Nonparametric estimation of aggregated Sobol' indices: application to a depth averaged snow avalanche model

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Abstract

Avalanche models are increasingly employed for elaborating landuse maps and designing defense structures, but they rely on poorly known parameters. Careful uncertainty assessment is thus required but difficulty arises from the nature of the outputs of these models, which are commonly both functional and scalar. Hence, so far in the avalanche field, few sensitivity analyses have been performed. In this work, we propose to determine the most influential inputs of an avalanche model by estimating aggregated Sobol' indices. We propose a nonparametric estimation procedure based on the Nadaraya-Watson kernel smoother, which allows to estimate the aggregated Sobol' indices from a given random sample of small to moderate size. Due to the limited size of the sample, the kernel estimation is biased. Therefore, we propose a bootstrap based bias correction before selecting the bandwidth by cross-validation. After different test-cases showing the efficiency of our approach, it is applied to a real avalanche case. Results show that the friction parameters and the snow depth in the release zone are the most influential parameters determining the avalanche characteristics.

1 Introduction

In mountain environments, snow avalanches are a constant threat for settlements and their inhabitants McClung and Schaerer, 2006 Ancey, 2006.

This creates conflict between development and safety and land-use planning is an efficient way to reduce death tolls Gruber and Margreth, 2001, Eckert et al., 2018. To this aim, avalanche flow dynamic models are increasingly employed for elaborating land-use maps and designing defense structures Naaim et al. 2010, Favier et al. 2014. However, all existing physicallybased snow avalanche models remain based on some parameters which are poorly known Ancey and Meunier 2004 Eckert et al. 2008. This applies, for instance, to friction parameters representing the behavior of snow in motion and to initial conditions corresponding to the avalanche release Jamieson et al. 2008 Eckert et al. 2010 Naaim et al. 2013. Thus, a careful assessment of the impact of the uncertainty of the inputs on the outputs should be carried out Fischer 2013. Difficulty arises from the nature of the outputs of these models, which are commonly both functional (e.g., the velocity and flow depth of the avalanche as function of space and time) and scalar (e.g., the runout distance, aka the point of further reach on the 2D topography of the avalanche flow path).

One of the main purposes of sensitivity analysis is to determine the inputs which are the most influential on the output or outputs of a model where the model can be of any nature, for example a black-box model or a complex computational code [Saltelli et al., 2000]. More specifically, [Saltelli et al., 2004] proposed four settings as a guide of objectives of a sensitivity analysis: factor prioritization, factor fixing, variance cutting and factor mapping [Saltelli et al., 2004] [Iooss and Prieur, 2017]. It depends on the analyst to define the objectives of its sensitivity analysis. In the global sensitivity (GSA) framework, the input parameters are modeled by random variables, which will be assumed independent in this paper. The probability distribution chosen to model the input vector is often guided by practitioner's belief. The output is then random as it depends on the inputs through the model. In this work, our objective is factor prioritization which consists in identifying which inputs or factors once fixed would reduce the variance of the output [Saltelli et al., 2008] at most.

There exist different sensitivity measures in the literature for quantifying the influence of each input on the output: variance based indices, also known as Sobol' indices [Sobol'] [1993], density based measures [Borgonovo et al.] [2016], entropy-based sensitivity measures [Auder and Iooss] [2008], etc. A detailed review of sensitivity measures can be found, e.g., in [Iooss] and Lemaître [2015] and [Borgonovo and Plischke] [2016].

We focus our study on variance based Sobol' indices Sobol', 1993 commonly used for factor prioritization. Moreover, Sobol' indices have a natural extension to multivariate or functional outputs [see, e.g., Lamboni et al.]

2009 Gamboa et al. 2013 which is the framework of the application that motivated this study. Another remarkable advantage of Sobol' indices is their easy interpretation: a high index shows the input is relevant and a value close to zero shows that it is not, all the indices are normalized between 0 and 1 and sum to 1.

In short, Sobol' indices are constructed as follows: if the output of a model is scalar, its total variance can be split into partial variances by using the Hoeffding decomposition [Hoeffding] 1948. If the inputs are independent, each of the partial variances is associated to an input or to an interaction between inputs through the ANOVA decomposition [Efron and Stein, 1981]. Then, the Sobol' indices [Sobol'] 1993] are calculated as the ratio of each partial variance and the total variance.

If the output is multivariate, it is possible to apply sensitivity analysis to each component of the multivariate output but this could lead to redundancies in the results, particularly in the setting of discretized functional outputs. It seems therefore interesting to turn to the so-called aggregated indices first introduced in Lamboni et al. [2009] which summarize the information. A preliminary step of output dimension reduction such as, e.g., principal component analysis (PCA) or partial least-squares may also be applied first [see, e.g., Campbell et al.] [2006]. For our real application in the avalanche field, dimension reduction was performed by simultaneous PCA introduced in Ramsay and Silverman [2005] [see also Nanty et al.] [2017], and references therein].

We now discuss the estimation of aggregated Sobol' indices. There are many methods to estimate Sobol' indices: the Fast Amplitude Sensitivity Test (FAST) [see, e.g., Saltelli et al., 1999] and references therein], Random Balance Design Tarantola et al., 2006], Sobol' pick-freeze schemes Sobol' 1993]. The main drawback of all the aforementioned methods Plischke 2010 is that they are based on sampling designs of particular type. Nevertheless, for many memory and time consuming real applications, the cost (in terms of number of model evaluations) of these approaches is prohibitive. For example, to estimate a single Sobol' index with an uncertainty of 10%, it could be required to perform 10⁴ model runs [looss and Lemaître, 2015].

To overcome the drawback of the aforementioned methods, authors use approaches not based on structured sampling designs to estimate the indices. These methods are known as given data or one sample methods. They also correspond to *green* sensitivity analysis because available data from previous model runs can be reused. Among these approaches, let us cite the effective algorithm for computing global sensitivity indices (EASI) method proposed by Plischke [2010], which is a spectral method based on the Fast

Fourier Transform. We also mention the work in Plischke et al. [2013], which relies on the notion of class-conditional densities, where a class is a sub-sample stemming from a suitable partition of the dataset. Much more recently, Antoniano-Villalobos et al. [2019] proposed a fully Bayesian given data procedure.

