

fun <- function(xx) {
  yy <- 3*xx[, 1]^2 + xx[, 2]*xx[, 3] - 2*xx[, 4]
  return(yy)
}

d <- 4
N <- 5000
R <- 1000
params <- paste("$X_{", 1:d, ", \"", sep = \"\"")
mat <- sobol_matrices(N = N, params = params)
Y <- fun(mat)
sensobol_ind <- sobol_indices(Y = Y, N = N, params = params,
  boot = TRUE, R = R)
cols <- colnames(sensobol_ind$results)[1:5]
sensobol_ind$results[, (cols):= round(.SD, 3), .SDcols = (cols)]
print(sensobol_ind)

##
## First-order estimator: saltelli | Total-order estimator: jansen
##
## Total number of model runs: 30000
##
## Sum of first order indices: 0.9938516
##
## original bias std.error low.ci high.ci sensitivity parameters
## 1: 0.677 0 0.016 0.645 0.709 Si $X_1$
## 2: 0.018 0 0.003 0.011 0.024 Si $X_2$
## 3: 0.018 0 0.003 0.012 0.024 Si $X_3$
## 4: 0.282 0 0.010 0.263 0.301 Si $X_4$
```
```r
## 5: 0.677 0 0.012 0.653 0.701 Ti $X_1$
## 6: 0.023 0 0.001 0.022 0.025 Ti $X_2$
## 7: 0.023 0 0.001 0.022 0.025 Ti $X_3$
## 8: 0.282 0 0.005 0.271 0.293 Ti $X_4$

sensitivity_ind <- sobolSalt(model = fun, X1 = mat[1:N, ],
                              X2 = mat[(N+1):(2*N), ], nboot = R)
print(round(sensitivity_ind$S, 3)) # First order indices

## original bias std. error min. c.i. max. c.i.
## X1 0.677 0 0.007 0.664 0.690
## X2 0.018 0 0.014 -0.007 0.047
## X3 0.017 0 0.014 -0.009 0.047
## X4 0.282 0 0.012 0.257 0.307

print(round(sensitivity_ind$T, 3)) # Total order indices

## original bias std. error min. c.i. max. c.i.
## X1 0.677 0 0.012 0.650 0.701
## X2 0.024 0 0.001 0.022 0.025
## X3 0.023 0 0.001 0.022 0.025
## X4 0.282 0 0.006 0.270 0.294

It is worth mentioning that the package `sensobol` offers several useful visualisation tools such as `plot_uncertainty()` and `plot_scatter()` relying on the package `ggplot2` (Wickham, 2016). The former plots the histogram of the model response and the latter gives an scatter plot against each input parameter. Figures 2 and 3 display the graphs obtained by `plot_uncertainty()` and `plot_scatter()` for the polynomial function, respectively. The function `plot_scatter()` divides the domain of each input $X_i$ into bins and computes the mean of $Y \mid X_i$ in every bin. The red dots in Figure 3 represent those means.

```r
library(ggplot2)
plot_uncertainty(Y = Y, N = N) + labs(y = "Counts", x = "Y")
```

![Figure 2: The empirical distribution of $Y$ for the polynomial function defined in (16) using the function `plot_uncertainty()` implemented in the `sensobol` package.](image)

plot_scatter(data = mat, N = N, Y = Y, params = params) +
  labs(y = "Y", x = "Variation range of input parameters")

Figure 3: The scatter plots obtained by the function `plot_scatter()` implemented in the `sensobol` package. The black dots are responses of the polynomial function given $X_i$. The domain of each factor is divided into bins and the red dots represent the mean of $Y | X_i$ in every bin.

### 3.2 Ishigami function

The Ishigami function (Ishigami & Homma, 1990) is commonly used as a benchmark example for sensitivity studies. It is a 3-dimensional, highly nonlinear function expressed by

$$
Y = \sin(X_1) + 7 \sin^2(X_2) + 0.1X_3^4 \sin(X_1), \quad X_1, X_2, X_3 \sim \mathcal{U}(-\pi, \pi).
$$

(20)

The scatter plot of the Ishigami’s input variables is demonstrated in Figure 4 using the function `plot_scatter()`. It is observed that the main effect of $X_3$ (i.e., $\mathbb{V}(\mathbb{E}[Y | X_3])$) is possibly zero as the red dots (the mean of $Y | X_i$ in the bins) has a flat pattern. The theoretical Sobol’ indices for the Ishigami function are calculated in (Ishigami & Homma, 1990; Sudret, 2008) and are summarised in Table 2.

