Aggregated Shapley effects: nearest-neighbor estimation procedure and confidence intervals. Application to snow avalanche modeling.

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Grenoble, 18 September 2020.

Natural phenomena are complex.

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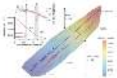

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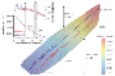

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Given some initial conditions:

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

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 $\Gamma = \|\vec{\mathbf{F}}\|$ is the Voellmy frictional force,

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

where μ and ξ are the friction parameters (see more detail in [Naaim et al., 2004]).

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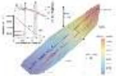

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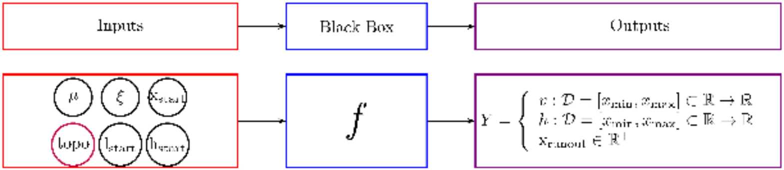
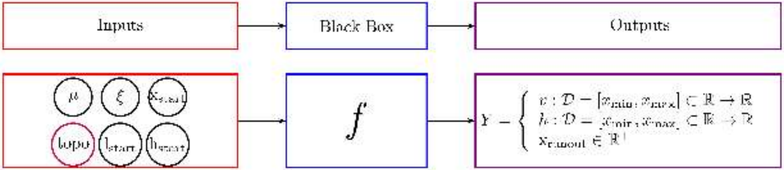
Black box model


Inputs
Black Box
Outputs
μ
ξ
x_{start}
topo
l_{start}
h_{start}
f
$Y = \begin{cases} u : \mathcal{D} = [x_{min}, x_{max}] \subset \mathbb{R} \to \mathbb{R} \\ h : \mathcal{D} = [x_{min}, x_{max}] \subset \mathbb{R} \to \mathbb{R} \\ x_{runout} \in \mathbb{R}^{+} \end{cases}$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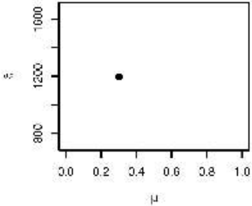
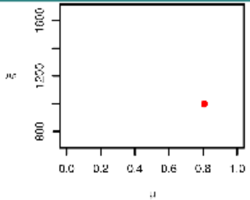

800
1200
1600
0.0
0.2
0.4
0.6
0.8
1.0
μ

$\Rightarrow$



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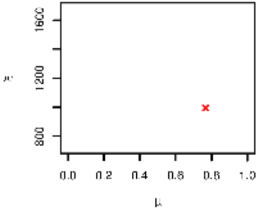

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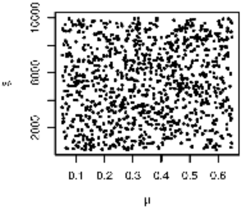
negligible snow avalanche

To get meaningful samples, we apply acceptance-rejection (AR) sampling:



AR sampling
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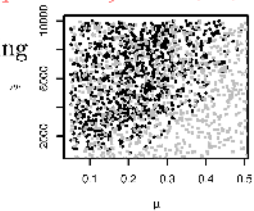

Framework of our application

The ingredients for our global sensitivity analysis (GSA) problem are:

- input parameters leading to significant snow avalanches are dependent,
- the sample is given from the AR sampling and not drawn based on a specific estimation strategy (pick-freeze, replicated designs,...),
- two of the three outputs are functional.

GSA framework

We aim at determining which input parameters contribute the most to a given quantity of interest (defined from the output of the model).

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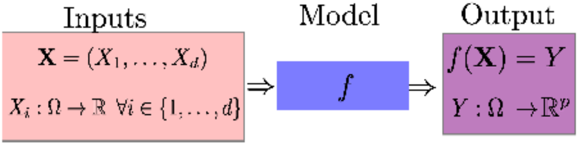

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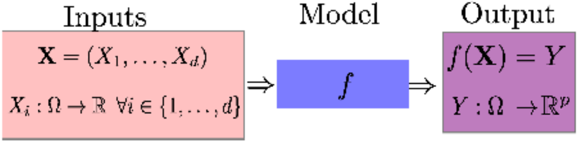

Depending on the quantities of interest:

- variance-based (Sobol' indices [Sobol', 1993], Shapley effects [Owen, 2014]),
- density-based indices or moment-free measures [Borgonovo, 2007, Da Veiga, 2015],
- derivative-based measures [Sobol' and Kucherenko, 2009, Lamboni et al., 2013].

