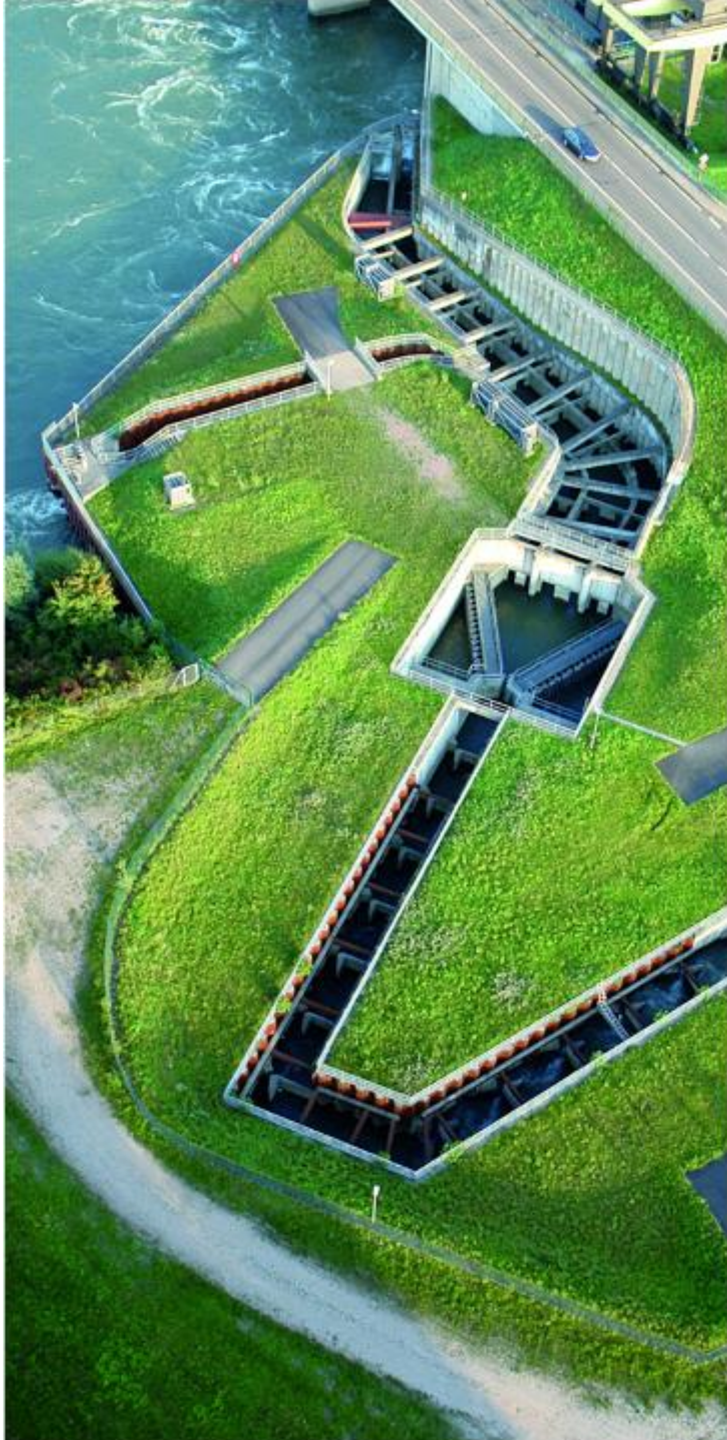
Formation MEXICO « Solutions à la Shapley pour l'analyse de sensibilité avec entrées dépendantes »

