Recent advances in Global Sensibility Analysis

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Part II

Global Sensitivity Analysis:
GSA for stochastic models, variance-based SA with dependent inputs.

Global sensitivity analysis for stochastic models

A first step to GSA for stochastic models

We assume that for any $\mathbf{x} = (x_1, \ldots, x_d) \in \mathcal{X} = \mathcal{X}_1 \times \ldots \mathcal{X}_d$, $\mathcal{M}(\mathbf{x})$ is random with values in $\mathcal{Y}$.

The stochastic model is fully described by the stochastic process $\{\mathcal{M}(\mathbf{x})\ ,\ \mathbf{x} \in \mathcal{X}\}$.

Typical stochastic models are agent-based models or models driven by stochastic differential equations.

A first way to perform global sensitivity analysis for stochastic models is to focus on deterministic quantities of interest (QoI) obtained by integrating the model output w.r.t. the intrisic noise, then to perform standard GSA (see, e.g., Etoré *et al.*, 2020 and references therein).

Let us rewrite the stochastic model in the form $\mathcal{M}(\mathbf{X}, D)$ with $\mathbf{X}$ the vector of uncertain inputs and D an extra unobserved random input (corresponding to the intrinsic noise).

Such a decomposition is exploited in Janon *et al.* (2014), to quantify the metamodeling error in the estimation of Sobol' indices.

Mazo (2021) studies two different variance-based indices.

1. The first approach consists in substituting $\mathcal{M}(\mathbf{X}, D)$ for $\mathcal{M}(\mathbf{X})$ in the definition of first order Sobol' indices, leading to

$$S_i = \frac{\mathrm{Var}[\mathbb{E}(\mathcal{M}(\mathbf{X}, D)|X_i)]}{\mathrm{Var}(\mathcal{M}(\mathbf{X}, D))}.$$

   In this case, D is considered as an additional input, even though it is not observable.

2. The second approach consists in substituting $\mathbb{E}(\mathcal{M}(\mathbf{X}, D)|\mathbf{X})$ for $\mathcal{M}(\mathbf{X})$ in the definition of first-order Sobol' indices. The model output is thus averaged w.r.t. the intrinsic noise.

In Hart *et al.* (2017), the authors consider random first-order Sobol' indices: $S_i(D)$, $i = 1, \dots, d$. From a set of n realizations $S_i(D^{(j)})$, $j = 1, \dots, n$, they compute r^{th} order empirical moments:

$$\hat{\mu}_{i,r} = \frac{1}{n} \sum_{j=1}^{n} \left(S_i(D^{(j)}) \right)^r .$$

Note that

$$\mathbb{E}_D[\hat{\mu}_{i,r}] = \mathbb{E}_D[(S_i)^r] \quad \text{and} \quad \mathrm{Var}_D(\hat{\mu}_{i,r}) = \frac{1}{n} \mathrm{Var}_D((S_i)^r).$$

Let us now assume that $\mathcal{Y} = \mathbb{R}$. In Fort *et al.*(2021), the authors note that to any stochastic model corresponds two deterministic applications:

1. $(\mathbf{x}, d) \mapsto \mathcal{M}(\mathbf{x}, d)$ which takes values in $\mathbb{R}$,
2. $\mathbf{x} \mapsto \mathcal{M}_2(\mathbf{x}) = \mu_{\mathbf{x}}$, with $\mu_{\mathbf{x}}$ the probability distribution of $\mathcal{M}(\mathbf{x}, D)$. This second application takes values in the set of probability distributions on $\mathbb{R}$.

On the set of probability measures on $\mathbb{R}$, one defines the 2-Wasserstein distance W_2 as:

$\forall$ μ, ν probability measures on $\mathbb{R}$ with c.d.f. F_μ and F_ν resp.,

$$W_2^2(\mu, \nu) = \int_0^1 (F_\mu^{-1}(t) - F_\nu^{-1}(t))^2 dt = \mathbb{E}[\big(F_\mu^{-1}(U) - F_\nu^{-1}(U)\big)^2]$$

with F_μ^{-1} (*resp.* F_ν^{-1}) the generalized inverse of F_μ (*resp.* F_ν) and $U \sim \mathcal{U}([0,1])$.