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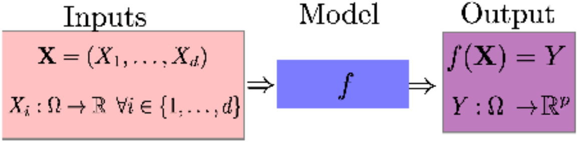

Shapley effects are the ideal framework to our problem!

- they are meaningful even for dependent inputs [Owen and Prieur, 2017, Iooss and Prieur, 2019],
- there exists a given data estimation method [Broto et al., 2020].

Moreover,

- we can extend them to multivariate and functional outputs adapting the propositions in [Campbell et al., 2006, Lamboni et al., 2009, Gamboa et al., 2013, Alexanderian et al., 2020],
- we propose a bootstrap strategy to build confidence intervals.

Shapley effects

If Y is scalar.
Shapley effect [Owen, 2014] (coopetative game theory [Shapley, 1953]) of i:

$$Sh_i = \frac{1}{d\mathrm{Var}(Y)} \sum_{\mathrm{u} \subseteq -\{i\}} \binom{d-1}{|\mathrm{u}|}^{-1} \left(\mathrm{Var}\left(\mathbb{E}(Y|\mathbf{X}_{\mathrm{u}\cup i})\right) - \mathrm{Var}\left(\mathbb{E}(Y|\mathbf{X}_{\mathrm{u}})\right)\right).$$

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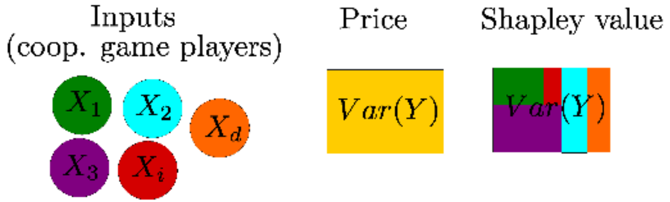

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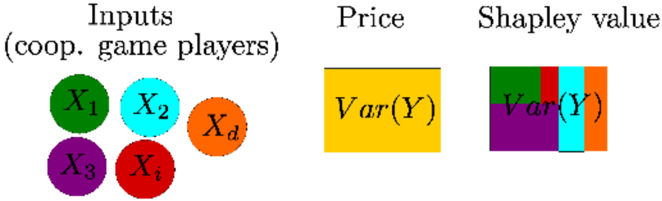

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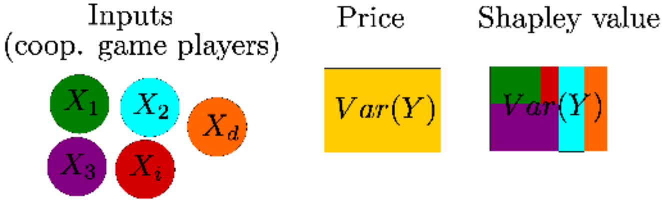

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Shapley effect properties:

- $0 \leq Sh_i \leq 1$ for all $i \in \{1, \ldots, d\}$,
- $\sum_{i=1}^{d} Sh_i = 1$.

Aggregated Shapley effects

If output is multivariate or the discretization of a functional output $\mathbf{Y} = (Y_1, \ldots, Y_p)$.

Aggregated Shapley effects of input X_i:

$$GSh_i = \frac{\sum_{j=1}^{p} \text{Var}(Y_j) Sh_i^j}{\sum_{j=1}^{p} \text{Var}(Y_j)},$$

Aggregated Shapley effects accomplish the natural requirements for a sensitivity measure [Heredia et al., 2020]:

- $0 \leq GSh_i \leq 1$,
- $GSh_i(\lambda f(\mathbf{X})) = GSh_i(f(\mathbf{X}))$ for all $\lambda \in \mathbb{R}$,
- $GSh_i(Of(\mathbf{X})) = GSh_i(f(\mathbf{X}))$ for all $O \in \mathbb{R}^{p \times p}$ and $O^t O = I$.