Partie 2
Les effets de Shapley
Cours 1



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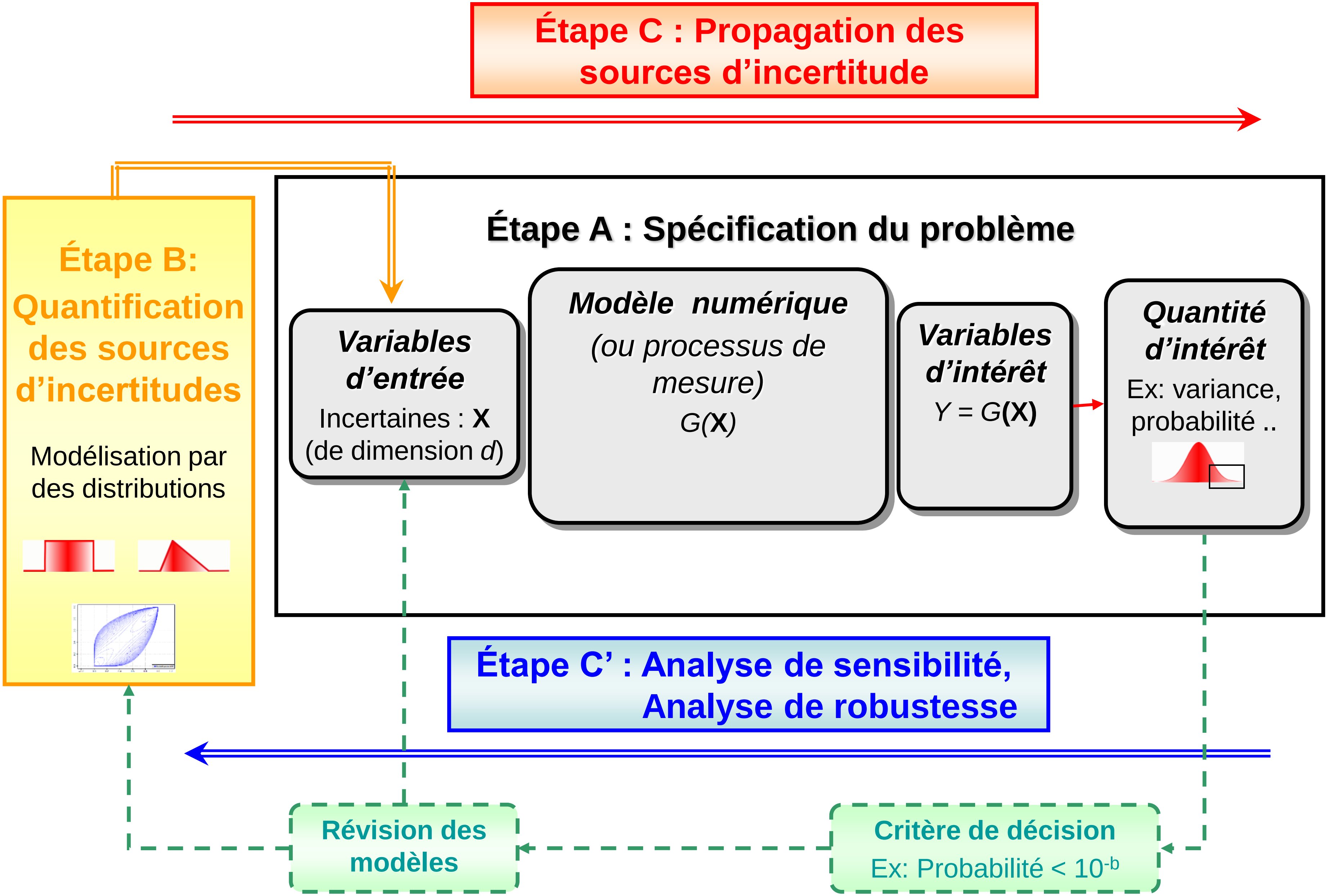
6 mai 2022

Méthodologie de traitement des incertitudes



Variance-based SA via Sobol' indices

First order: $S_i = \frac{\mathrm{Var}[\mathrm{E}(Y|X_i)]}{\mathrm{Var}(Y)}$; second order: $S_{ij} = \frac{\mathrm{Var}[\mathrm{E}(Y|X_i X_j)]}{\mathrm{Var}(Y)} - S_i - S_j$; ...

More generally, if $\mathcal{P}_d = \mathcal{P}(\{1, \dots, d\})$ (i.e. set of all subsets) and $\forall\, A \in \mathcal{P}_d, X_A = (X_i)_{i \in A}$:

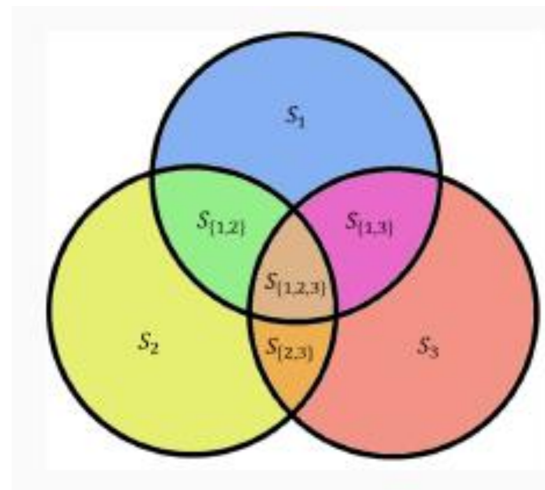
$$\forall\, A \in \mathcal{P}_d, S_A = \frac{\sum_{B \subset A} (-1)^{|A|-|B|} \mathrm{Var}[\mathrm{E}(Y|X_B)]}{\mathrm{Var}(Y)}$$

[Sobol 1990]

Under independence between inputs assumption, S_A represents a variance share:

$$\begin{cases} S_A \geq 0, \quad \forall A \in \mathcal{P}_d. \\ \sum_{A \in \mathcal{P}_d} S_A = 1. \end{cases}$$

$X = (X_1, \dots, X_3)$



Not true in the dependent case!
Sobol' indices can be negative and thus do not consist in a variance decomposition anymore

[see the state of the art about the dependent case in Da Veiga et al 2021]

Indices de sensibilité dans le cas non linéaire

- **<u>Cas indépendant</u>** : indices de Sobol' (extension SRC²)

