Proportional marginal effects

for sensitivity analysis with correlated inputs

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GSA FRAMEWORK - NOTATIONS

- **Inputs**: $X = (X_1, ..., X_d)$ real-valued random vector of joint probability measure P_X and marginal probability measures P_{X_i};
- **Model**: $G : \begin{cases} \mathbb{R}^d \longrightarrow \mathbb{R} \\ X \longmapsto G(X) \end{cases} , \quad G \in \mathbb{L}^2(P_X)$;
- **Output**: $Y = G(X)$.

$$\mathcal{P}_d = \mathcal{P}(\{1, ..., d\}).$$

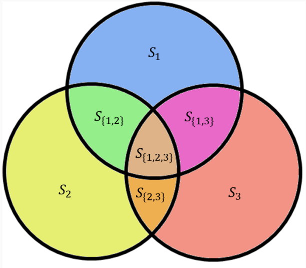
$$\forall u \in \mathcal{P}_d, \quad X_u = (X_i)_{i \in u}.$$

Sobol' Indices (Sobol 1990)

$$\forall A \in \mathcal{P}_d, \quad S_A = \frac{\sum_{B \subset A} (-1)^{|A|-|B|} \mathbb{V}(\mathbb{E}[G(X)|X_B])}{\mathbb{V}(G(X))}$$

Under independence assumption ($P_X = \prod_i P_{X_i}$), S_A represents a variance share:

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



Not true in the general case!

The Sobol' indices can be negative and thus do not consist in a variance decomposition anymore.

(Da Veiga et al. 2021)

SHAPLEY EFFECTS: COOPERATIVE GAME SOLUTION

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

- A set of players $D = \{1, ..., d\}$;
- A value function $v : \mathcal{P}_d \rightarrow \mathbb{R}^+$ 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 $(\phi)_{i=1,\dots,d}$.

Shapley values (Shapley 1951)

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

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

Shapley effects (Owen 2014) (Song, Nelson, and Staum 2016)

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

SHAPLEY EFFECTS: COOPERATIVE GAME SOLUTION

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

$$\Downarrow$$

- variance decomposition in the correlated case;
- input ranking according output variance contribution;
- factor fixing:
  $Sh_i = 0 \Rightarrow \forall A \subseteq D \backslash \{i\}, \;\; S^T_{A \cup \{i\}} - S^T_A = 0.$
  $\Rightarrow X_i$ does not contribute to output variance.

PB: partial factor fixing since an exogenous variable can get non zero Shapley effect.

Shapley's joke example

(Iooss and Prieur 2019)

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

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

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

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

Marginal proportional values (PMV) (Feldman 2005)

For all cooperative game (D, v) with v valued in $\mathbb{R}^{+*}$ (extension to $\mathbb{R}^{+}$ provided in this work)

$$\mathrm{PV}_i\left((D, v)\right) = \frac{R(D, v)}{R(D \setminus \{i\}, v)}$$

where R is defined recursively by:

$$\forall A \in \mathcal{P}(D), \;\; R(A, v) = v(A) \left(\sum_{j \in A} \frac{1}{R(A \setminus \{j\}, v)} \right)^{-1} \quad and \quad R(\emptyset, v) = 1$$

.

Proportional Marginal Effects (PME)

$$\forall i \in D, \; \mathrm{PME}_i = \mathrm{PV}_i\left((D, S^T)\right)$$

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

PME = Shapley effects alternative to provide variance decomposition with correlated input.

Balanced contribution property

$$\forall i,j \in D,\ \ \mathrm{Sh}_i - \mathrm{Sh}_{i,-j} = \mathrm{Sh}_j - \mathrm{Sh}_{j,-i}$$

Equal proportional gain property

$$\forall i,j \in D, \qquad \frac{\mathrm{PME}_i}{\mathrm{PME}_{i,-j}} = \frac{\mathrm{PME}_j}{\mathrm{PME}_{j,-i}}$$

where $\phi_{i,-j}$ refer to the variance share of X_i without including the variance due to the interaction with X_j.

Illustration for $D = \{1,2\}$: $\quad \forall i \in D,\ \ D = \{i,\bar{i}\},\ \ \phi_{i,-\bar{i}} = S_i^T$ (individual value)

$$\prod = \frac{\mathrm{PME}_i}{\mathrm{PME}_{i,-\bar{i}}} = \frac{1}{S_1^T + S_2^T}$$

$$\sum = \mathrm{Sh}_i - Sh_{i,-\bar{i}} = \frac{1}{2}(1 - S_1^T - S_2^T)$$

$$\Rightarrow$$

$$\mathrm{PME}_i = \prod . S_i^T = S_i^T + \frac{S_i^T}{S_1^T + S_2^T}(1 - S_1^T - S_2^T)$$

$$\mathrm{Sh}_i = \sum + S_i^T = S_i^T + \frac{1}{2}(1 - S_1^T - S_2^T)$$

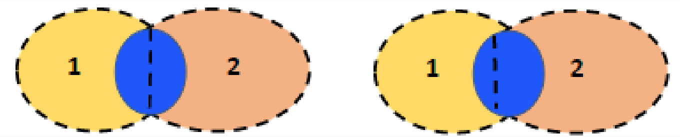


Figure 1: Schematic illustration of the interaction distribution (left: Shapley effects/ right : PME).