In the present paper, we propose a new given data method to estimate first-order Sobol' indices, based on a nonparametric Nadaraya-Watson Nadaraya, 1964, Watson, 1964 bias corrected kernel regression [Racine] 2001. Our approach is close to the one introduced in Solís [2019]. The main difference is in the formula we apply to correct the bias, which seems to be more efficient, at least in the results of our simulation study. We then extend this estimation procedure to the estimation of the aggregated Sobol' indices [Lamboni et al., 2009]. To our knowledge, it is the first time a nonparametric given data procedure is proposed in this framework. In the framework of the estimation of non aggregated usual Sobol' indices, Da Veiga et al. [2009] proposed a methodology based on local linear regression. The Nadaraya-Watson estimator can be seen as a particular case of the wider class of nonparametric estimators, called local polynomial estimators used in Da Veiga et al. 2009. Specifically, it corresponds to performing a local constant fit. However the procedure in Da Veiga et al. [2009] is clearly different from ours, as it consists in spliting the sample in two disjoint sub-samples, the first one used to emulate the conditional expectation, the second one used to estimate each first-order Sobol' index, replacing the conditional expectation with its corresponding emulator. More recently, Broto et al. 2018 proposed to estimate Shapley effects introduced by Owen 2014 in the framework of sensitivity analysis with a nonparametric estimator based on nearest neighbours.

Within the avalanche field, only a few studies have analyzed the influence of inputs on the outputs of dynamic propagation models. For example, Barbolini and Savi [2001] used a Monte Carlo approach to analyze the sensitivity of runout distances and impact pressures in the VARA model. Jamieson et al. [2008] discussed the main sources of uncertainty in the inputs of avalanche models. Borstad and McClung [2009] developed a sensitivity analysis of an avalanche model with a Coulomb-type friction law. [Bühler et al. [2011]] explored the influence of the digital elevation models resolution on the outputs of the RAMMS avalanche model. Eventually, [Bühler et al. [2018]] developed a sensitivity analysis of released volumes, runout distances and avalanche velocities in the runout zone with respect to the initial released volume with the RAMMS avalanche model. However, the previous studies did not apply formal statistical methods to quantify the respective

importance of the inputs. Moreover, authors considered only scalar outputs in their approaches. By contrast, in our paper, we focus on the avalanche model proposed by Naaim et al. 2004 and we quantify the importance of its inputs on its outputs by estimating the aggregated Sobol' indices with our new nonparametric procedure. The uncertainty on the input parameters was defined based on data obtained from an avalanche released on 13 February 2013 at the Lautaret full-scale test-site Thibert et al. 2015.

In summary, the aims of this study are: (i) to propose a nonparametric estimation method for the aggregated Sobol' indices in a given data framework when sample size is small (ii) to quantify the input importance in avalanche models, having complex outputs (e.g., a mix of functional and scalar outputs). The approach can be easily adapted to other avalanche models and more widely in environmental sciences in the frequent case of complex models with outputs which are both functional and scalar. This work is organized as follows: the aggregated Sobol' indices and the estimation method are described in Section [2] In Section [3], we test the estimation method on toy functions. Then, in Section [4] the avalanche model is described and the results are presented. Finally, in Section [5] the conclusions and perspectives are discussed.

2 Aggregated Sobol' indices

Let us denote by f the model which takes as inputs the vector $\mathbf{X} = (X_1, \dots, X_d)$. The inputs X_1, \dots, X_d are modeled by random variables defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and valued in a measurable space $E = E_1 \times E_2 \dots \times E_d$. The output of the model f is the p multivariate vector $\mathbf{Y} = (Y_1, \dots, Y_p)^T$. It means, we have:

$$f(\mathbf{X}) = f(X_1, \dots, X_d) = \mathbf{Y} = (Y_1, \dots, Y_p)^T$$

In the following, we assume that $\mathbb{E}(Y_1^2 + \ldots + Y_p^2) < \infty$ and that the random variables X_1, \ldots, X_d are independent from each other. This condition guarantees the unicity of the ANOVA decomposition [Sobol'], [1993]. To summarize the importance of each input X_i on the multivariate output \mathbf{Y} , we aim at computing the aggregated Sobol' index GS_i introduced in Lamboni et al. [2009] [see also [Gamboa et al.], [2013] defined as:

$$GS_i = \frac{\sum_{j=1}^p \operatorname{Var}(Y_j) S_i^j}{\sum_{j=1}^p \operatorname{Var}(Y_j)},$$

where S_i^j is the first-order Sobol' index of the output Y_j with respect to the input X_i namely

$$S_i^j = \frac{\operatorname{Var}(\mathbb{E}(Y_j|X_i))}{\operatorname{Var}(Y_j)} \tag{1}$$

Notice that $GS_i \in [0,1]$. As in the case of the scalar indices, the main advantage of the aggregated indices is their easy interpretation: a high value means the input is important, a value close to zero means it is not, and $\sum_{i=1}^{d} GS_i = 1$.

In the following, we propose to estimate nonparametrically GS_i from given data, proposing a new procedure based on the Nadaraya-Watson kernel smoother Nadaraya, [1964] Watson, [1964].

2.1 Nonparametric estimation procedure

Let $(X_i^{\ell}, Y_j^{\ell})_{1 \leq \ell \leq n}$ be an independent identically distributed random sample of (X_i, Y_j) . The Nadaraya-Watson kernel smoother consists in estimating the conditional mean of $\mathbb{E}(Y_i|X_i)$ at a point x in the domain of X_i by:

$$\mathbb{E}(Y_j|X_i = x) = m_h(x) = \sum_{\ell=1}^n Y_j^{\ell} W_{\ell,h}(x),$$
 (2)

where

$$W_{\ell,h}(x) = \frac{K\left(\frac{x - X_i^{\ell}}{h}\right)}{\sum_{\ell=1}^{n} K\left(\frac{x - X_i^{\ell}}{h}\right)},\tag{3}$$

with K a kernel function and h a bandwidth. In Equation 3, different weights $W_{\ell,h}$ can be used, as for example, local linear regression proposed in Da Veiga et al., 2009 and nearest neighbor smoothers as proposed by Broto et al. 2018.