Let's assume that for any $\mathbf{x}$, the probability measure $\mu_{\mathbf{x}}$ belongs to $\mathcal{Y} = \mathcal{W}_2(\mathbb{R})$ the space of all probability distributions on $\mathbb{R}$ with finite second-order moment w.r.t. the 2-Wasserstein distance W_2. We consider the r.v. $\mu_{\mathbf{X}}$ with values in $\mathcal{Y}$. We denote by $\mathbb{P}$ its probability distribution.

Let $\tilde{\mu}$ and $\tilde{\tilde{\mu}}$ be two elements in $\mathcal{W}_2(\mathbb{R})$. The general metric space indices in this framework $S_{2,W_2}^{\mathbf{u}}$ can be defined as in (Fort *et al.*, 2021):

$$\frac{\int_{\mathcal{W}_2(\mathbb{R})\times\mathcal{W}_2(\mathbb{R})} \mathrm{Var}\left[\mathbb{E}\left(\mathbb{1}_{W_2(\tilde{\mu},\mu_{\mathbf{X}})\leq W_2(\tilde{\mu},\tilde{\tilde{\mu}})}|X_{\boldsymbol{u}}\right)\right] d\mathbb{P}^{\otimes 2}(\tilde{\mu},\tilde{\tilde{\mu}})}{\int_{\mathcal{W}_2(\mathbb{R})\times\mathcal{W}_2(\mathbb{R})} \mathrm{Var}(\mathbb{1}_{W_2(\tilde{\mu},\mu_{\mathbf{X}})\leq W_2(\tilde{\mu},\tilde{\tilde{\mu}})}) d\mathbb{P}^{\otimes 2}(\tilde{\mu},\tilde{\tilde{\mu}})}.$$

In practice one can only obtain an empirical approximation of the measure $\mu_{\mathbf{x}}$ computed from n evaluations $\mathcal{M}(\mathbf{x}, d^{(j)})$, $j = 1, \dots, n$. Note that in general, the $d^{(j)}$ are not observed.

Finally, the general design of experiments is the following:

$$\mathbf{x}^{(1)}, d^{(1,1)}, \dots, d^{(1,n)} \longrightarrow \mathcal{M}(\mathbf{x}^{(1)}, d^{(1,1)}), \dots, \mathcal{M}(\mathbf{x}^{(1)}, d^{(1,n)})$$

$$\dots$$

$$\mathbf{x}^{(N)}, d^{(N,1)}, \dots, d^{(N,n)} \longrightarrow \mathcal{M}(\mathbf{x}^{(N)}, d^{(N,1)}), \dots, \mathcal{M}(\mathbf{x}^{(N)}, d^{(N,n)})$$

For any $k = 1, \dots, N$, we define the approximations of $\mu_{\mathbf{x}^{(j)}}$ as:

$$\widehat{\mu}_{\mathbf{x}^{(k)}} = \frac{1}{n} \sum_{j=1}^{n} \delta_{\mathcal{M}(\mathbf{x}^{(k)}, d^{(k,j)})} .$$

Then the indices $S^{\mathbf{u}}_{2,W_2}$ can be estimated either with a pick-freeze scheme, either with U-statistics or with a rank-based approach (for $\mathbf{u}$ a singleton and for scalar inputs).