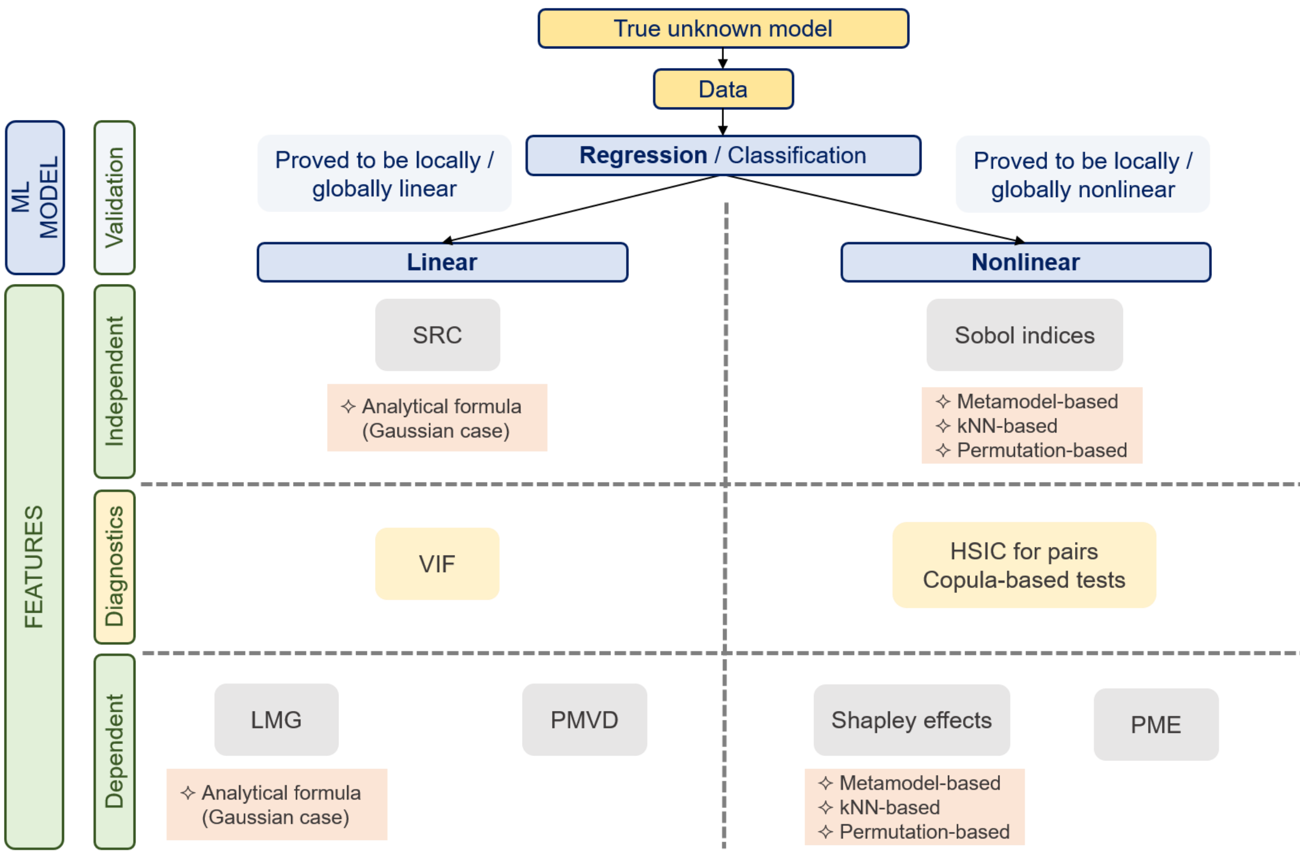
$$S_i = \mathrm{Var}[\mathrm{E}(Y|X_i)]/\mathrm{Var}(Y)$$
$$T_i = \mathrm{E}\left[\mathrm{Var}(Y|X_{-i})\right]/\mathrm{Var}(Y)$$

- **<u>Cas dépendant</u>** : ANCOVA : je déconseille (indices négatifs)

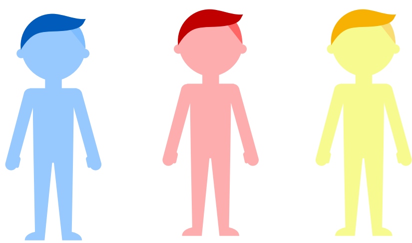
  => indices de Shapley (extension des LMG, indices de Sobol à la place du R^2

  => NEW (en cours de consolidation) : PME (extension PMVD)

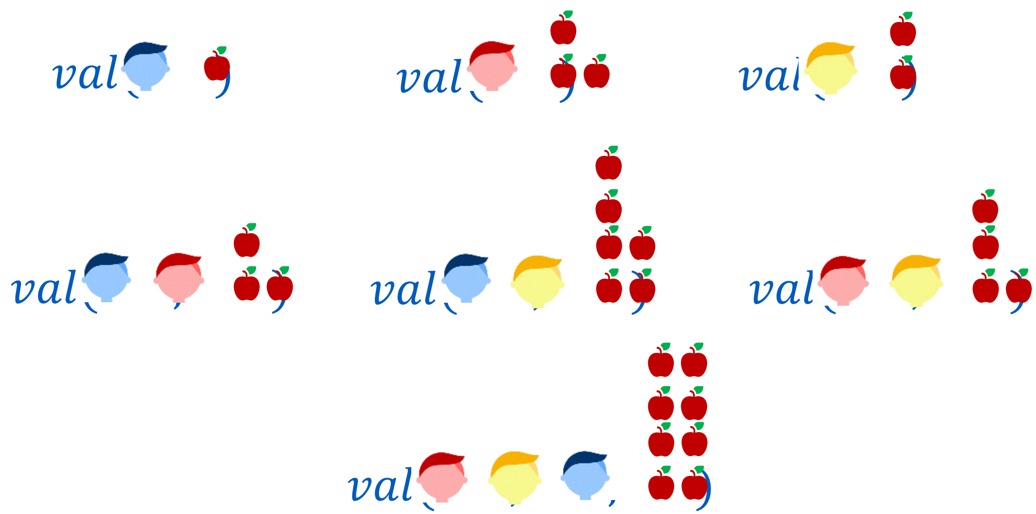
- <u>Synthèse</u> :



Les valeurs de Shapley par l'exemple



Comment redistribuer leur production de manière coopérative ?