When the sample size is small, the selection of the bandwidth h is critical. Indeed, to avoid undersmoothing or oversmoothing, an optimal value of h which balances bias and variance must be found Tsybakov, 2008 page 17]. An option widely used to select h is cross-validation but if the sample size is small, the estimator will suffer of finite-sample bias [see Racine 2001 Solís, 2019]. Therefore, if the sample size is small, it is recommended to perform a bias correction to the kernel smoother estimator preliminary to the bandwidth selection.

It is important to underline that the criterion we introduce here to select the badwidth is different from the one proposed in Solís [2019], which was based on bagging minimization. The selection of the bandwidth we propose to apply in our paper is described in the next section.

Once the bandwidth h has been chosen, the estimation of the aggregated Sobol' index is straightforward: given a n sample $(x_i^{\ell}, y_i^{\ell})_{1 < \ell < n}$ of (X_i, Y_i) ,

$$\widehat{GS}_i = \frac{\sum_{j=1}^p \widehat{\operatorname{Var}} \left[(y_j^{\ell})_{1 \le \ell \le n} \right] \hat{S}_i^j}{\sum_{j=1}^p \widehat{\operatorname{Var}} \left[(y_j^{\ell})_{1 \le \ell \le n} \right]},\tag{4}$$

where \hat{S}_{i}^{j} is the estimation of the first-order Sobol' index:

$$\hat{S}_i^j = \frac{\widehat{\mathrm{Var}}\left[\left(\widehat{m}_{\mathrm{h}}(x_i^\ell)\right)_{1 \leq \ell \leq n}\right]}{\widehat{\mathrm{Var}}\left[(y_j^\ell)_{1 \leq \ell \leq n}\right]},$$

with $\widehat{\text{Var}}$ denoting empirical variance.

Note that the same sample $(x_i^{\ell}, y_j^{\ell})_{1 \leq \ell \leq n}$ is used for both the estimators \hat{m}_h and $\widehat{\text{Var}}$.

2.2 Bandwidth selection h with bias correction

As mentioned previously, cross-validation is one option to select the bandwidth. In more details, given a n sample $\mathbf{x} = (x^1, \dots, x^n)$ of X_i and the corresponding evaluations $\mathbf{y} = (y^1, \dots, y^n)$ of Y_j , the bandwidth can be selected as:

$$h_{\text{cv}} = \operatorname{argmin}_{h>0} \frac{1}{n} \sum_{k=1}^{n} \left(y^k - \frac{\sum_{\substack{\ell=1\\\ell \neq k}}^{n} y^\ell K_h(x^\ell - x^k)}{\sum_{\substack{\ell=1\\\ell \neq k}}^{n} K_h(x^\ell - x^k)} \right)^2, \tag{5}$$

for notation simplicity, $K_h(.)$ denotes $K(\frac{.}{h})$ and we dropped all the i and j subindices, but keep in mind that we refer to a sample of X_i and Y_j .

If the sample size is small, it is better to apply a bias correction before performing bandwidth selection. In our framework of sensitivity analysis, we adapt the procedure introduced in Racine 2001 to select the bandwidth. The different steps of our procedure are described hereafter:

1. Given a n sample $\mathbf{x} = (x^1, \dots, x^n)$ of X_i and the corresponding evaluations $\mathbf{y}_j = (y^1, \dots, y^n)$ of Y_j and a bandwidth h > 0 (for example,

an initial bandwidth value could be $h = h_{cv}$ given by Equation (5), we calculate the Nadaraya-Watson kernel regression estimate:

$$\widehat{m}_h(x^k) = \frac{\sum_{\substack{\ell=1\\\ell\neq k}}^n y^{\ell} K_h(x^{\ell} - x^k)}{\sum_{\substack{\ell=1\\\ell\neq k}}^n K_h(x^{\ell} - x^k)}.$$
(6)

If
$$\sum_{\substack{\ell=1\\\ell\neq k}}^{n} K(x^{\ell} - x^{k}) = 0$$
, we set $\widehat{m}_{h}(x^{k}) = 0$.

2. We calculate the errors:

$$\hat{\epsilon}^{\ell} = y^{\ell} - \widehat{m}_h(x^{\ell}), \qquad \ell = 1, \dots, n.$$

These errors are heteroscedastic because Y_j depends also on $X_1, \ldots, X_{i-1}, X_{i+1}, \ldots, X_d$, therefore, a standardization of the errors must be applied before bootstraping.

3. The errors $\{\hat{\epsilon}^{\ell}\}_{1 \leq \ell \leq n}$ are standardized as:

$$\hat{v}^{\ell} = \frac{\hat{\epsilon}^{\ell} - \bar{\epsilon}}{r(x^{\ell})}, \qquad \ell = 1, \dots, n$$

where $\bar{\epsilon}$ is the empirical mean of $\{\hat{\epsilon}^\ell\}_{1 \leq \ell \leq n}$ and $r(x^\ell)$ is an estimation of the conditional standard deviation of the random variable $\epsilon | X_i |$ at x. $r(x^\ell)$ is estimated using kernel smoother nonparametric estimation.

4. A bootstrap sample $\mathbf{y}^{(b)}$ of \mathbf{y} is created as:

$$y^{(b)\ell} = \widehat{m}_h(x^{\ell}) + r(x^{\ell})v^{(b)\ell}, \qquad \ell = 1, \dots, n,$$

where $v^{(b)\ell}$ is a bootstrap sample of $\{\hat{v}^{\ell}\}_{1 \leq \ell \leq n}$.