If the output dimension $p >> 1$, dimension reduction techniques such as pca, fpca [Yao et al., 2005] [Ramsay and Silverman, 2005] should be performed.

Estimation using nearest neighbors

For all $1 \leq i \leq d$ and all $1 \leq j \leq p$ to estimate Sh_i^j and GSh_i, we need to estimate

$$\mathrm{Var}\left(\mathbb{E}(Y_j|\mathbf{X}_{\mathfrak{u}})\right) \qquad \text{or} \qquad \mathbb{E}\left(\mathrm{Var}(Y_j|\mathbf{X}_{-\mathfrak{u}})\right)$$

for all $\mathfrak{u} \subseteq \{1,\ldots,d\}$, with $-\mathfrak{u} = \{1,\ldots,d\} \setminus \mathfrak{u}$.
In our context, we have to estimate from the given data $(\mathbf{X}, \mathbf{Y})$ obtained from the AR sampling.

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[Broto et al., 2020] proposed to estimate $E_{\mathfrak{u}} = \mathbb{E}\left(\mathrm{Var}(Y_j|\mathbf{X}_{-\mathfrak{u}})\right)$ using nearest-neighbors. The estimator $\widehat{E}_{\mathfrak{u}}$ converges in probability to $E_{\mathfrak{u}}$ under mild assumptions (theorem 6.6 of [Broto et al., 2020]).

Combining what they call the subset W-aggregation procedure with the estimates $\widehat{E}_u$, [Broto et al., 2020, proposition 6.12] propose a consistent estimator for each Shapley effect.

Adaptation to the estimation of both Shapley and aggregated Shapley effects, with the construction of bootstrap confidence intervals:

Inputs: **(i)** a n sample $(\mathbf{x},\mathbf{y})$, **(ii)** N_{tot} the estimation cost, **(iii)** $1 \leq N_{\text{u}} \leq n$, the cost for estimation of E_{u} (N_{u} depends on N_{tot} and can be chosen in order to minimize the variance of the estimation), **(iv)** a N_{u} random sample $(s_\ell)_{1\leq\ell\leq N_{\text{u}}}$ from $\{1,\dots,n\}$, **(v)** N_I number of neighbors.

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1 For all $\mathrm{u} \subset \{1,\ldots,d\}$ and for all $1 \leq \ell \leq N_{\mathrm{u}}$, compute:

$$\widehat{E}^j_{\mathrm{u},s_\ell} = \frac{1}{N_I - 1} \sum_{v:\mathbf{x}^v{}_u \in \mathscr{B}_{-\mathrm{u},\ell}} \left(y^v_j - \frac{1}{N_I} \bar{y}_{s_\ell} \right)^2 \text{ with } \bar{y}_{s_\ell} = \frac{1}{N_I} \sum_{v:\mathbf{x}^v{}_u \in \mathscr{B}_{\mathrm{u},\ell}} y^v_j$$

with $\mathscr{B}_{-\mathrm{u},\ell}$ the set of N_I closest neighbors of $x^{s_\ell}_{-\mathrm{u}}$ where $x^{s_\ell}_{-\mathrm{u}} = (x^{s_\ell}_{w_1},\ldots x^{s_\ell}_{w_k})$ with $-\mathrm{u} = \{w_1,\ldots,w_k\}$ and $k = |-\mathrm{u}|$.