Pick-freeze estimation procedure

1. Generate two samples $\mathbf{x}^{(k)}, d^{(k,j)}$ and $\mathbf{x}'^{(k)}, d'^{(k,j)}$, $k = 1, \ldots, N$, $j = 1, \ldots, n$.
2. Generate a pick-freeze sample of size N: $\left(\mathbf{x}^{(k)}, \mathbf{x}^{\mathbf{u},(k)}\right) = \left(\mathbf{x}^{(k)}, \mathbf{x}_{\mathbf{u}}^{(k)} : \mathbf{x}'^{(k)}_{-\mathbf{u}}\right)$, $k = 1, \ldots, N$.
3. For each input, compute the corresponding output n times: $\mathcal{M}(\mathbf{x}^{(k)}, d^{(k,j)})$, $\mathcal{M}(\mathbf{x}^{\mathbf{u},(k)}, d'^{(k,j)})$, $k = 1, \ldots, N$, $j = 1, \ldots, n$.
4. Approximate the measures by empirical measures:
$$\mu^{(k)} \approx \widehat{\mu}^{(k)} = \frac{1}{n} \sum_{j=1}^{n} \delta_{\mathcal{M}(\mathbf{x}^{(k)}, d^{(k,j)})},$$
$$\mu^{\mathbf{u},(k)} \approx \widehat{\mu}^{\mathbf{u},(k)} = \frac{1}{n} \sum_{j=1}^{n} \delta_{\mathcal{M}(\mathbf{x}^{\mathbf{u},(k)}, d'^{(k,j)})}.$$
5. We also need two additional samples of the output, indendent from the pick-freeze scheme:
$\mathcal{M}(\tilde{\mathbf{x}}^{(k)}, \tilde{d}^{(k,j)})$, $\mathcal{M}(\tilde{\tilde{\mathbf{x}}}^{(k)}, \tilde{\tilde{d}}^{(k,j)})$, $k = 1, \ldots, N$, $j = 1, \ldots, n$ leading to $\widehat{\tilde{\mu}}^{(k)}$, $\widehat{\tilde{\tilde{\mu}}}^{(k)}$, $k = 1, \ldots, N$.

Pick-freeze estimation procedure

The cost in terms of number of evaluations of $\mathcal{M}$ is $4Nn$.

In order to compute explicitly our estimator, it remains to compute terms of the form:

$$W_2(\widehat{\mu}^{(\ell)}, \widehat{\mu}^{(k)}).$$

The quantity $W_2(\nu_1, \nu_2)$ is easy to compute if ν_1 and ν_2 are two discrete measures on $\mathbb{R}$ supported on a same number of points. Namely, for

$$\nu_1 = \frac{1}{n}\sum_{k=1}^{n} \delta_{a_k},\ \nu_2 = \frac{1}{n}\sum_{k=1}^{n} \delta_{b_k},$$

the Wasserstein distance between ν_1 and ν_2 simply writes

$$W_2^2(\nu_1, \nu_2) = \frac{1}{n}\sum_{k=1}^{n} (a_{(k)} - b_{(k)})^2,$$

where $z_{(k)}$ is the k-th order statistics of z.

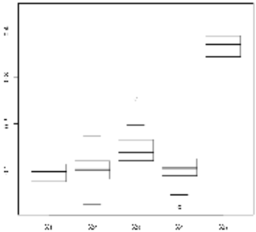
Illustration on a toy model

Let us define the stochastic simulator (see Da Veiga, 2021; Moutoussamy *et al.*, 2015) as

$$Y = (X_1 + 2X_2 + U_1)\sin(3X_3 - 4X_4 + G) + U_2 + 5X_5\, B + \sum_{i=1}^{5} i\, X_i$$

where the intrisic noise is modeled by $U_1 \sim \mathcal{U}([0,1])$, $U_2 \sim \mathcal{U}([1,2])$, $G \sim \mathcal{N}(0,1)$ and $B \sim$ Bernoulli$(1/2)$, and the uncertain parameters X_i are uniformly distributed on $[0,1]$.