- 5. B bootstrap samples of \mathbf{y} are created using Step 4. For each bootstrap sample $(\mathbf{x}, \mathbf{y}^{(b)})$, we estimate the kernel smoother $\hat{m}_h^{(b)}$ using Equation [6].
- 6. The bias of $\hat{m}_h(x^{\ell})$ is estimated as:

$$\frac{1}{B} \sum_{h=1}^{B} \widehat{m}_h^{(b)}(x^{\ell}) - \hat{m}_h(x^{\ell}).$$

Then, the corrected bias kernel smoother $\hat{m}_h^c(x^{\ell})$ is calculated as:

$$\hat{m}_h^c(x^{\ell}) = \hat{m}_h(x^{\ell}) - \left(\frac{1}{B} \sum_{h=1}^B \hat{m}_h^{(b)}(x^{\ell}) - \hat{m}_h(x^{\ell})\right)$$
(7)

$$= 2\hat{m}_h(x^{\ell}) - \frac{1}{B} \sum_{b=1}^{B} \hat{m}_h^{(b)}(x^{\ell})$$
 (8)

7. Finally, the bandwidth h is selected as

$$\hat{h}_{\text{boot}} = \operatorname{argmin}_{h>0} \frac{1}{n} \sum_{\ell=1}^{n} \left(y^{\ell} - \hat{m}_{h}^{c}(x^{\ell}) \right)^{2}.$$

Once \hat{m}_{boot}^c is calculated, the aggregated Sobol' index GS_i is estimated from \P . In what follows, our estimator with bias correction is denoted by \P and the same estimator without bias correction, for which the bandwidth is selected by solving \P , is denoted by \P .

2.3 Dimension reduction based on principal component analvsis

If the output is high-dimensional or even functional, it may be computationally interesting to reduce the output dimension in a preliminary step. There are different reduction techniques. Principal component analysis, also known as Karhunen-Loève decomposition in the functional framework, consists in projecting the output on a new basis so that most information is concentrated in the first few components [see, e.g., Pearson, 1901] Loève, 1963]. Note that if the outputs are the descretization of more than one functional random variable (e.g., velocity and flow depth), simultaneous PCA may provide efficient reduction. For more details, see e.g., the work of Nanty et al. [2017] and reference therein.

In brief, simultaneous PCA consists in applying PCA to the matrix composed by the concatenation of the discretized functions divided by a normalization factor. Nanty et al. [2017] show that using the maximum of each functional as normalization factor provides the best results. Thus, in the avalanche application, we follow their procedure.

There exist dimension reduction tools specific to functional data, such as the regularized functional PCA described in Chapter 9 of Ramsay and Silverman [2005] [see also the work of Yao et al., [2005] which has been

applied in different fields [e.g., Locantore et al.] [1999] Antoniadis et al.] [2012]. Also, it has been shown that in some applications, functional PCA provides better results than usual PCA applied after a discretization of the functional data [e.g., Viviani et al., 2005]. On our test cases, usual PCA applied on the discretized data set and functional PCA provided similar results. The results we show in this paper are the ones obtained by applying usual PCA on discretized data.

The PCA consists in decomposing the variance-covariance matrix of the output. More precisely, let us denote by Σ the variance-covariance matrix of the output vector \mathbf{Y} . The principal component decomposition of \mathbf{Y} is based on the expansion:

$$\Sigma = \sum_{j=1}^{p} \lambda_j \mathbf{v}_j \mathbf{v}_j^T,$$

where $\lambda_1 \geq \ldots \geq \lambda_p$ are the eigenvalues and $\mathbf{v}_1, \ldots \mathbf{v}_p$ are the orthonormal eigenvectors of Σ . Therefore, \mathbf{Y} can be decomposed as:

$$\mathbf{Y} = \mathbb{E}(\mathbf{Y}) + \sum_{j=1}^{p} ((\mathbf{Y} - \mathbb{E}(\mathbf{Y}))^{T} \mathbf{v}_{j}) \mathbf{v}_{j}$$
$$= \mathbb{E}(\mathbf{Y}) + \sum_{j=1}^{p} \mathbf{h}_{j} \mathbf{v}_{j}$$

where \mathbf{h}_j is the *jth* principal component of \mathbf{Y} . The output can be approximated using the $q \leq p$ first components which capture the major part of the output variance:

$$\mathbf{Y} pprox \mathbb{E}(\mathbf{Y}) + \sum_{j=1}^{q} \mathbf{h}_{j} \mathbf{v}_{j}.$$

Then, the aggregated Sobol' indices can be computed in the first q principal components. For example, for input X_i :

$$GS_i \approx \frac{\sum_{j=1}^q \lambda_j S_i(\mathbf{h}_j)}{\sum_{j=1}^q \lambda_j} \tag{9}$$

where $S_i(\mathbf{h}_j)$ denotes the Sobol' index of \mathbf{h}_j with respect to input X_i . The estimation of the aggregated Sobol' indices will be done for the reduced output $\mathbf{H} = (h_1, \dots, h_q)^T$.

3 Test cases

The cnp method is tested on three toy functions and then, it is applied to an avalanche dynamic model. The cnp accuracy is compared with np (bandwidth selected with cross-validation and without bias correction), Solis2019 Solís 2019, and sobolroalhs Tissot and Prieur 2015 implemented in R. The estimator implemented in sobolroalhs is a pick-and-freeze method, which is particularly interesting in terms of number of model evaluations required for an accurate estimation of Sobol' indices.

Because of its regularity properties, the Epanechnikov kernel of order 2 is used:

$$K(u) = \frac{3}{4}(1 - u^2)I_{(|u| \le 1)},$$

where I denotes the indicator function. All the computations were performed in R Core Team [2019].

3.1 Toy functions

For each toy function, to test the accuracy of the method, the Sobol' indices were estimated with N=100 independent samples of sizes $n\in\{100,200,300\}$. For cnp, the number of bootstrap samples was set to B=100.

3.1.1 Scalar g-sobol function

The scalar g-Sobol function is defined as:

$$Y = f(X_1, \dots, X_d) = \prod_{i=1}^d \frac{|4X_i - 2| + a_i}{1 + a_i}, \ a_i \in \mathbb{R}, i \in \{1, \dots d\}$$

where $(X_1, ..., X_d) \sim \mathcal{U}([0, 1]^d)$.

An analytical expression of the scalar Sobol' indices is available for this test case:

$$S_i = \frac{\frac{1}{3(1+a_i)^2}}{\prod_{i=1}^d \left(\frac{3(a_i)^2 + 6a_i + 4}{3(1+a_i)^2}\right) - 1}, \quad i \in \{1, \dots, d\}.$$

For this first test case, we chose d=8 and $\mathbf{a}=(0,1,4.5,9,99,99,99,99)$. The indices were estimated for N=100 independent samples of sizes $n \in \{100, 200, 300\}$ using the four methods cnp, np, sobolroalhs and Solis2019. The results can be seen in Figures 1 and 2

We remark that the cnp procedure we have proposed in this work behaves well even for small data sets. The bias correction seems to outperform the usual np procedure, except maybe for n = 100.