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1 For all $u \subset \{1, \ldots, d\}$ and for all $1 \leq \ell \leq N_u$, compute:

$$\widehat{E}^j_{u,s_\ell} = \frac{1}{N_I - 1} \sum_{v:\mathbf{x}^v{}_u \in \mathcal{B}_{-u,\ell}} \left(y^v_j - \frac{1}{N_I} \bar{y}_{s_\ell} \right)^2 \text{ with } \bar{y}_{s_\ell} = \frac{1}{N_I} \sum_{v:\mathbf{x}^v{}_u \in \mathcal{B}_{u,\ell}} y^v_j$$

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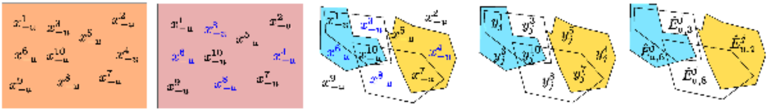

2.1 Compute for all $\mathfrak{u} \subset \{1, \ldots, d\}$.

$$\widehat{E}^{j}_{\mathfrak{u}} = \frac{1}{N_u} \sum_{\ell=1}^{N_u} \widehat{E}^{j}_{u,s_\ell}. \tag{1}$$

2.2 Compute B bootstrap samples (the idea of block-bootstrap is adapted from [Benoumechiara and Elie-Dit-Cosaque, 2019]) from (1):

2.2.1 Create $N_{\mathfrak{u}}$ bootstrap samples from $\widehat{E}^{j}_{\mathfrak{u},s_\ell}$ by sampling with replacement from $\left(\widehat{E}^{j}_{u,s_\ell}\right)_{1 \leq \ell \leq N_{\mathfrak{u}}}$.

2.2.2 Compute for all $b \in \{1, \ldots, B\}$:

$$\widehat{E}^{j,(b)}_{\mathfrak{u}} = \frac{1}{N_{\mathfrak{u}}} \sum_{\ell=1}^{N_{\mathfrak{u}}} \widehat{E}^{j,(b)}_{\mathfrak{u},s_\ell}. \tag{2}$$

3.1. Compute $\widehat{Sh}_i^j$ for all $j \in \{1, \ldots, p\}$ according to:

$$\widehat{Sh}_i^j = \frac{1}{d\hat{\sigma}_j^2} \sum_{\mathfrak{u} \subset -i} \binom{d-1}{|\mathfrak{u}|}^{-1} \left(\widehat{E}^j_{\mathfrak{u} \bigcup \{i\}} - \widehat{E}^j_{\mathfrak{u}}\right), \tag{3}$$

where $\hat{\sigma}_j^2$ is the empirical variance of y_j.

3.2 Compute B bootstrap samples of $\widehat{Sh}_i^j$ using (2) in (3):

$$\widehat{Sh}_i^{j,(b)} = \frac{1}{d\hat{\sigma}_j^{2(b)}} \sum_{\mathfrak{u} \subset -i} \binom{d-1}{|\mathfrak{u}|}^{-1} \left(\widehat{E}^{j,(b)}_{\mathfrak{u} \bigcup \{i\}} - \widehat{E}^{j,(b)}_{\mathfrak{u}}\right),$$

where $\hat{\sigma}_j^{2(b)}$ is the empirical variance of a bootstrap sample of y_j.

4.1 Compute $\widehat{GSh}_i$ for all $i \in \{1, \dots, d\}$ according to:

$$\widehat{GSh}_i = \frac{1}{d \sum_{j=1}^{p} \hat{\sigma}_j^2} \sum_{j=1}^{p} \sum_{\mathfrak{u} \subset -i} \binom{d-1}{|\mathfrak{u}|}^{-1} \left(\widehat{E}^j_{\mathfrak{u} \cup \{i\}} - \widehat{E}^j_{\mathfrak{u}} \right),$$

4.2 compute B bootstrap samples of $\widehat{Gh}_i$:

$$\widehat{GSh}_i^{(b)} = \frac{1}{d \sum_{j=1}^{p} \hat{\sigma}_j^{2,(b)}} \sum_{j=1}^{p} \sum_{\mathfrak{u} \subset -i} \binom{d-1}{|\mathfrak{u}|}^{-1} \left(\widehat{E}^{j,(b)}_{\mathfrak{u} \cup \{i\}} - \widehat{E}^{j,(b)}_{\mathfrak{u}} \right).$$

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5 Compute simultaneous bootstrap confidence intervals (correction of Bonferroni) with bias correction (see e.g., [Efron, 1981]).