__4 Axiomes :__

1. ***(Efficacité)*** La somme des valeurs réparties doit être égale à la production totale

2. ***(Symétrie)*** Si, pour toute coalition, l'apport marginal de deux joueurs est égale, leur part doit être égale.

3. ***(Joueur nul)*** Si, pour toute coalition, l'apport marginal d'un joueur est nul, sa part est nulle.

4. ***(Additivité)*** Si un jeu peut être décomposé en deux sous-jeux distincts, les valeurs de Shapley de ce jeu sont la somme de ceux des deux sous-jeux.

L'unique solution est :

$$\phi_j = \frac{1}{d} \sum_{A \subset -j} \binom{d-1}{|A|}^{-1} \left(val(A \cup \{j\}) - val(A)\right)$$

Shapley effects for sensitivity analysis

In a cooperative game, Shapley values allocate the earnings to each actor of the game

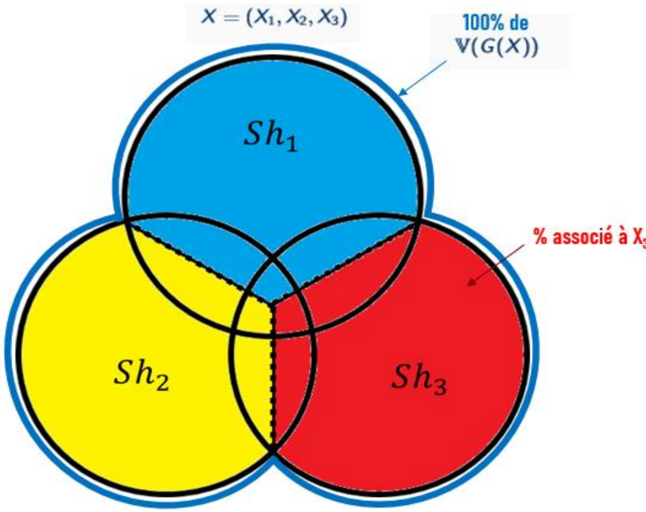
Let val(.) be the cost function and $\mathcal{D} = \{1,\ldots,d\}$

$$\boxed{Sh_i = \sum_{u \subseteq \mathrm{D} \setminus \{i\}} \frac{(d-|u|-1)!\,|u|!}{d!} |\mathrm{val}(u \cup \{i\}) - \mathrm{val}(u)|}$$

[Shapley 1953]

Variance-based SA => Shapley effects as sensitivity indices

by taking $\mathrm{val}(u) = S_u = \mathrm{Var}[\mathrm{E}(Y|X_u)]/\mathrm{Var}(Y)$ *[Owen 14]*



Important properties:

1) $Sh_i \geq 0 \forall i = 1,\ldots,d$ and $\sum_{i=1}^{d} Sh_i = 1$

2) In case of independent inputs: $Sh_i = \sum_{u \supset i} \frac{S_u}{|u|}$

then $S_i \leq Sh_i \leq T_i$ (not respected in general case)

+	−
• Ne requiert pas d'hypothèse d'indépendance. • Permet une décomposition interprétable de la variance de la variable d'intérêt.	• Les parts dues aux interactions, et celles dues à la dépendance ne sont pas explicites.

Plus formellement avec la théorie des jeux coopératifs

A **cooperative game** (D, v) consists of:

- A set of players $D = \{1, ..., d\}$;
- A value function $v : \mathcal{P}_d \to \mathbb{R}^+$ s.t. $v(\emptyset) = 0$.

hyp : $\forall A_1, A_2 \in \mathcal{P}_d \;\; s.t. \;\; A_1 \subseteq A_2, \;\; v(A_1) \leq v(A_2)$.

An **allocation rule** is a real-valued function ϕ that associates to any cooperative game (D, v) a real-valued vector $(\phi_i)_{i=1,\dots,d}$.