The variances of both cnp and np are improved with respect to pick-freeze procedure sobolroalhs based on replicated sampling of Tissot and Prieur 2015 and even to the nonparametric bagging approach in Solís 2019. At least, we remark a decrease of the efficiency of our approach for very small Sobol' indices.

3.1.2 Multivariate g-sobol function

To test our estimation method on a multivariate function, we use a multivariate version of the g-Sobol function. The function is defined as:

$$(Y_1, \ldots, Y_p)^T = f(X_1, \ldots, X_d)$$
 with $(X_1, \ldots, X_d) \sim \mathcal{U}([0, 1]^d)$

where

$$Y_j = \prod_{i=1}^d \frac{|4X_i - 2| + a_i^j}{1 + a_i^j}, \ a_i^j, \text{ with } j \in \{1, \dots, p\}, i \in \{1, \dots d\}.$$

An analytical expression of aggregated Sobol' indices is available for this test case:

$$GS_i = \frac{\sum_{j=1}^p \frac{1}{3(1+a_i^j)^2}}{\sum_{j=1}^p \prod_{i=1}^d \left(\frac{3(a_i^j)^2 + 6a_i^j + 4}{3(1+a_i^j)^2}\right) - 1}.$$

We chose p=2, d=6 and the coefficients $a_i^j, i \in \{1, ..., 6\}, j \in \{1, 2\}$ are coded in the matrix $A_2 \in \mathbb{R}^{6 \times 2}$:

$$A_2^T = \begin{pmatrix} 0 & 0.5 & 3 & 9 & 99 & 99 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$

Figure 3 shows the estimation of the Sobol' indices using cnp, np and sobolroalhs in N = 100 independent samples of sizes $n \in \{100, 200, 300\}$. The bias accuracy of cnp compared to the other two methods is the best (see Figure 3). Furthermore, the variance of cnp estimation is lower than

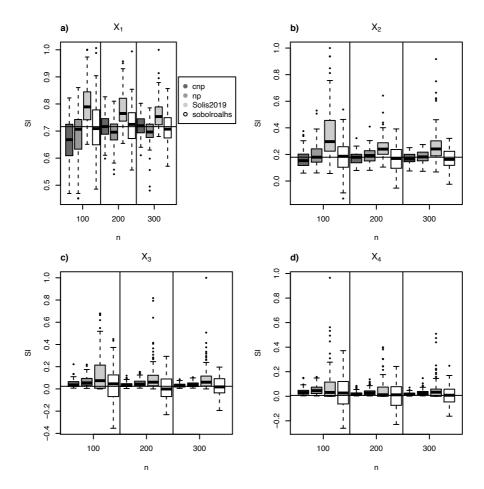


Figure 1: Scalar g-Sobol function: estimation of the first-order Sobol' indices for X_1 , X_2 , X_3 and X_4 using four estimation methods: cnp, np, Solis2019 and sobolroalhs. To draw the boxplots, the indices were computed in N=100 independent samples of sizes $n \in \{100,200,300\}$. For each iteration of cnp and Solis2019, we used B=100 bootstrap samples.

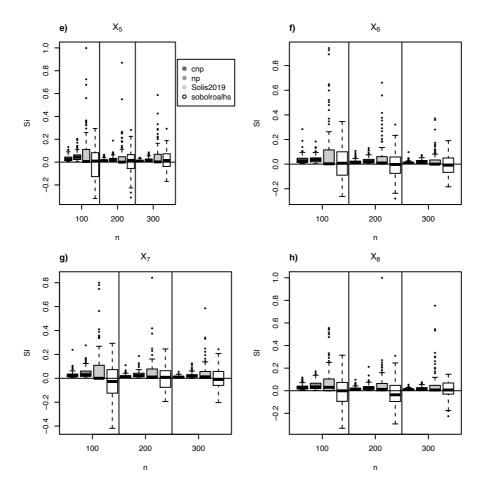


Figure 2: Scalar g-Sobol function: estimation of the first-order Sobol' indices for X_5 , X_6 , X_7 and X_8 using four estimation methods: cnp, np, Solis2019 and sobolroalhs. To draw the boxplots, the indices were computed in N=100 independent samples of sizes $n \in \{100,200,300\}$. For each iteration of cnp and Solis2019, we used B=100 bootstrap samples.

Input	Description	Distribution
m	mass (kg)	U[10, 12]
c	damping constant $(Nm^{-1}s)$	U[0.4, 0.8]
k	spring constant (Nm^{-1})	U[70, 90]
l	initial elongation (m)	$\mathcal{U}[-1, -0.25]$

Table 1: Mass spring model: Inputs description and uncertainty intervals.

the other two methods (see Figure 3). Additionally, for this test case, the bias correction performance is more evident than in the previous case (see Figures 1 and 2 compared to Figure 3).

3.2 A functional example: the mass-spring model

Before applying our procedure to the avalanche application, we illustrate its performance on a test case with discretized functional output: the functional mass-spring model proposed by Gamboa et al. [2013], where the displacement of a mass connected to a spring is considered:

$$mx''(t) + cx'(t) + kx(t) = 0, (10)$$

with initial conditions x(0) = l, x'(0) = 0, and $t \in [1, 40]$. There exists an analytical solution of Equation (10). This model has four inputs (see more details in Table 1). The model output is the vector:

$$\mathbf{Y} = f(\mathbf{X}) = (x(t_1), \dots, x(t_{800})), \quad t_i = 0.05i \text{ with } i \in \{1, \dots, 800\}.$$

The discretized output is high-dimensional (p = 800). Therefore, we first reduce the dimension of the output by using PCA before estimating the aggregated Sobol' indices in the first q principal components with $q \ll p$.

The indices were estimated for N = 100 independent samples of size $n \in \{100, 200, 300\}$. Each sample was also used for PCA. We tested if the results were more accurate if we used two independent samples, one for PCA and the other one for the estimation of the Sobol' indices. At a constant cost in terms of model evaluations, the results were even better using only one sample (see Figure 12 in the Appendix in Section 6).