With Sébastien's code we compute, for each input X_i, 50 independent realizations of the pick-freeze estimator of S^i_{2,W_2} with $N = 200$ and $n = 100$.



see Jupyter notebook Code–Sto

To go further . . . note that alternative kernel-based procedures can be applied to perform GSA for stochastic models (see Da Veiga, 2021).

Variance-based sensitivity analysis with dependent inputs

Introduction

In this talk, we consider

$$\mathcal{M}\colon \begin{cases} \mathcal{X} = \mathcal{X}_1 \times \ldots \mathcal{X}_d & \to & \mathcal{Y} \\ \boldsymbol{x} = (x_1, \ldots, x_d) & \mapsto & y = \mathcal{M}(\boldsymbol{x}) \end{cases}$$

with

- $\mathcal{M}$: mathematical or numerical model,
- $\boldsymbol{x}$: uncertain input parameters,
- y : output.

We model the uncertain input parameters by a probability distribution P on $\mathcal{X}$ and get

$$Y = \mathcal{M}(X_1, \ldots, X_d)$$

with the vector $\mathbf{X} = (X_1, \ldots, X_d)$ distributed as P.

Introduction

Independent framework: $P(d\boldsymbol{x}) = P_1(dx_1)\dots P_d(dx_d)$

Why is the independent framework not always the right one?

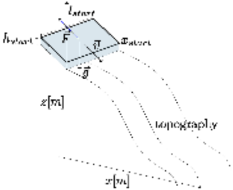
In the following, we consider an application to long-term avalanche hazard assessment. The model under consideration is:

- a snow avalanche model, joint work with INRAE (Grenoble, FRANCE).

Snow avalanche modeling

Model based on depth-averaged Saint-Venant equations (see [Heredia et al., 2020] for more details)

$$\begin{aligned} \frac{\partial h}{\partial t} + \frac{\partial hv}{\partial x} &= 0 \\ \frac{\partial hv}{\partial t} + \frac{\partial}{\partial x}\left(hv^2 + \frac{h^2}{2}\right) &= h\left(g\sin\theta - \mathsf{F}\right) \end{aligned}$$



with $v = \|\vec{\mathbf{v}}\|$ the flow velocity, h the flow depth, θ the local angle, t the time, g the gravity constant and $\mathsf{F} = \|\vec{\mathbf{F}}\|$ a frictional force. The model uses the Voellmy frictional force $\mathsf{F} = \mu g cos\theta + g/(\xi h)v^2$, where μ and ξ are friction parameters.

The equations are solved with a finite volume scheme [Naaim, 1998]. The topography is the one of a path located in Bessans, France.

Let us present one of the two scenarii presented in [Heredia et al., 2020].

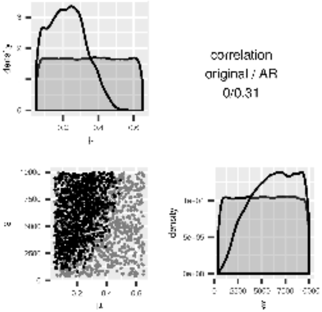
Input	Description	Distribution
μ	Static friction coefficient	$\mathcal{U}[0.05, 0.65]$
ξ	Turbulent friction [m/s^2]	$\mathcal{U}[400, 10000]$
l_{start}	Length of the release zone [m]	$\mathcal{U}[5, 300]$
h_{start}	Mean snow depth in the release zone [m]	$\mathcal{U}[0.05, 3]$
x_{start}	Release abscissa [m]	$\mathcal{U}[0, 1600]$

Let's $\mathrm{vol}_{start} = l_{start} \times h_{start} \times 72.3/\cos(35^\circ)$ instead of h_{start} and l_{start}.

AR rules:

- avalanche simulation is flowing in $[1600m, 2412m]$,
- $vol > 7000m^3$,
- runout distance $< 2500m$ (end of the path).

From $n_0 = 100\,000$ initial runs, we keep $n_1 = 6152$ constrained ones.