Efficiency: $\sum_i \phi_i = v(D)$

Shapley values:

[Shapley 1953]

For all cooperative game (D, v), for all $i \in D$:

$$\mathrm{Shap}_i\Big((D, v)\Big) = \sum_{A \subseteq D \setminus \{i\}} \frac{(d - |A| - 1)!|A|!}{d!}\Big(v(A \cup \{i\}) - v(A)\Big).$$

Shapley effects:

[Owen 2014; Song et al. 2016]

$$\forall i \in D, \; \mathrm{Sh}_i = \mathrm{Shap}_i\Big(\Big(D, S^T\Big)\Big) \quad \text{where} \quad \forall A \in \mathcal{P}_d, \;\; S_A^T = \frac{\mathbb{E}[\mathbb{V}(G(X)|X_{\bar{A}})]}{\mathbb{V}(G(X))}.$$

Shapley effects in SA

$$\begin{cases} \sum_i \mathrm{Sh}_i = 1 \quad (\textbf{Efficiency property}) \\ \forall i \in D, \quad \mathrm{Sh}_i \geq 0 \end{cases}$$

⬇

Variance decomposition (valid in correlated cases)
$\Rightarrow$ Quantitative partitioning setting

$\mathrm{Sh}_i = 0$ means that X_i does not contribute to the output variance
$\Rightarrow$ Screening setting

BUT: the screening setting is not fully attained because an exogeneous variable can get a non-zero Shapley effect (Shapley's joke)
The exclusion property is not fulfilled

Shapley's joke example
(Iooss and Prieur 2019)

$$Y = G(X) = X_1$$

$$(X_1, X_2) \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}\right)$$

$$\mathrm{Sh}_1 = 1 - \frac{\rho^2}{2}$$

$$\mathrm{Sh}_2 = \frac{\rho^2}{2}$$

Simple linear models: Shapley = LMG

$\mathbf{X} \sim \mathcal{N}_2(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ and $Y = \beta_0 + \boldsymbol{\beta}^\mathsf{T}\mathbf{X}$, with

$$\boldsymbol{\mu} = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix}, \boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}, \rho \in [-1, 1], \sigma_i > 0.$$

We have $\sigma^2 = V[Y] = \beta_1^2\sigma_1^2 + 2\rho\beta_1\beta_2\sigma_1\sigma_2 + \beta_2^2\sigma_2^2$. Then

$$\begin{cases} \sigma^2 Sh_1 = \beta_1^2\sigma_1^2(1 - \frac{\rho^2}{2}) + \rho\beta_1\beta_2\sigma_1\sigma_2 + \beta_2^2\sigma_2^2\frac{\rho^2}{2}, \\ \sigma^2 S_1 = \beta_1^2\sigma_1^2 + 2\rho\beta_1\beta_2\sigma_1\sigma_2 + \rho^2\beta_2^2\sigma_2^2 \text{ and } \sigma^2 S_1^{\text{tot}} = \beta_1^2\sigma_1^2(1 - \rho^2). \end{cases}$$