The explained variance as a function of the number of PCs q is shown in Figure 4. Notice that 70% of the variance is explained with a small number of PCs (q = 3) and almost all the variance (95%) is explained by 6 PCs. Thus, the aggregated Sobol' indices are estimated using the first 6 PCs.

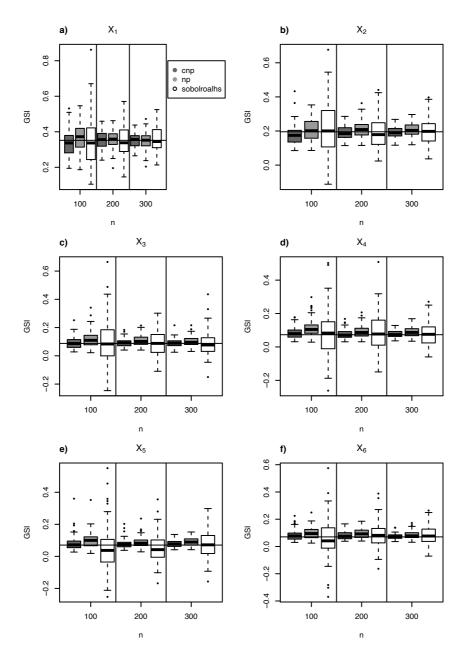


Figure 3: Multivariate g-Sobol function: estimation of the aggregated Sobol' indices using cnp, np and sobolroalhs. Boxplots were drawn from N=100 samples of sizes $n \in \{100, 200, 300\}$. To use cnp, we set B=100.

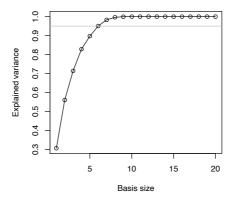


Figure 4: Mass-spring model: Explained variance as a function of the decomposition basis size (number of PCs). The gray line is displayed at the 95% of the variance explained which corresponds to 6 PCs.

The true aggregated Sobol' indices for this instance are unknown but they are considered close to the values estimated with a sample of large size $n = 100\,000$ using sobolroalhs.

The evolution of the estimation of the aggregated Sobol' indices using the three methods in function of the sample size $n \in \{100, 200, 300\}$ are shown in Figure 5. The cnp estimation has a much smaller variance than the sobolroalhs estimation. The bias correction allows to correct the bias of the np estimation procedure, even if a residual bias seems to persist. The bias decreases as n increases, as expected. As it was mentioned before, our aim is factor prioritization and this objective is achieved with the cnp method in the sense that the most influential factor X_3 is clearly identified.

In general, the cnp method has a better accuracy compared to the other methods np, sobolroalhs and Solis2019 in all the test cases we considered. Therefore, in the following section we apply the cnp method to estimate the aggregated Sobol' indices of an avalanche model.

4 Application: the avalanche model

The avalanche model used in this study represents the avalanche motion as a fluid. The model is based on depth-averaged Saint-Venant equations and it was proposed by Naaim et al. [2004].

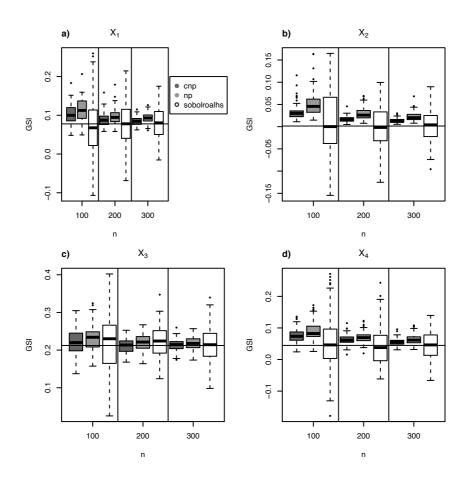


Figure 5: Mass-spring model: Estimation of the aggregated Sobol' indices using cnp, np and sobolroalhs. Boxplots were drawn from N=100 samples of different sizes $n \in \{100, 200, 300\}$. To use cnp, we set B=100.

In short, the model considers only the dense layer of the avalanche. The depth of the flow is then small compared to its length. Under this assumption, shallow-water approximations of the mass and momentum equations can be used. Also, the model assumes the avalanche is flowing on a curvilinear profile z = l(x), where z is the elevation and x is the projected runout length distance measured from the starting abscissa point of the avalanche. The mass and momentum conservation equations of the Saint-Venant avalanche model are:

$$\frac{\partial h}{\partial t} + \frac{\partial hv}{\partial x} = 0$$

$$\frac{\partial hv}{\partial t} + \frac{\partial}{\partial x} \left(hv^2 + \frac{h^2}{2} \right) = h \left(g \sin \phi - F \right)$$

where $v = \|\vec{\mathbf{v}}\|$ is the flow velocity, h is the flow depth, ϕ is the local angle, t is the time, g is the gravity constant and $\mathbf{F} = \|\vec{\mathbf{F}}\|$ is a frictional force. The F frictional force considered in the model is the Voellmy frictional force:

$$F = \mu g cos\phi + \frac{g}{\xi h} v^2,$$

where μ and ξ are the friction parameters (see more details of the avalanche model in Naaim et al. [2004]). For keeping the same notation in the document, the avalanche model is hereafter denoted by f.

4.1 The inputs

The avalanche model depends on six inputs: the friction parameters μ and ξ , the length l_{start} of the avalanche release zone, the snow depth h_{start} within the release zone, the release position of the avalanche denoted by $\mathbf{x}_{\text{start}}$ and the discretized topography of the flow path, denoted by $D = (\mathbf{x}, \mathbf{z}) \in \mathbb{R}^{T \times 2}$ where $\mathbf{x} \in \mathbb{R}^T$ is the vector of projected runout length from the starting point of the avalanche and $\mathbf{z} = l(\mathbf{x}) \in \mathbb{R}^T$ is the elevation vector. T is the number of points of the discretized path.