Shapley's joke example

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

$$S_1^T > 0, \quad Sh_1 = 1 - \frac{\rho^2}{2}, \quad PME_1 = 1.$$
$$S_2^T = 0, \quad Sh_2 = \frac{\rho^2}{2}, \quad PME_2 = 0.$$

Proposition

Suppose that there exists a subset of endogenous variable $D^* \subseteq D$ of size d^* such that $\forall i \in D^*, \ \ S_i^T > 0$ and such that one can find a measurable function f that verifies $Y = G(X) = f(X_{D^*})$. Then:

$$\forall i \notin D^*, \quad PME_i = 0.$$

CONSEQUENCE : ROBUSTNESS TO CORRELATION (EXAMPLE II)

Linear gaussian case:

$$Y = X_1 + \beta_2 X_2 + X_3$$

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

$$Sh_1 = PME_1 \underset{\rho \to 1}{\longrightarrow} \frac{1}{2 + \beta_2^2 + 2\beta_2} \underset{\beta_2 >> 1}{\sim} 0$$

$$Sh_2, Sh_3 \underset{\rho \to 1}{\longrightarrow} \frac{\frac{1}{2}\beta_2^2 + \beta_2 + \frac{1}{2}}{2 + \beta^2 + 2\beta_2} \underset{\beta_2 >> 1}{\sim} \frac{1}{2}$$

$$PME_2 \underset{\rho \to 1}{\longrightarrow} \frac{\beta_2^2(1 + \beta_2^2 + 2\beta_2)}{(2 + \beta^2 + 2\beta_2)(1 + \beta_2^2)} \underset{\beta_2 >> 1}{\sim} 1$$

$$PME_3 \underset{\rho \to 1}{\longrightarrow} \frac{(1 + \beta_2^2 + 2\beta_2)}{(2 + \beta^2 + 2\beta_2)(1 + \beta_2^2)} \underset{\beta_2 >> 1}{\sim} 0$$

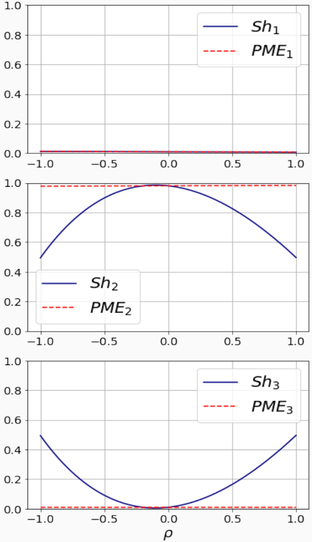


Figure 2: Shapley effects and PME indices w.r.t to ρ for $\beta_2 = 10$. Input X_1,X_2,X_3 from up to down.

2-step estimation procedure (similar to the Shapley effects estimation):

- Estimation of the conditional elements $S_A^T, \forall A \in \mathcal{P}_{\mathcal{D}}$:
  - Monte Carlo estimation (Song, Nelson, and Staum 2016);
  - Data-given estimation using a nearest-neighbor procedure (Broto, Bachoc, and Depecker 2020).
- Aggregation procedure by plugging-in the estimated conditional elements in the PME recursive formula.

$\longrightarrow$ package sensitivity in R

APPLICATION A TO REALISTIC MODEL

Robot arm model (An and Owen 2001)

- inputs: angles (A_i) and lengts (L_i) of 4 segments of the arm;
- output : extension of the arm

$$Y = \left\{ \left[\sum_{i=1}^{4} L_i \cos\left(\sum_{j=1}^{i} A_j \right) \right]^2 + \left[\sum_{i=1}^{4} L_i \sin\left(\sum_{j=1}^{i} A_j \right) \right]^2 \right\}^{1/2}$$

- The inputs are artificially correlated:
  - $\forall A_i \sim \mathcal{U}[0, 2\pi]$, pairwise correlated with Gaussian copula with a 95% correlation coeff;
  - $L_1 \sim \mathcal{U}[0, 1], \forall i > 1,\ L_i \sim \mathcal{U}[0, L_{i-1}]$