Simple linear models: examples

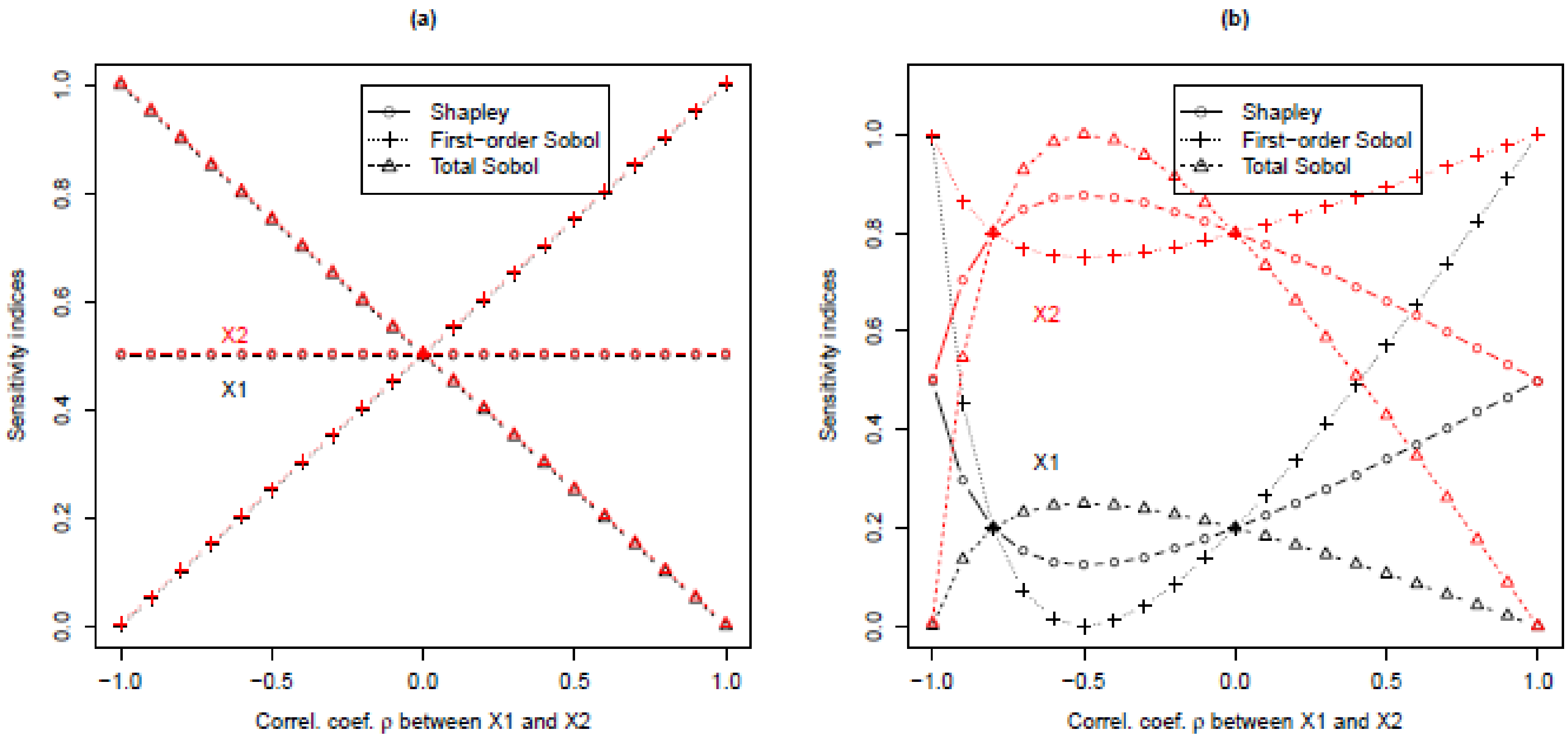


Figure: Sensitivity indices on the linear model ($\beta_1 = 1$, $\beta_2 = 1$) with two Gaussian inputs. (a): $(\sigma_1, \sigma_2) = (1, 1)$. (b): $(\sigma_1, \sigma_2) = (1, 2)$.

Another simple example

$$G(X) = X_1 + X_2X_3,$$

$$\begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & \rho \\ 0 & 1 & 0 \\ \rho & 0 & 1 \end{pmatrix} \right).$$

The three Inputs have Shapley effects:

$$\mathrm{Sh}_1 = 0.5 - 2\rho^2/12$$

$$\mathrm{Sh}_2 = 0.25 + \rho^2/12$$

$$\mathrm{Sh}_3 = 0.25 + \rho^2/12$$

The Shapley effects can be understood as an averaging index over the interaction and dependence effects

Numerical estimation algos in the general case

$$Sh_i = \frac{1}{d!} \sum_{\pi \in \Pi(\mathrm{D})} |\mathrm{val}(P_i(\pi) \cup \{i\}) - \mathrm{val}(P_i(\pi))|$$

$\Pi(\mathcal{D})$ = set of all permutations, $P_i(\pi)$ variables that precede X_i in π

Instead of $\mathrm{val}(u) = S_u$, take $\mathrm{val}(u) = T_u = \mathrm{E}[\mathrm{Var}(Y|X_{-u})]/\mathrm{Var}(Y)$

[Song et al. 2016]

<u>Tuning parameters:</u>

Nv : sample size for Var(*Z*) estimation ; *m* : number of permutations

Ni : inner loop size (conditional variance) ; *No* : outer loop size (expectation)

=> Cost = *Ni No m* (*d*-1) + *Nv*

1) Exact permutation algorithm: *m* = *d*!

   Optimal with *Ni*=3 => Cost: *N* = 3 *d*! *No* (*d*-1) + *Nv*

2) Random permutation algorithm: Monte Carlo (MC) on permutation loop

   Optimal with *Ni*=3 and *No*=1 => Cost: *N* = 3 *m* (*d*-1) + *Nv*

Rem1: Bootstrap confidence intervals can be computed [Benoum. & Elie-Dit-Cosaque 19]

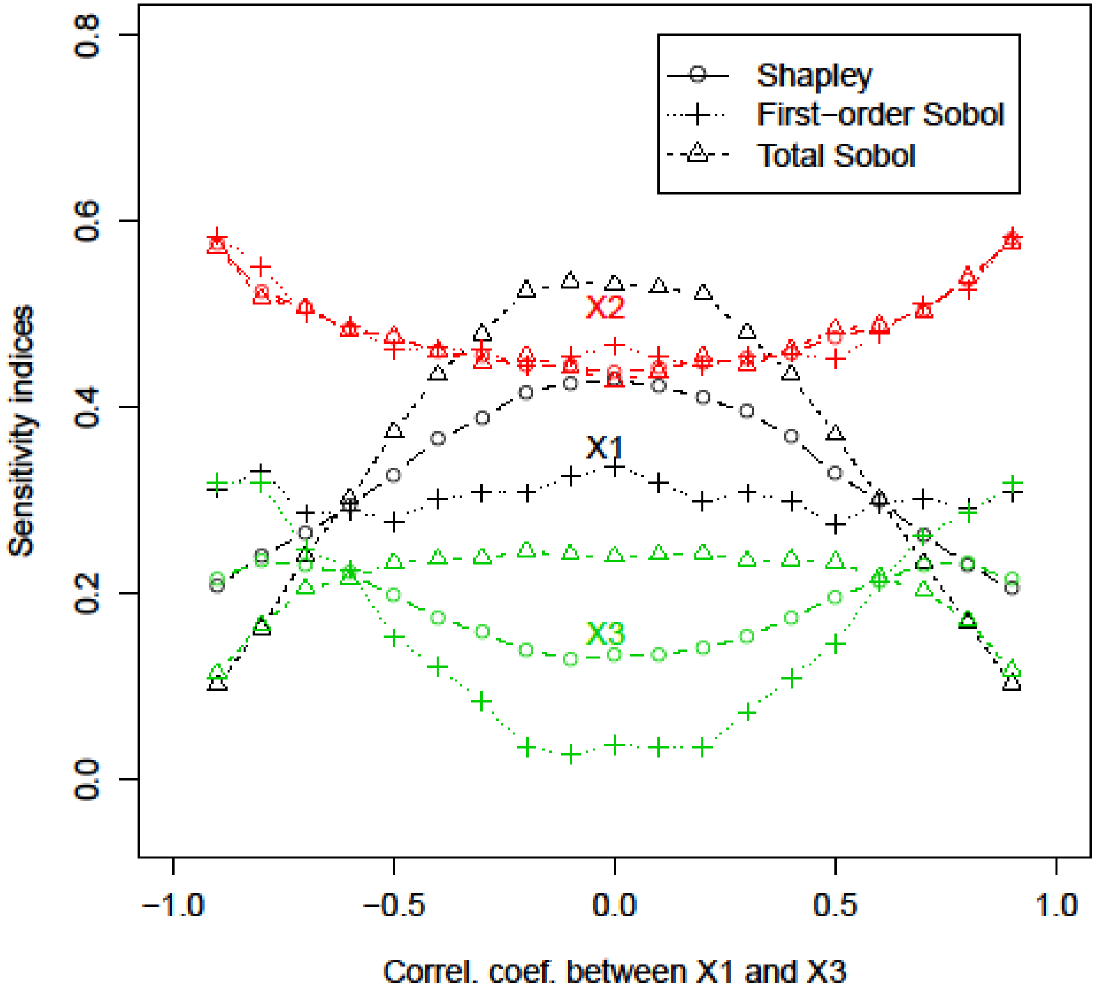
Rem 2: A costly model can be replaced by a metamodel