Variance based SA in the general framework

We still consider $\mathcal{M}: \begin{cases} \mathbb{R}^d & \rightarrow & \mathbb{R} \\ \boldsymbol{x} = (x_1, \ldots, x_d) & \mapsto & y = \mathcal{M}(\boldsymbol{x}) \end{cases}$

Uncertain parameters are no longer assumed independent, thus $P(d\boldsymbol{x})$ is not necessarily equal to $P_1(dx_1) \ldots P_d(dx_d)$. We have $F_{\mathbf{X}}(\boldsymbol{x}) = C\left(F_{X_1}(x_1), \ldots, F_{X_d}(x_d)\right)$ (Sklar's Theorem) with $F_{X_i}(\cdot)$ and $F_{\mathbf{X}}(\cdot)$ the cdf of X_i, $\boldsymbol{X}$. If the F_{X_i} are continuous, then the copula C is unique.

We still define, for any $i \in \{1, \ldots, d\}$: $S_i = \dfrac{V\left[\mathbb{E}\left[Y|X_i\right]\right]}{V\left[Y\right]}$ and

$S_i^{\text{tot}} = \dfrac{\mathbb{E}\left[V\left[Y|\boldsymbol{X}_{-i}\right]\right]}{V\left[Y\right]}$.

However, nice properties due to orthogonality are lost.

An alternative, the Shapley effects

Let $\mathcal{D} = \{1, \ldots, d\}$. Let team $u \subseteq \mathcal{D}$ create value $\mathbf{val}(u)$. Total value is $\mathbf{val}(\mathcal{D})$. We attribute ϕ_i of this to $i \in \mathcal{D}$.

Shapley axioms [Shapley, 1953]

- Efficiency $\sum_{i=1}^{d} \phi_i = \mathbf{val}(\mathcal{D})$
- Dummy If $\mathbf{val}(u \cup \{i\}) = \mathbf{val}(u)$ for all $u \subseteq \mathcal{D}$, then $\phi_i = 0$
- Symmetry If $\mathbf{val}(u \cup \{i\}) = \mathbf{val}(u \cup \{j\})$ for all $u \cap \{i, j\} = \emptyset$, then $\phi_i = \phi_j$
- Additivity If games **val**, **val'** have values ϕ, ϕ', then $\mathbf{val} + \mathbf{val'}$ has value $\phi + \phi'$

Unique solution

$$\phi_i = \frac{1}{d} \sum_{u \subseteq -\{i\}} \binom{d-1}{|u|}^{-1} \left(\mathbf{val}(u + i) - \mathbf{val}(u) \right)$$

Let $X_1, \dots, X_d$ be the team members trying to explain the variability of $\mathcal{M}$. The value of any $u \in \mathcal{D}$ is how much can be explained by $\boldsymbol{X}_u$.

We choose $\mathbf{val}(u) = \dfrac{V\left[\mathbb{E}\left[Y|\boldsymbol{X}_u\right]\right]}{V\left[Y\right]}$ which leads to the definition of Shapley effects [Owen, 2014]:

$$\phi_i = \frac{1}{d} \sum_{u \subseteq -\{i\}} \binom{d-1}{|u|}^{-1} \left(\frac{V\left[\mathbb{E}\left[Y|\boldsymbol{X}_u, X_i\right]\right]}{V\left[Y\right]} - \frac{V\left[\mathbb{E}\left[Y|\boldsymbol{X}_u\right]\right]}{V\left[Y\right]} \right)$$

It is equivalent to consider to choose $\widetilde{\mathbf{val}}(u) = \dfrac{\mathbb{E}\left[V\left[Y|\boldsymbol{X}_{-u}\right]\right]}{V\left[Y\right]}$ [Song et al., 2016].