Additionally to these parameters, we included the term σ to code the error of the digital elevation model \mathbf{z} on the path's topography. To do so, a Gaussian error term is added to each element of \mathbf{z} to construct a new topography $D' = (\mathbf{x}, \mathbf{z}')$ for each new model run, whose elevation is calculated as follows:

Input	Description	Distribution
$\overline{\mu}$	Static friction coefficient	$\mathcal{U}[0.177, 0.498]$
ξ	Turbulent friction [m.s ⁻²]	$\mathcal{U}[306.97, 1475.67]$
h_{start}	Snow depth within the release zone [m]	$\mathcal{U}[0.17, 0.33]$
l_{start}	Length of the release zone [m]	U[24, 34]
σ	Digital Elevation Model error [m]	$\mathcal{U}[0, 0.15]$

Table 2: Avalanche model: Input description and uncertainty intervals. $\mathcal{U}[a,b]$ denotes an uniform distribution in the interval [a,b].

$$\mathbf{z}' = \mathbf{z} + \mathcal{N}(0, \mathbb{I}_T \sigma^2)$$

where \mathbb{I}_T is the $T \times T$ identity matrix. This error codes the imprecision of the digital elevation model which allows analysing how it affects the simulation results.

In this study, we analyzed precisely the sensitivity of the model for the simulations of a single avalanche event. The input uncertainty intervals are those corresponding to an avalanche released at the Lautaret full-scale test-site on 13 February 2013. More details about this avalanche event can be found in Pulfer et al. 2013 Heredia et al. 2020. Thus parameter (x,z) is not uncertain anymore.

For this avalanche event, the release position of the avalanche x_{start} is precisely known because it was fixed by the experimental team (artificial avalanche release). Thanks to the sophisticated equipment of the test-site, the uncertainty of this input can therefore be neglected. The l_{start} and h_{start} input uncertainty intervals could be determined thanks to measures taken during the experiment. By contrast, the inputs μ and ξ cannot be measured. In another study, we developed a Bayesian calibration approach to infer these inputs from the measurements made along the flow. Thus, the uncertainty intervals of μ and ξ considered here correspond to the 95% credibility intervals of the posterior distribution we obtained Heredia et al. [2020]. However, to avoid privileging some values in the sensitivity analysis, uniform distributions were chosen to model the d=5 inputs, including the friction parameters (i.e. we did not directly use their posterior distribution). The uncertain inputs of the model and their uncertainty intervals are summarized in Table [2]

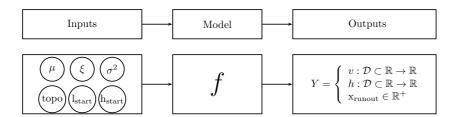


Figure 6: Avalanche model: Inputs and outputs. x_{start} is fixed. All other quantities are taken as random and considerd in the sensitivity analysis.

4.2 The outputs

The outputs of the avalanche model are the functional maximal velocity \vec{v} and the functional maximal flow depth \vec{h} of the avalanche on the discretized grid corresponding to the topography D, and the runout distance of the avalanche denoted by $\mathbf{x}_{\text{runout}}$. In other words, the model has two vectorial and one scalar outputs.

The vectors whose components are the evaluations on the discretized topography D of the velocity and flow depth functional outputs are denoted $\mathbf{v} = (v_1, \dots, v_T)$ and $\mathbf{h} = (h_1, \dots, h_T)$, respectively. Note that we have $p = 2 \times T + 1$ outputs. A brief summary of our framework is drawn in Figure $\boxed{6}$

The global sensitivity analysis is conducted only on a section of the path where all the avalanche simulations are flowing. More precisely, considering e.g., the velocity, our sensitivity analysis is performed on a subset of length n, $\mathbf{v} = \{v_1^{\ell}, \dots, v_{T_1}^{\ell}\}_{\ell \in \{1, \dots, n\}}$, with $T_1 \leq T$ and such that $v_k^{\ell} > 0$ for all $k \in \{1, \dots, T_1\}$.

Figure 7 shows the functional high density region (HDR) boxplots of 300 velocity (a) and snow depth curves (b) and the boxplot for the runout distance (c). The functional HDR plots are a tool for visualizing large amounts of functional data based in the estimation of the bivariate kernel density function of the two first components of the decomposition of the functional data [see Hyndman and Shang, 2010] for more details]. The HDR boxplots show the 50% HDR and the 100% HDR in light and dark gray, respectively. The modal curve is plotted with a solid line. These Figures were obtained using the R package rainbow developed by Hyndman and Shang [2010].

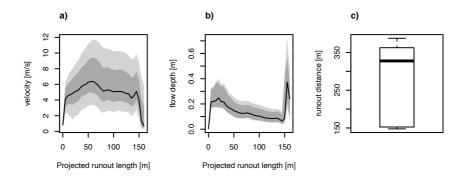


Figure 7: Avalanche model: a) functional high density region boxplots for the velocity b) functional high density region boxplots for the flow depth and, c) boxplot for the runout distance.

4.3 Sobol' indices

To estimate the sensitivity indices, we developed n=300 model simulations using the random input distributions shown in Table 2 Figure 8 shows the topography of the avalanche path and the gray box shows the region where all the avalanche simulations are flowing. The output values in this subset are used in the sensitivity analysis. Also, in Figure 8 we show the percentage of avalanches flowing in the path as function of the position along the topography.

4.4 Scalar Sobol' indices

The scalar Sobol' indices were calculated using n=300 samples and they are shown in Figure $\centsymbol{9}$ For the velocity output, in the first 50 m of the path, the input μ is the most important, then it is followed by ξ . For the rest of the path, the input ξ is the most important. For the flow depth output, the h_{start} input is the most important. The input σ^2 is the less important parameter for both outputs. The scalar sensitivity indices for the runout distance are shown in Figure $\centsymbol{10}$ For this output, the h_{start} input is the most important. These three figures give us valuable information about the model. However, it could also be interesting to get a summarized information by computing aggregated sensitivity indices and this is done in the following section.

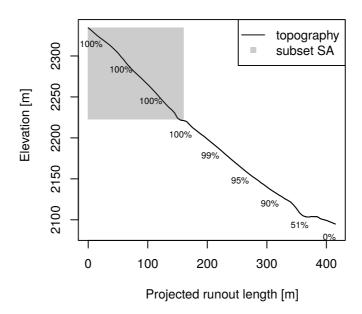


Figure 8: Avalanche model: path's topography (black line) with T=84 discretization points and the subset of the path in gray box ($T_1=33$ discretization points) where the sensitivity analysis is performed. The panel highlights the percentage of avalanche flowing as function of the position within the path.