Rem. 3: Smart so. with kriging [Benoum. & EDC 19] *& random forests* [Bénard 2021]

Rem 4: Nearest-neighbors estimation (=> given-data algo which does not require to know & simulate conditional input distributions) [Broto et al. 2020] [cf. Marouane]

Numerical test on Ishigami function

$$\begin{cases} f(X_1, X_2, X_3) = \sin X_1 + 7(\sin X_2)^2 + 0.1 X_3^4 \sin X_1 \\ X_i \sim U_{[-\pi;\pi]} \quad \text{for} \quad i = 1, \ldots, 3 \end{cases}$$



Random permut. algo

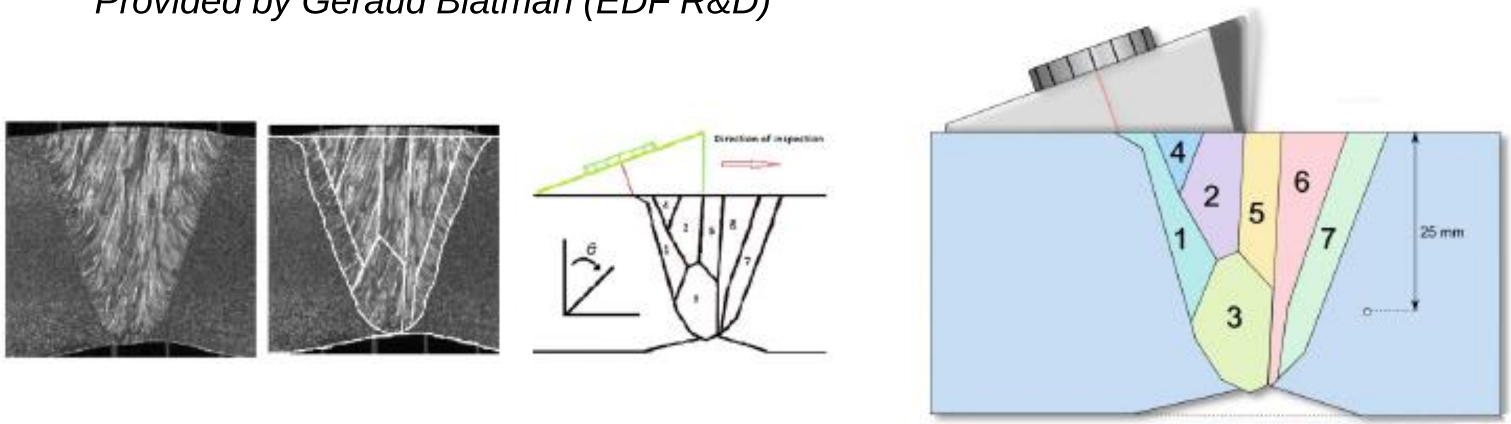
Nv = 1e4
Ni = 3
No = 1
m = 5e4

Industrial application

Non Destructive Control for a weld inspection with ultrasonic waves

Provided by Géraud Blatman (EDF R&D)

[Rupin et al. 14]
[Iooss & Prieur 21]



Numerical simulations by Finite Element model (ATHENA 2D)

Output: signal amplitude

Inputs (11):
- 4 non-correlated elastic constants (Gaussian)
- 7 correlated orientations (Gaussian)