Now we use the two packages to estimate the sensitivity indices and compare them with their actual values; see the code chunk below. The Ishigami function is implemented in the package `sensitivity` and can be called via `ishigami.fun()`. The results show that the two packages have a good performance in estimating the sensitivity indices.
Table 2: Theoretical values of the first and total order sensitivity indices for the Ishigami function.

|     | First order | Total order |
|-----|-------------|-------------|
| $X_1$ | 0.314       | 0.558       |
| $X_2$ | 0.442       | 0.442       |
| $X_3$ | 0           | 0.244       |

Figure 4: The scatter plots obtained by `plot_scatter()` for the Ishigami function. The red dots are the mean of $Y \mid X_i$ in the bins created over the domain of $X_i$. 
d <- 3
params <- paste("X", 1:d, sep = "")
mat <- sobol_matrices(N = N, params = params)
mat <- 2*pi*mat - pi
Y <- ishigami.fun(mat)
sensobol_ind <- sobol_indices(Y = Y, N = N, params = params, boot = TRUE, R = R)
cols <- colnames(sensobol_ind$results)[1:5]
sensobol_ind$results[, (cols)]= round(.SD, 3), .SDcols = (cols)]
print(sensobol_ind)

##
## First-order estimator: saltelli | Total-order estimator: jansen
##
## Total number of model runs: 25000
##
## Sum of first order indices: 0.7677866
## original bias std.error low.ci high.ci sensitivity parameters
## 1: 0.316 0.001 0.021 0.274 0.355 Si X_1
## 2: 0.446 0.000 0.017 0.412 0.480 Si X_2
## 3: 0.007 0.000 0.017 -0.026 0.039 Si X_3
## 4: 0.561 0.001 0.020 0.520 0.599 Ti X_1
## 5: 0.444 0.000 0.010 0.425 0.462 Ti X_2
## 6: 0.244 0.000 0.006 0.232 0.257 Ti X_3

sensitivity_ind <- sobolSalt(model = ishigami.fun, X1 = mat[1:N, ],
X2 = mat[(N+1):(2*N), ], nboot = R)
print(round(sensitivity_ind$S, 3))

## original bias std. error min. c.i. max. c.i.
## X1 0.313 0 0.012 0.289 0.336
## X2 0.442 0 0.011 0.421 0.465
## X3 -0.002 0 0.019 -0.040 0.035

print(round(sensitivity_ind$T, 3))

## original bias std. error min. c.i. max. c.i.
## X1 0.552 0 0.017 0.515 0.584
## X2 0.445 0 0.011 0.423 0.465
## X3 0.243 0 0.006 0.232 0.255

4 SA in the case of correlated inputs

In many applications such as epidemiology it happens that the input parameters are correlated. In this situation, the Sobol’ indices are not reliable sensitivity measures because they may over/underestimate the contribution of each input parameter on the output variability (Owen, 2014) since the variance decomposition in (4) relies on the assumption that the factors are independent. More precisely, Equation (12) may not hold in the case of dependent inputs, e.g. \( \sum_{i=1}^{d} S_i > 1 \)
A cooperative game is characterised by a set of players. As can be seen, if the correlation coefficient we have obtained for each input making the interpretation easier than the Sobol’ method. Besides, the sum of the Shapley values is equal to one even if there is a strong correlation among the factors. In the following, we first introduce briefly the game theory idea behind the Shapley value and then focus on its application in SA of simulators with dependent inputs.