Linear Gaussian model with two inputs

Model from [Iooss and Prieur, 2019].

$$Y = \beta_0 + \boldsymbol{\beta}^t \mathbf{X}$$

with $\mathbf{X}_i \sim \mathcal{N}(0,1)$, $\beta_1 = 1$, $\beta_2 = 0$, X_1 and X_2 correlated $\rho = 0.4$.

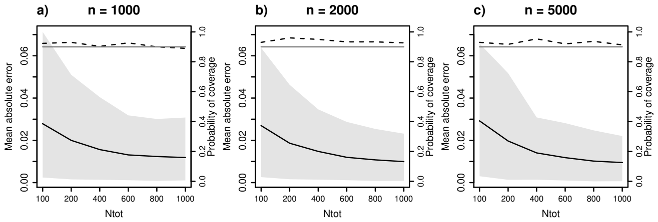


Figure: *Mean absolute error of the estimation of scalar Shapley effects in N=300 i.i.d. samples in function of N_{tot}. $N_I = 3$. The 0.05 and 0.95 pointwise quantiles of the absolute error are drawn with gray polygons. The probability of coverage of the 90% bootstrap simultaneous intervals (Bonferroni correction) is displayed with dotted lines. The theoretical probability of coverage 0.9 is shown with a plain gray line. The bootstrap sample size is fixed to $B = 500$.*

Multivariate Linear Gaussian model with two inputs

$$\mathbf{Y} = (Y_1, Y_2, Y_3) = \beta_0 + \boldsymbol{\beta}^t \mathbf{X}$$

with $\mathbf{X}_i \sim \mathcal{N}(0,1)$, X_1 and X_2 correlated $\rho = 0.4$, and $\boldsymbol{\beta} \in \mathbb{R}^{2\times 3}$:

$$\boldsymbol{\beta} = \begin{bmatrix} 1 & 4 & 0.1 \\ 1 & 3 & 0.9 \end{bmatrix}.$$

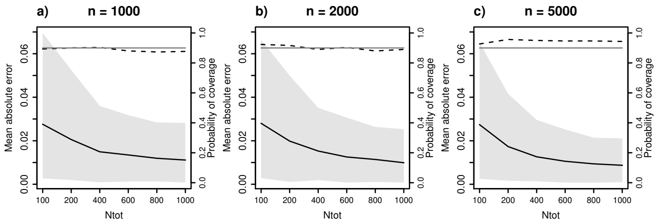


Figure: *Mean absolute error of the estimation of aggregated Shapley effects in N=300 i.i.d. samples in function of N_{tot}. N_I. The 0.05 and 0.95 pointwise quantiles of the absolute error are drawn with gray polygons. The probability of coverage of the 90% bootstrap simultaneous intervals (Bonferroni correction) is displayed with dotted lines. The theoretical probability of coverage 0.9 is shown with a plain gray line.*

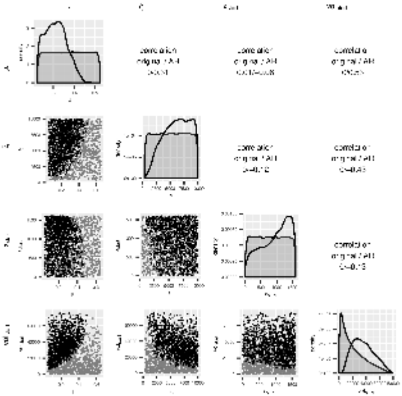
Input	Description	Distribution
μ	Static friction coefficient	$\mathscr{U}[0.05, 0.65]$
ξ	Turbulent friction [m/s^2]	$\mathscr{U}[400, 10000]$
$\mathrm{l}_{\mathrm{start}}$	Length of the release zone [m]	$\mathscr{U}[5, 300]$
$\mathrm{h}_{\mathrm{start}}$	Mean snow depth in the release zone [m]	$\mathscr{U}[0.05,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

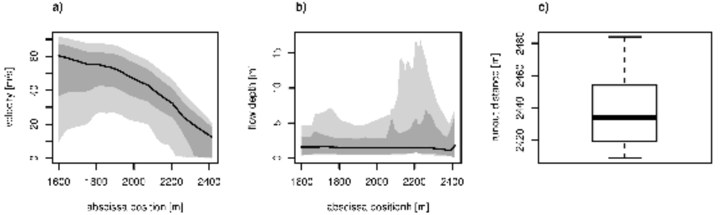
We consider $\mathrm{vol}_{\mathrm{start}} = l_{start} \times h_{start} \times 72.3/\cos(35^\circ)$ instead of $\mathrm{h}_{\mathrm{start}}$ and $\mathrm{l}_{\mathrm{start}}$.