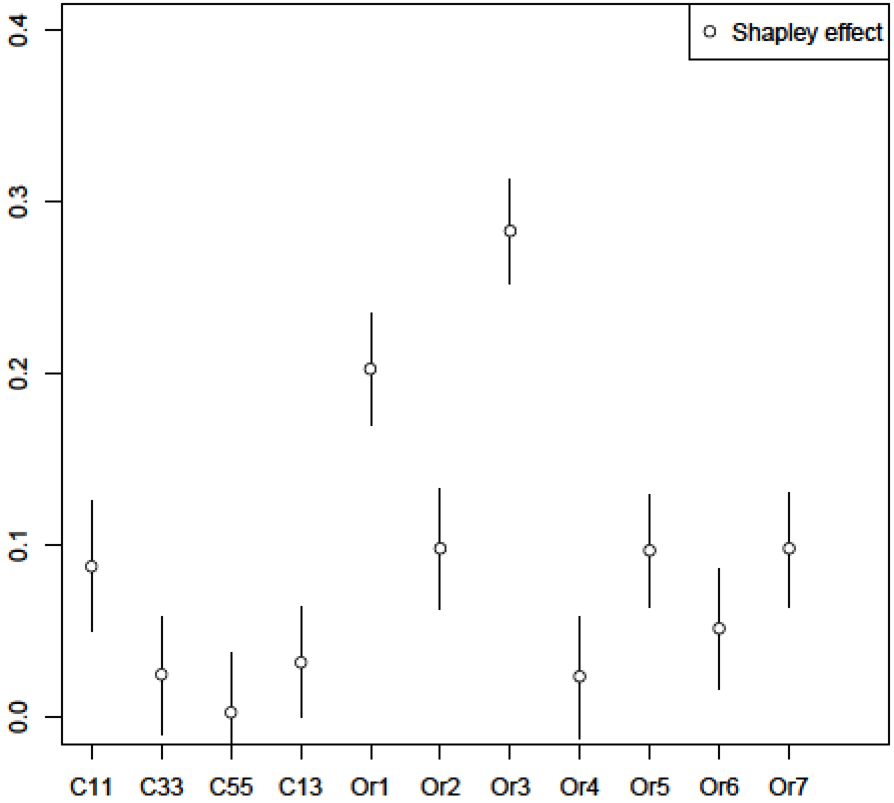
$$\begin{pmatrix} 1 & 0.80 & 0.74 & 0.69 & 0.31 & 0.23 & 0.20 \\ & 1 & 0.64 & 0.53 & 0.59 & 0.51 & 0.46 \\ & & 1 & 0.25 & 0.60 & 0.57 & 0.54 \\ & & & 1 & -0.25 & -0.34 & -0.33 \\ & & & & 1 & 0.96 & 0.84 \\ & & & & & 1 & 0.95 \\ & & & & & & 1 \end{pmatrix}$$

500 numerical experiments (Sobol' sequence)
3 h of cpu-time on a HPC cluster

Results: Kriging-predictor based Shapley effects

Linear model: $R^2 = 25\%$

Kriging metamodel: $Q^2=86.5\%$



$Nv = 1e4$
$Ni = 3$
$No = 1$

$m = 1e4$
(R memory allocation problem with larger m values)

Travaux récents sur les valeurs proportionnelles : Analogie avec LMG/PMVD => Shapley/PME

- La valeur de Shapley est la seule allocation **efficace** vérifiant la propriété « **contributions équilibrées »** : la présence simultanée de deux joueurs *i* et *j* **ajoute une même valeur** aux valeurs qu'ils auraient obtenues en l'absence l'un de l'autre

  Autrement dit, le gain apporté par l'interaction de *i* et *j* est additionnel.

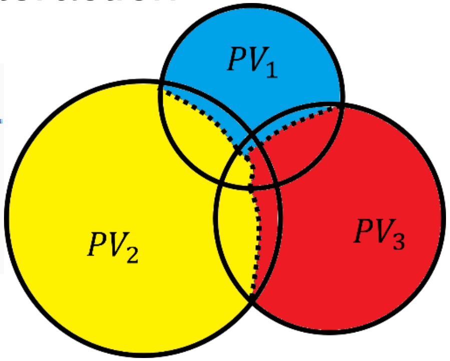
- La valeur proportionnelle est l'unique allocation **efficace** vérifiant la propriété « **gains proportionels égaux »** : la présence simultanée de deux joueurs *i* et *j* **multiplie par une même valeur** les valeurs qu'ils auraient obtenues en l'absence l'un de l'autre

  Autrement dit, le gain apporté par l'interaction de *i* et *j* est multiplicatif

=> C'est un partage différent du surplus de valeur créée par leur *interaction*

$$PV\big((\{1,2\},v)\big)_i = v(\{i\}) + \frac{v(\{i\})}{v(\{1\})+v(\{2\})}\big(v(\{1,2\})-v(\{1\})-v(\{2\})\big), \quad i=1,2.$$

$$Shap\big((\{1,2\},v)\big)_i = v(\{i\}) + \frac{1}{2}\big(v(\{1,2\})-v(\{1\})-v(\{2\})\big), \quad i=1,2.$$



[Hérin et al. 2021]

PV => Proportional Marginal Effects (PME), qui résolvent la blague de Shapley

Les effets d'interaction restent à approfondir (cf. notion de synergie)

Merci - Références

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