A cooperative game is characterised by a set of players \( D = \{1, \ldots, d\} \) called the “grand coalition” and a characteristic function \( \nu : 2^D \rightarrow \mathbb{R} \). The coalition \( D \) can be viewed as the set of all input factors in the SA paradigm. The characteristic function maps subsets of players \( I \subseteq D \) to a real number \( \nu(I) \) which reflects the payoff that the members of the coalition \( I \) can achieve by cooperation. Notice that the empty set \( (I = \emptyset) \) is also a coalition with a zero payoff \( \nu(\emptyset) = 0 \). Now let \( J \subseteq D \setminus \{i\} \) represent a coalition of \( |J| \) players not containing the player \( i \). The marginal contribution of the player \( i \) with respect to \( \nu(\cdot) \) is given by \( \nu(J \cup \{i\}) - \nu(J) \) which indicates the incremental value for including the player \( i \) in the coalition \( J \). The Shapley value is then expressed by

\[
\phi_i = \sum_J \frac{|J|!(d-|J|-1)!}{d!}[\nu(J \cup \{i\}) - \nu(J)], \quad i = 1, \ldots, d,
\]

that is a weighted average of the marginal contribution of the player \( i \) over all possible coalitions, including \( J = \emptyset \). The Shapley value can be computed in a different manner, which is based on the permutations of \( D \)

\[
\phi_i = \frac{1}{d!} \sum_{\pi \in \Pi} [\nu(P_i(\pi) \cup \{i\}) - \nu(P_i(\pi))], \quad i = 1, \ldots, d,
\]

where \( \Pi \) is the set of all \( d! \) permutations of players and \( P_i(\pi) \) is the set of players that precedes player \( i \) in the permutation \( \pi \) in \( \Pi \).

The main disadvantage of the Shapley value is its enormous computational burden, especially when \( d \) is large. The reason is that computing the Shapley effect requires all possible subsets of players. To overcome this complexity, various approximation methods have been developed. For example, Castro et al. (Castro et al., 2009) proposed the following expression relying on Equation (26) to approximate the Shapley value

\[
\hat{\phi}_i = \frac{1}{M} \sum_{m=1}^{M} [\nu(P_i(\pi_m) \cup \{i\}) - \nu(P_i(\pi_m))], \quad i = 1, \ldots, d.
\]
In the above equation, \( \pi_1, \ldots, \pi_M \) are \( M \) random permutations in \( \Pi \).

Now we describe how the Shapley values can be used for the sensitivity study of computer codes specially if the inputs are dependent. In this framework, the model factors are deemed as players of a game with the total payoff \( \mathbb{V}(Y) \) (or one in the normalized case). Also, for a set of inputs \( I \subseteq D \), \( \nu(I) \) returns the output uncertainty caused by the uncertainty of those inputs. Thus, the Shapley value is a variance-based method and serves as a global sensitivity metric.

Two possible choices of the characteristic function are (Iooss & Prieur, 2019)

\[
\begin{align*}
\nu_1(I) &= \frac{\mathbb{V}_{X_I}(\mathbb{E}[Y | X_I])}{\mathbb{V}(Y)}, \\
\nu_2(I) &= \frac{\mathbb{E}_{X_I}(\mathbb{V}[Y | X_{\sim I}])}{\mathbb{V}(Y)}
\end{align*}
\]

(28) (29)

where the former is interpreted as the first order and the latter as the total order effect in the Sobol’ formulation. Although it is proved that both characteristic functions yield the same Shapley value (Song et al., 2016), the MC estimation to \( \nu_2 \) is always unbiased making it a more popular choice. In contrast, the estimator of \( \nu_1 \) can be badly biased if the number of MC samples used to evaluate the conditional expectation (i.e. \( \mathbb{E}[Y | X_I] \)) is small (Radaideh et al., 2019; Sun et al., 2011). As recommended in (Song et al., 2016; Sun et al., 2011), the estimation of \( \nu_2 \) is performed via a two-level MC: an inner loop for the conditional variance and an outer loop for the expectation estimation. According to the theoretical analysis in (Song et al., 2016), it is suggested that a suitable size for the inner and outer loops is one and three, respectively. This algorithm is implemented in the package sensitivity with the characteristic function \( \nu_2 \). More recent algorithms (see e.g., (Broto et al., 2020, 2022; Da Veiga et al., 2021)) for the estimation of the Shapley effects are also included in the sensitivity package. They are implemented in the functions shapleySubsetMc(), shapleysobol_knn(), and sobolshap_knn().