Main properties

Independent framework: $\forall\, i = 1, \ldots, d$, $\phi_i = \displaystyle\sum_{\mathbf{u} : i \in \mathbf{u}} \frac{1}{|\mathbf{u}|} S_{\mathbf{u}}$

We also have: $\forall\, i = 1, \ldots, d$, $0 \leq S_i \leq \phi_i \leq S_i^{\text{tot}} \leq 1$ and $\sum_{i=1}^{d} \phi_i = 1$.

Main properties

Independent framework: $\forall\, i = 1, \dots, d$, $\phi_i = \sum_{\mathbf{u}: i \in \mathbf{u}} \frac{1}{|\mathbf{u}|} S_{\mathbf{u}}$

We also have: $\forall\, i = 1, \dots, d$, $0 \leq S_i \leq \phi_i \leq S_i^{\text{tot}} \leq 1$ and $\sum_{i=1}^d \phi_i = 1$.

Dependent framework:

In this framework, we still have $0 \leq \phi_i \leq 1$ and $\sum_{i=1}^d \phi_i = 1$

We do not necessarily have $S_i \leq \phi_i \leq S_i^{\text{tot}}$

The Shapley allocation rule is based on an equitable principle, which ensures that $\phi_i \approx 0 \Rightarrow X_i$ has no significant contribution to $\text{Var}[Y]$, neither by its interactions nor by its dependencies with other inputs.

If output is multivariate or the discretization of a functional output $\mathbf{Y} = (Y_1, \ldots, Y_p)$, we define aggregated Shapley effects as:

$$\forall\, 1 \leq j \leq p\,,\ \forall\, 1 \leq i \leq d\,,\ \phi_i^{\text{agg}} = \frac{\sum_{j=1}^{p} V[Y_j]\phi_i^j}{\sum_{j=1}^{p} V[Y_j]}$$

with ϕ_i^j defined as the Shapley effect of Y_j associated to input X_i [Heredia et al., 2020] (see also [Lamboni et al., 2011]).

Proposition [Heredia et al., 2020, Prop. 2.1]

The set of aggregated Shapley effects $\left(\phi_i^{\text{agg}},\ i \in \{1, \ldots, d\}\right)$ *correspond to the set of Shapley values with characteristic function:*

$$u \subseteq \{1, \ldots, d\} \mapsto \boldsymbol{val}(u) = \frac{\sum_{j=1}^{p} V[Y_j]\boldsymbol{val}_j(u)}{\sum_{j=1}^{p} V[Y_j]}$$

with $\boldsymbol{val}_j(u) = \dfrac{V\left[\mathbb{E}\left[Y_j|\mathbf{X}_u\right]\right]}{V\left[Y_j\right]}$ *or* $\boldsymbol{val}_j(u) = \dfrac{\mathbb{E}\left[V\left[Y_j|\mathbf{X}_{-u}\right]\right]}{V\left[Y_j\right]}$.

What about algorithms?

Algorithms to compute Shapley effects [Castro et al., 2009] are based on the value function $u \mapsto \frac{\mathbb{E}[V[Y|\mathbf{X}_{-u}]]}{V[Y]}\cdot$ Note that

$$\phi_i = \frac{1}{d\,!} \sum_{\pi \in \Pi(\{1,\ldots,d\})} \left(\widetilde{\mathbf{val}}(P_i(\pi) \cup \{i\})) - \widetilde{\mathbf{val}}(P_i(\pi)) \right)$$

with $\Pi(\{1,\ldots,d\})$ the set of all possible permutations of the inputs and for a permutation $\pi \in \Pi(\{1,\ldots,d\})$, the set $P_i(\pi)$ is defined as the inputs that precede input i in π.

Exact permutation algo. (moderate d) all possible permutations are covered.

Random permutation algo. ($d >> 1$) it randomly sample permutations of the inputs.

In [Song et al., 2016], $\widetilde{\mathbf{val}}(u) \to \widehat{\widetilde{\mathbf{val}}}(u)$.

For each iteration of the loop on the inputs' permutations, the expectation of a conditional variance must be computed.