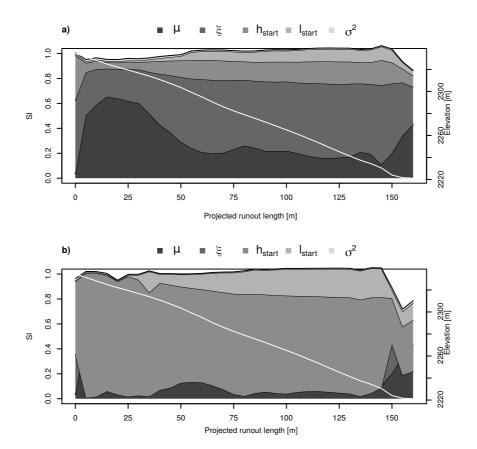


Figure 9: Avalanche model: **a)** scalar Sobol' indices for the velocity and **b)** flow depth outputs. The white line corresponds to the path's topography.

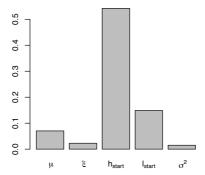


Figure 10: Avalanche model: scalar Sobol' indices for the runout distance output.

4.5 Aggregated Sobol' indices

To estimate the aggregated indices, we used two ways of aggregating the output information. In the first one, we performed two PCAs separately: one for the velocity output and the other one for the flow depth output. And in the second one, we used simultaneous PCA to estimate the indices of the three outputs. The results of the aggregated indices using two PCAs are shown in the panel a) of Figure 11 and using simultaneous PCA in the panel b) of Figure 11. This summarizes the importance of the inputs.

Let us analyze the results of the aggregated indices calculated when performing a PCA on each functional output: for the velocity output, the ξ and μ inputs are the most relevant and for the flow depth output, the h_{start} input is by far the most important. These results are consistent with findings of other studies [e.g., Barbolini and Savi] [2001] [Borstad and McClung, [2009] [Fischer et al., [2015]].

Finally, let us analyze the results of the aggregated indices calculated when performing a simultaneous PCA for the whole set of outputs(he two functional ones and the scalar runout distance): the most important inputs are ξ , h_{start} and μ .

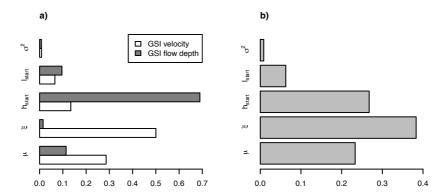


Figure 11: Avalanche model: aggregated indices estimated with two ways of aggregating the information. a) Two PCAs performed separately for the two functional outputs: one for the velocity output and the other one for the flow depth output. b) Simultaneous PCA to estimate the indices of the three outputs (the two functional ones and the scalar runout distance) altogether.

5 Conclusions and perspectives

In this work, we proposed a nonparametric method to estimate the aggregated Sobol' indices from a given random sample with small size, we called this method cnp. The method is based on the Nadaraya-Watson kernel smoother. Due to the small size of the sample at hand, the kernel estimation is biased. Therefore, to remove the bias of the estimation, we proposed a bias correction using bootstrapping samples based on the works of Racine [2001] and Solís [2019] before bandwidth selection based on cross-validation.

We tested the accuracy of the method on a scalar and two multivariate test cases. In general, the method cnp is accurate, even if the sample size is low (n=300). Also, by comparing cnp with its no bias correction np variant, the results have shown that the bias is successfully removed. Nevertheless, it still exhibits small bias for very small Sobol' indices. However, the objective of our sensitivity analysis was factor prioritization and this aim is well achieved with our method.

The method was developed to estimate the aggregated indices for an avalanche model which has three outputs: the functional velocity and flow depth discretized on a given topography and the runout distance of the

avalanche. In this work, we developed a sensitivity analysis of a single avalanche event. The event corresponds to an avalanche released at the Lautaret test-site the 13 February 2013. The results have shown that for this particular avalanche event: for the velocity output, the μ and ξ inputs are the most relevant and for the snow depth output, h_{start} is the most important. Finally, for the runout distance output, h_{start} is the most important. We also showed how this information can be aggregated in one single set of indices summing up the model sensitivity which could be a very useful information for avalanche practitioners.

Note that in this work we proposed a method to quantify the importance of the inputs of a particular avalanche model but this method can be widely applied to other avalanche models. Moreover, the method could be applied to other avalanche events with the same model to generalize the results. Eventually, it could be adapted to various problems for which complex models with outputs which are both functional and scalar are employed.

In this paper, we did not provide confidence intervals (CI) associated to the estimation of Sobol' or aggregated Sobol' indices. This would be an interesting task for a future work. Bootstrap based CI are costly in that framework as they would involve two boostrap stages: one for the bias correction and one for the computation of CI.

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6 Appendix

In this appendix, we want to compare the accuracy of Sobol' index estimation for the mass-spring test case when using a single sample of size n=200 for both PCA and Sobol' index estimation or two independent samples of size n=100, one for PCA, the other one for Sobol' index estimation. Boxplots presented in Figure 12 were obtained with N=100 independent replications.

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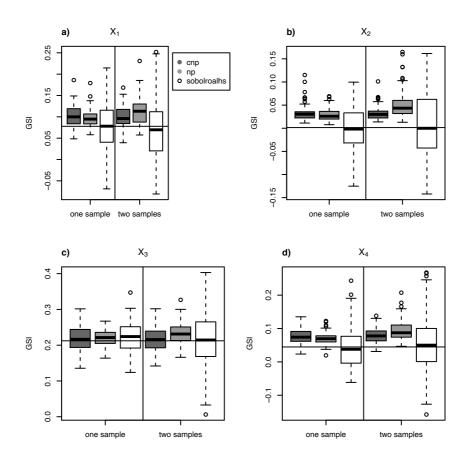


Figure 12: Mass-spring model: Estimation of the aggregated Sobol' indices using cnp, np and sobolroalhs. Boxplots were drawn from N=100 samples of sizes 200. The estimation results using the same sample to estimate the indices and the PCs (one sample) and to estimate the indices and the PCs using two samples are shown. To use cnp, we set B=100.

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