5 Case of stochastic models

Stochastic simulators such as agent-based models are ubiquitous in the social and biological sciences (Binois et al., 2018). In stochastic models, contrary to deterministic ones, different observations are attained at an identical input due to the inclusion of a random number seed in their code (O’Hagan, 2006). To characterise the response distribution at a specific input, we need to run the code with the same input repeatedly. Hence, applying SA to stochastic simulators requires a larger number of model evaluations than the case of deterministic codes. If the stochastic model is computationally expensive, conducting SA becomes impossible. To address this issue, one can replace the simulator with a cheap-to-evaluate surrogate model and perform SA on it. In this framework, there are different classes of surrogate models; see e.g., (Sudret, 2008; Zhu & Sudret, 2021). Here, we only consider Gaussian processes (GP) emulators (Rasmussen & Williams, 2005). GPs have become the gold standard surrogate model in the field of the design and analysis of computer experiments due to their statistical properties (Santner et al., 2003). For example, the GP prediction is equipped with an estimation of uncertainty that reflects the accuracy of the prediction. Some applications of GPs in modelling computer experiments can be found in (Beck & Guillas, 2016; Mohammadi et al., 2019; Vernon et al., 2018). The statistical background of GPs is presented below.
5.1 Gaussian process emulators

We consider the output of a stochastic model to be of the following form

\[ y(x) = f(x) + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \tau(x)). \]  

(30)

The above expression represents the general heteroscedastic case as the noise variance \( \tau(x) \) (also referred to as the nugget (Binois et al., 2018)) changes across the input space. If the noise variance is constant, the model is called homoscedastic. In the GP paradigm, the prior belief about the form of \( f \) is modelled via the stochastic process

\[ Z_x = \mu(x) + \eta_x, \]  

(31)

where \( \mu(x) \) is the trend function and \( \eta_x \) is a centred (or zero mean) GP. Without loss of generality, we assume that the trend function is a constant denoted by \( \mu_0 \). The covariance structure of \( \eta_x \) is determined by its positive definite covariance function/kernel \( c(\cdot, \cdot) \) defined as

\[ c : \mathbb{R}^d \times \mathbb{R}^d \mapsto \mathbb{R}, \quad c(x, x') = \text{Cov}(\eta_x, \eta_{x'}). \]  

(32)

Although there are many options available for the choice of the covariance function, the Matern or squared exponential kernels (Rasmussen & Williams, 2005) are typically adopted in the computer experiments literature. Traditionally, a parameterized family of \( c \) is specified and its parameters are estimated from the data by e.g., maximum likelihood (Roustant et al., 2012).

Now let \( X_n = \left( x^{(1)}, \ldots, x^{(n)} \right)^\top \) be \( n \) locations (called the design points) in the input space with the corresponding noisy output observations \( Y_n = \left( y(x^{(1)}), \ldots, y(x^{(n)}) \right)^\top \). Often, the elements of \( X_n \) are selected according to a space-filling design. Given that all parameters in Equation (31) are known, the predictive distribution at any site \( x^* \) is driven by the posterior distribution \( Z_{x^*} \mid Y_n \) which is Gaussian characterised by

\[ \mu(x^*) = \mathbb{E}[Z_{x^*} \mid Y_n] = \mu_0 + c^\top C^{-1} (X_n - \mu_0 1), \]  

(33)

\[ \sigma^2(x^*) = \mathbb{V}[Z_{x^*} \mid Y_n] = c(x^*, x^*) + \tau(x^*) - c^\top C^{-1} c. \]  

(34)

Here, \( c = \left( c(x^*, x^{(1)}), \ldots, c(x^*, x^{(n)}) \right)^\top \) and \( C \) is an \( n \times n \) covariance matrix whose elements are \( C_{kl} = c(x^{(k)}, x^{(l)}) + \delta_{lk} \tau(x^{(k)}) \) where \( \delta_{lk} \) is the Kronecker delta function, for \( 1 \leq l, k \leq n \). The GP predictive mean and variance expressions for deterministic codes are analogous to Equations (33) and (34) except that the noise variance term is discarded.