The cost C of these algorithms is the following:

$$C = N_v + m(d-1)N_0 N_i$$

with N_v the sample size for the variance computation, N_0 the outer loop size for the expectation, N_i the inner loop size for the conditional variance and m the number of permutations according to the selected method.

Bootstrap confidence intervals can be computed. A costly model can be replaced by a metamodel. [Iooss and Prieur, 2019, Benoumechiara and Elie-Dit-Cosaque, 2019]

Those algorithms require the ability to sample from the distribution of $\mathbf{X}_u \mid \mathbf{X}_{-u}$, $\forall u \subsetneq \{1, \ldots, d\}$. In [Broto et al., 2020], a given data procedure based on nearest neighbors is introduced.

It is possible to plug algorithms presented in [Castro et al., 2009, Song et al., 2016, Broto et al., 2020] in the estimation of aggregated Shapley effects [Heredia et al., 2020].

Application: snow avalanche modeling

Model based on depth-averaged Saint-Venant equations (see [Heredia et al., 2020] for more details)

$$
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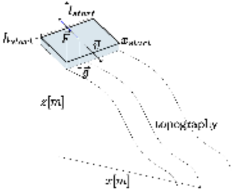
\end{aligned}
$$



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Objective: better understanding the numerical model.

Input	Description	Distribution
μ	Static friction coefficient	$\mathcal{U}[0.05, 0.65]$
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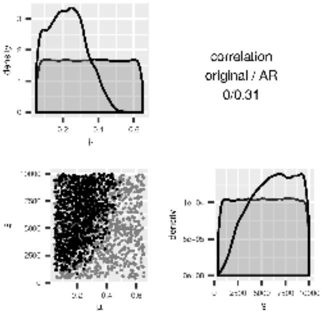
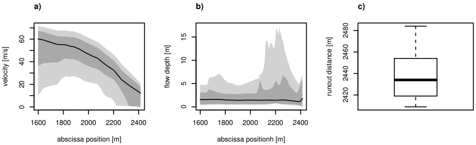
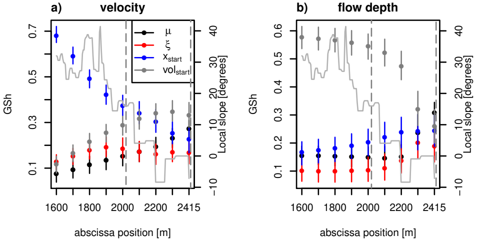




Aggregated Shapley effects of velocity and flow depth curves calculated over space intervals $[x, 2412m]$ where $x \in \{1600m, 1700m, \ldots, 2412m\}$



We have $n = 6152$, $N_{\text{tot}} = 2002$, $B = 500$. Effects are estimated using the first (2, *resp.* 4) fPCs [Yao et al., 2005, Ramsay and Silverman, 2005] explaining more than 95% of the variance. Local slope is drawn with a gray line. A gray dotted rectangle is drawn at $[2017m, 2412m]$ where avalanche return periods vary from 10 to 10 000 years.

In summary,

- it is fundamental to have a good approximation of the released volume and abscissa for velocity forecasting, while for flow depth forecasting, a good approximation of released volume is desirable;
- nevertheless, none of the other inputs are negligible.

To outperform the estimation accuracy at the end of the path generating a larger initial sample of avalanches is possible, but the computational burden is prohibitive.

Conclusion, perspectives

Conclusion: Shapley effects present an alternative to allocate parts of variance in the correlated framework. It is possible to define aggregated Shapley indices. There exist algorithms to estimate these indices, see Jupyter notebook Dependent–Inputs.

Open questions

- What about goal-oriented Shapley effects? (see recent work in [Da Veiga, 2021])
- Nearest neighbor algorithm depends on many parameters to tune (number of neighbors, total cost…)? Is it possible to propose an adaptive choice of these parameters?
- How can Shapley effects be related to gradient-based measures of sensitivity?
- …

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