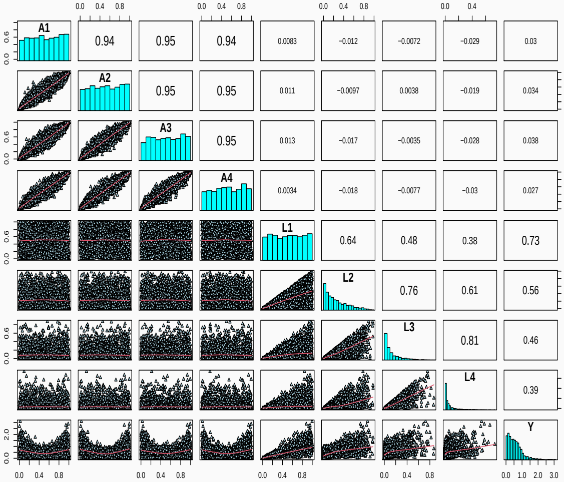


Figure 3: Pair plots of a 2000-size Monte Carlo sample for the robot arm model.

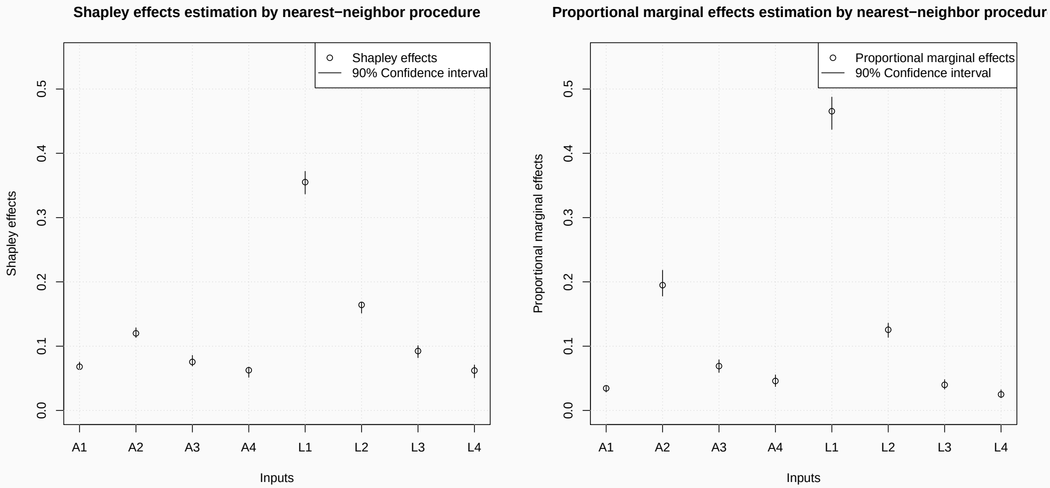
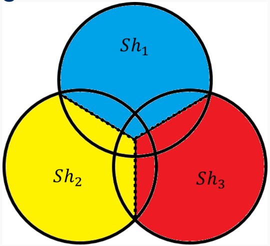


Figure 4: Shapley effects (left) and PME (right) for the robot arm model.

CONCLUSION

PME indices allow for another variance decomposition in the correlated case with new properties:

- **Equal proportional gain : interaction is shared proportionaly to individual power. The three following points can be seen as valuable consequences of this property.**
- **Robustness to correlation when interaction = correlation;**
- **No Shapley's joke: an exogenous input always get zero % variance share, even if it is correlated to endogenous variable;**
- **Strong discrimination between inputs.**



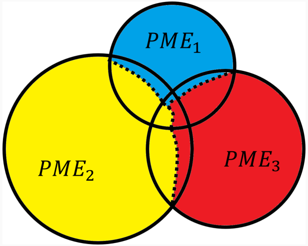


Figure 5: Schematic illustration of PME (right) and Sh (left) indices for d = 3.

PERSPECTIVES

- Finite sample properties of the estimator?
- A PME equivalent of the Shapley-Owen indices (Rabitti and Borgonovo 2019) (Shapley effects quantifying group importance)?

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Proportional values extension

$$\forall i \in D,\ \widetilde{\mathrm{PV}}_i((D,v)) = \begin{cases} \dfrac{\sum\limits_{\substack{S \subset D_{-i} \\ |S| = k_M \\ v(S)=0}} R(D_{-i} \backslash S, v_S)^{-1}}{\sum\limits_{\substack{S \subset D \\ |S| = k_M \\ v(S)=0}} R(D \backslash S, v_S)^{-1}} & \text{if } \exists S \subseteq D_{-i}\ s.t\ |S| = k_M,\ v(S) = 0, \\ 0 & \text{else,} \end{cases}$$

where k_M is the size of the largest null coalition, i.e., $k_M = k_M((D,v)) = \max\limits_{T \subseteq D} \{|T|\ |v(T) = 0\}$

Allocation reduce game:

$$\phi_{i,-j} = \phi_i(D\backslash\{j\}, v), \quad \sum_{i \neq j} \phi_{i,-j} = v(D\backslash\{j\})$$