In practice, the true value of \( \tau(x) \) is unknown. The noise variance can be estimated at the design points by repeatedly running the simulator there and computing the sample variances. This method is called the stochastic kriging (Ankenman et al., 2010); it only works if there are enough replicated observations at \( x^{(k)}, k = 1, \ldots, n \). Yet, it is not possible to estimate \( \tau(x^*) \) in the GP predictive variance (Equation (34)) as no observations are available at \( x^* \). To overcome this problem, Binois et al. (Binois et al., 2018) proposed a computationally efficient method such that a joint GP model is used to fit the mean response and noise variance. In this approach, the noise variances at the design points, \( \left( \tau(x^{(1)}), \ldots, \tau(x^{(n)}) \right) \), are treated as latent variables that can be learnt together with the kernel parameters through a joint likelihood. An implementation of this method is available in the 

\texttt{R} package \texttt{hetGP} (Binois & Gramacy, 2021). Figure 5 visualises a heteroscedastic example in which the true function and the noise variance are \( f(x) = \sin(x) \) and \( \tau(x) = 0.01x^2 \), respectively.
On the left picture of Figure 5, the emulator (red) is built based on 100 noisy observations (black circles): predictive mean (solid) and confidence interval (dashed). The red line on the right panel shows the noise variance prediction, $\hat{\tau}(x)$.

```r
library(hetGP)
set.seed(123)
tau <- function(xx) 0.01*xx^2  # Noise variance function
fun <- function(xx) {
    yy <- sin(xx) + rnorm(1, 0, sqrt(tau(xx)))
    return(yy)
}
X_n <- as.matrix(runif(100, 0, 6))  # Design points
Y_n <- apply(X_n, 1, fun)  # Outputs at X_n
emulator <- mleHetGP(X = X_n, Z = Y_n, lower = 0.1, upper = 20, maxit = 1000, covtype = "Gaussian")
x <- as.matrix(seq(0, 6, 0.01))
P <- predict(object = emulator, x = x)
CI <- 2*sqrt(P$sd2 + P$nugs)  # Confidence interval
#P$sd2: predictive variance, P$nugs: noise variance prediction
par(mfcol = c(1, 2))
par(mar = c(4, 4, .1, .1))
plot(X_n, Y_n, col = "black", xlab = "Input", ylab = "Output", ylim = c(-2, 1.3))
lines(x, sin(x), type = "l", lwd = 1.5)
lines(x, P$mean, col = "red", lwd = 1.5)  # P$mean: predictive mean
lines(x, P$mean + CI, col = "red", lty = 2, lwd = 1.5)
lines(x, P$mean - CI, col = "red", lty = 2, lwd = 1.5)
legend("bottomleft", lwd=c(1,1.5,1.5,1.5), lty=c(NA,1,1,2), pch=c(1,NA,NA,NA),
        legend=c("Observations","f(x) = sin(x)","Predictive mean","Confidence interval"),
        col = c("black", "black", "red", "red", "red"), cex = 0.75)
plot(x, tau(x), type = "l", lwd = 1.5, xlab = "Input", ylab = "")
lines(x, P$nugs, col = "red", lwd = 1.5)
legend("topleft", legend = c("Noise variance", "Noise variance prediction"),
        col = c("black", "red"), lwd = 1.5, lty = 1, cex = 0.75)
```