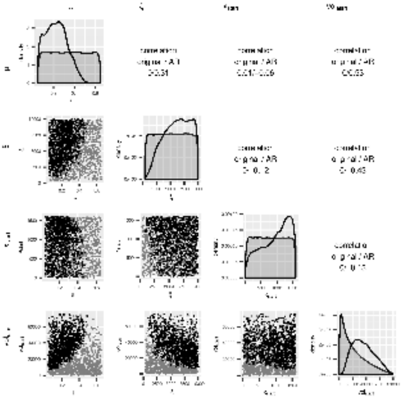
AR rules:

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

From $n_0 = 100000$, AR sample size $n_1 = 6152$.







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Ubiquitous Shapley effects

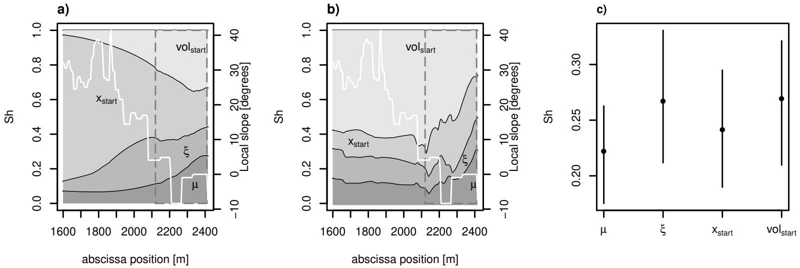

Figure: *Shapley effects are estimated with a sample of size 6152 and Ntot=2002. The local slope is displayed with a white line. A gray dotted rectangle box is displayed at interval [2017, 2412] where snow avalanche return periods vary from 10 to 10 000 years. The bootstrap sample size is fixed to* $B = 500$.

Aggregated Shapley effects

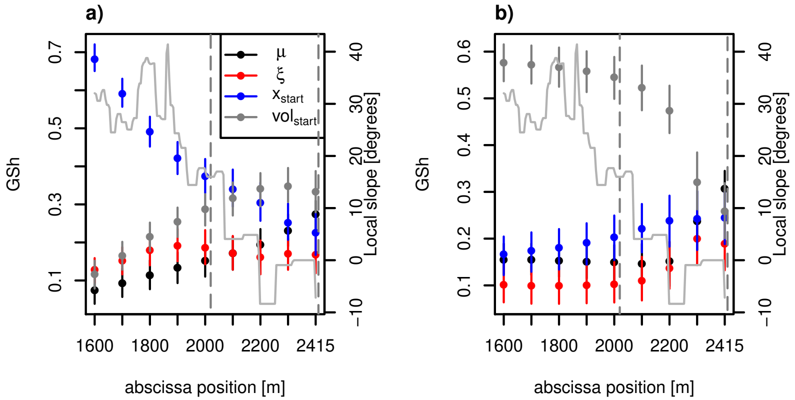

Figure: *Aggregated Shapley effects are estimated with a sample of size 6152 and Ntot=2002. Effects are estimated using the first fPCs explaining more than 95% of the output variance. The local slope is displayed with a gray line. A gray dotted rectangle is displayed at [2017m, 2412m] where snow avalanche return periods vary from 10 to 10 000 years. The bootstrap sample size is fixed to* $B = 500$.

Conclusions

- We extended Shapley effects to models with multivariate or functional outputs.
- We proposed an algorithm to construct bootstrap confidence intervals for estimation.
- The bootstrap confidence intervals have accurate coverage probability.
- Aggregated Shapley effects are more stable and easier to interpret (observed by [Alexanderian et al., 2020] for Sobol' indices).