### 5.2 SA of stochastic models

One way to conduct SA for stochastic simulators is to extend the set of the input parameters $\mathbf{X}$ by an extra variable $\mathbf{X}_\varepsilon$ which denotes the uncontrollable parameter governed by the simulator itself (Iooss & Ribatet, 2009). The new variable $\mathbf{X}_\varepsilon$ is called the “seed variable” and is independent of the other inputs. Accordingly, one can write the output variable as

$$Y = f(\mathbf{X}, \mathbf{X}_\varepsilon),$$

meaning that the response variability consists of intrinsic randomness caused by the seed variable and uncertainty in the inputs. In this framework, the mean ($Y_m$) and variance ($Y_v$) function of stochastic simulators are given by

$$Y_m(\mathbf{X}) = \mathbb{E}_{\mathbf{X}_\varepsilon}[Y | \mathbf{X}],$$

$$Y_v(\mathbf{X}) = \mathbb{V}_{\mathbf{X}_\varepsilon}(Y | \mathbf{X}) = \mathbb{E}_{\mathbf{X}_\varepsilon}[(Y - Y_m(\mathbf{X}))^2 | \mathbf{X}].$$

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Figure 5: Left: a heteroscedastic stochastic model defined by: $y(x) = \sin(x) + \varepsilon, \varepsilon \sim \mathcal{N}(0, \tau(x) = 0.01x^2), x \in [0, 6]$. There are 100 observations (black circles) taken from $y(x)$. The GP emulator (red) is constructed using the function `mleHetGP` implemented in the package `hetGP`. Right: the noise variance (black) and its prediction, $\hat{\tau}(x)$ (red).
It is shown that the first order effect of each $X_i (S_i)$ and the total order index of $X_t (S_T)$ can be expressed in terms of $Y_m$ and $Y_v$ (Iooss & Ribatet, 2009; Marrel et al., 2012). Thanks to the law of total expectation, we have

$$E_{X_{-i}}[Y | X_i] = E_{X_{-i}}[E_{X_t}[Y | X_t] | X_i] = E_{X_{-i}}[Y_m(X) | X_i].$$

Consequently, the first order effect of $X_i$ can be rewritten as

$$S_i = \frac{\nabla_{X_i} (E_{X_{-i}}[Y | X_i])}{\nabla(Y)} = \frac{\nabla_{X_i} (E_{X_{-i}}[Y_m(X) | X_i])}{\nabla(Y)},$$

which relies on the mean response function. The total order effect of $X_t$ takes the following form

$$S_T = \frac{E_X[\nabla_{X_t}(Y | X)]}{\nabla(Y)} = \frac{E_X[Y_v(X)]}{\nabla(Y)},$$

referring to the total sensitivity index defined in Equation (11). Moreover, the output variance can be expressed as a function of $Y_m$ and $Y_v$ thanks to the law of total variance:

$$\nabla(Y) = \nabla_X (E_{X_t}[Y | X]) + E_X[\nabla_{X_t}(Y | X)] = \nabla_X (Y_m(X)) + E_X[Y_v(X)].$$

The advantage of expressing the sensitivity indices in terms of $Y_m$ and $Y_v$ is that they can be approximated by GP emulators. This leads to a significant reduction in the computational cost of conducting SA for stochastic simulators. While $Y_m$ is approximated by the GP predictive mean (Equation (33)), the prediction of $Y_v$ in the heteroscedastic case needs more careful attention. To tackle this problem, (Marrel et al., 2012) suggested a joint surrogate modelling approach which requires constructing several GP emulators. However, one can use the noise variance prediction offered by the package hetGP (Binois & Gramacy, 2021) to approximate $Y_v$ as explained in Section 5.1. Finally, it is worth mentioning recent alternatives for SA of stochastic codes such as SA in Wasserstein spaces (Fort et al., 2021), or kernel-based SA (Da Veiga, 2021).

6 Conclusion

In this report, we investigated various aspects of sensitivity analysis of numerical models that one can encounter in real-world applications. This includes the Sobol’ indices, SA of stochastic simulators and those with dependent inputs. The latter is tackled via the Shapley effect since the Sobol’ indices are not reliable measures when the inputs are correlated. The Shapley effect is a concept in cooperative game theory. In the case of stochastic simulators, we first employed a GP to emulate the model and then applied SA on the emulator. GPs are commonplace surrogate models in the field of computer experiments to alleviate the computational burden. The analysis is carried out (mainly) with R packages sensitivity and sensobol. We provided several illustrative examples that help the user to learn the packages easily. All the results are reproducible making the report important from a practical point of view.

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