Perspectives

- In order to estimate with samples of higher size, build a surrogate model of our avalanche model.
- To perform a GSA in several corridors in order to see if there exist correlations between the local slope and the ubiquitous effects.
- To study theoretically the asymptotic properties of our estimator.

Thanks! Questions?

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Appendix

Shapley value [Shapley, 1953]

Given a set of d players in a coalitional game and a charateristic function $\mathrm{val} : 2^d \to \mathbb{R}$, $\mathrm{val}(\emptyset) = 0$, the Shapley value $(\phi_1, \ldots, \phi_d)$ is the only distribution of the total gains $\mathrm{val}(\{1, \ldots, d\})$ to the players satisfying the desirable properties listed below:

1. (Efficiency) $\sum_{i=1}^{d} \phi_i = \mathrm{val}(\{1, \ldots, d\})$.
2. (Symmetry) If $\mathrm{val}(\mathfrak{u} \cup \{i\}) = \mathrm{val}(\mathfrak{u} \cup \{\ell\})$ for all $\mathfrak{u} \subseteq \{1, \ldots, d\} - \{i, j\}$, then $\phi_i = \phi_\ell$.
3. (Dummy) If $\mathrm{val}(\mathfrak{u} \cup \{i\}) = \mathrm{val}(\mathfrak{u})$ for all $\mathfrak{u} \subseteq \{1, \ldots, d\}$, then $\phi_i = 0$.
4. (Additivity) If val and val' have Shapley values ϕ and ϕ' respectively, then the game with characteristic function val + val' has Shapley value $\phi_i + \phi'_i$ for $i \in \{1, \ldots, d\}$.

It is proved in [Shapley, 1953] that according to the Shapley value, the amount that player i gets given a coalitional game (val, d) is:

$$\phi_i = \frac{1}{d} \sum_{\mathfrak{u} \subseteq -\{i\}} \binom{d-1}{|\mathfrak{u}|}^{-1} (\mathrm{val}(\mathfrak{u} \cup \{i\}) - \mathrm{val}(\mathfrak{u})) \;\; \forall i \in \{1, \ldots, d\}.$$

Functional principal component analysis [Yao et al., 2005]

We have a collection of n independent trajectories of a smooth random function $f(.,\mathbf{X})$ with unknown mean $\mu(s) = \mathbb{E}(f(s,\mathbf{X})), s \in \tau$, where τ is a bounded and closed interval in $\mathbb{R}$, and covariance function:

$$G(s_1, s_2) = \mathrm{Cov}(f(s_1,\mathbf{X}), f(s_2,\mathbf{X})), s_1, s_2 \in \tau.$$

We assume that G has a L^2 orthogonal expansion in terms of eigenfunction ξ_k and non increasing eigenvalues λ_k such that:

$$G(s_1, s_2) = \sum_{k\geq 1} \lambda_k \xi_k(s_1,\mathbf{X})\xi_k(s_2,\mathbf{X}), s_1, s_2 \in \tau.$$

The Karhunen-Loève orthogonal expansion of $f(s,\mathbf{X})$ is:

$$f(s,\mathbf{X}) = \mu(s) + \sum_{k\geq 1} \alpha_k(\mathbf{X})\xi_k(s) \approx \mu(s) + \sum_{k=1}^{q} \alpha_k(\mathbf{X})\xi_k(s), s \in \tau, \tag{4}$$

where $\alpha_k(\mathbf{X}) = \int_\tau f(s,\mathbf{X})\xi_k(s)\,ds$ is the k-th functional principal component (fPC) and q is a truncation level.

For fPCs estimation, the authors in [Yao et al., 2005] propose first to estimate $\hat{\mu}(s)$ using local linear smoothers and to estimate $\widehat{G}(s_1, s_2)$ using local linear surface smoothers ([Fan and Gijbels, 1996]).

The estimates of eigenfunctions and eigenvalues correspond then to the solutions of the following integral equations:

$$\int_{\tau} \widehat{G}(s_1, s)\widehat{\xi}_k(s_1)\,ds_1 = \widehat{\lambda}_k \widehat{\xi}_k(s), s \in \tau,$$

with $\int_{\tau} \widehat{\xi}(s)\,ds = 1$ and $\int_{\tau} \widehat{\xi}_k(s)\widehat{\xi}_m(s) = 0$ for all $m \neq k \leq q$. The problem is solved by using a discretization of the smoothed covariance (see further details in [Rice and Silverman, 1991] and [Capra and Müller, 1997]). Finally, fPCs $\hat{\alpha}_k(\mathbf{X}) = \int_{\tau} f(s, \mathbf{X})\widehat{\xi}_k(s)\,ds$ are solved by numerical integration. Aggregated Shapley effects are computed with only the q first fPCs:

$$\widetilde{GSh}_i = \frac{1}{d\sum_{k=1}^{q} \lambda_k} \sum_{k=1}^{q} \sum_{\mathfrak{u} \subseteq -i} \binom{d-1}{|\mathfrak{u}|}^{-1} \left(\mathbb{E}(\mathrm{Var}(\alpha_k(\mathbf{X})|\mathbf{X}_{\mathfrak{u}\cup\{i\}})) - \mathbb{E}(\mathrm{Var}(\alpha_k(\mathbf{X})|\mathbf{X}_{\mathfrak{u}}))\right). \tag{5}$$

Theorem (Theorem 6.6 [Broto et al., 2020])

If f is bounded, the $\widehat{E}_{\mathfrak{u}}$ converges to $E_{\mathfrak{u}}$ in probability when n and $N_{\mathfrak{u}}$ if:

- *For all $i \in \{1, \ldots, d\}$, $(\mathscr{X}_i, d_i)$ is a Polish space with metric d_i, with $\mathscr{X}_i$ the domain of X_i, and $\boldsymbol{X} = (X_1, \ldots, X_d)$ has a density $f_{\boldsymbol{X}}$ with respect to a finite measure $\mu = \bigotimes_{i=1}^{d} \mu_i$ which is bounded and $\mathbb{P}_X$ almost everywhere continuous.*
- *The closest neighbors in $\mathscr{B}_{-\mathfrak{u},\ell}$ are two by two distinct.*

The bias-corrected percentile method [Efron, 1981]

Given bootstrap samples B of $\widehat{GSh}_i$, $\mathscr{R}_i = \{\widehat{GSh}_i^{(1)}, \ldots, \widehat{GSh}_i^{(B)}\}$.
We compute a bias correction constant z_0:

$$\hat{z}_0 = \Phi^{-1}\left(\frac{\#\{\widehat{GSh}_i^{(b)} \in \mathscr{R}_i \text{ s. t. } \widehat{GSh}_i^{(b)} \leq \widehat{GSh}_i\}}{B}\right)$$

where Φ the standard normal cumulative distribution function.
The corrected quantile estimate $\hat{q}(\beta)$:

$$\hat{q}_i(\beta) = \Phi(2\hat{z}_0 + z_\beta),$$

where z_β satisfies $\Phi(z_\beta) = \beta$.
To guarantee the validity of the previous BC corrected confidence interval $[\hat{q}_i(\alpha/2), \hat{q}_i(1-\alpha/2)]$, there must exist an increasing transformation g, $z_0 \in \mathbb{R}$ and $\tau > 0$ such that $g(\widehat{GSh}_i) \sim \mathcal{N}(GSh_i - \tau z_0, \tau^2)$ and $g(\widehat{GSh}_i^*) \sim \mathcal{N}(\widehat{GSh}_i - \tau z_0, \tau^2)$ where $\widehat{GSh}_i^*$ is the bootstrapped $\widehat{GSh}_i$ for fixed sample (see [Efron, 1981]).

Probability of coverage with Bonferroni correction

The probability of coverage with Bonferroni correction is the probability that $[\hat{q}_i(\alpha/(2d)), \hat{q}_i(1-\alpha/(2d))]$ contains GSh_i for all $i \in \{1, \dots, d\}$ simultaneously.

The POC is estimated as

$$\widehat{POC} = \sum_{k=1}^{N} \frac{w^k}{N}, \tag{6}$$

where w^k is equal to 1 if $\hat{q}_i(\alpha/(2d)) \leq GSh_i \leq \hat{q}_i(1-\alpha/(2d))$ for all i, and 0 otherwise.