Cooperative Game Theory and Global Sensitivity Analysis

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Introduction

Sobol' indices (Sobol 1990) allow for a powerful tool in order to assess **input importance** on the **variability of the output** of a numerical model. They can be interpreted as **shares of the output's variance**, due to **individual input effects**, or due to **their interaction**.

However, it relies on an **independence assumption** on the probabilistic modelling of the inputs, which may be **ill-suited in practice**. Whenever **dependence comes into play**, there exists **solutions** (Chastaing, Gamboa, and Prieur 2012; Mara and Tarantola 2012), but **no general decomposition of the output's variance**.

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Goal of the presentation:

Build meaningful model output variance decompositions in the context of dependent inputs using cooperative game theory.

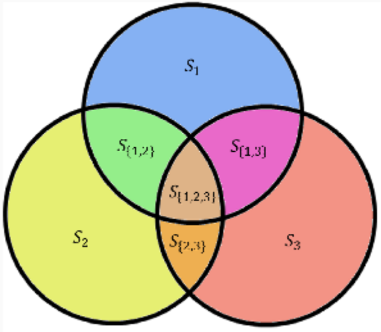
Shapley effects (Owen 2014) are a particular example of such a decomposition.

Sobol' indices and dependence

For a model $G \in \mathbb{L}^2(P_X)$, where P_X is the distribution of d inputs assumed **independent**, the **Sobol' indices** for a subset of variable $A \in \{1, \dots, d\}$, are defined as:

$$S_A = \frac{\sum_{B \subset A} (-1)^{|A|-|B|} \mathbb{V}\left(\mathbb{E}[G(X)|X_B]\right)}{\mathbb{V}(G(X))}, \quad \text{and allow for} \sum_{C \subset \{1,\dots,d\}} S_C = 1. \tag{1}$$

They can be interpreted as the **individual effects** (i.e.,$|A| = 1$) and the **interaction effects** (i.e.,$|A| > 1$) of the input on the variability of the output.



When **inputs are dependent**, it would be ideal to quantify a third effect: the **dependence effects** (i.e., the effect of the dependence structure on the variability of the output).

However, whenever **correlation comes into play**, the line between **"interaction effects"** and **"dependence effects"** is blurred.

Sobol' indices and dependence: illustration

Let's take an example (Iooss and Prieur 2019):

$$G(X) = X_1 + X_2 X_3, \quad X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & \rho \\ 0 & 1 & 0 \\ \rho & 0 & 1 \end{pmatrix}\right) \tag{2}$$

Independent case ($\rho = 0$)

$$S_1 = 0.5 \quad S_2 = 0, \quad S_3 = 0,$$
$$S_{\{1,2\}} = 0, \quad S_{\{1,3\}} = 0, \quad S_{\{2,3\}} = 0.5,$$
$$S_{\{1,2,3\}} = 0$$

Correlated case ($\rho \neq 0$)

$$S_1 = 0.5 \quad S_2 = 0, \quad S_3 = \rho^2/2,$$
$$S_{\{1,2\}} = \rho^2/2, \quad S_{\{1,3\}} = -\rho^2/2, \quad S_{\{2,3\}} = 0.5,$$
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How can one interpret **negative output variance percentages**?
Should X_1 and X_2 be given an **interaction effect**? Should X_3 be given an **individual effect**?

Cooperative game theory

In a nutshell, cooperative game theory can be summarized as **“the art of cutting a cake”**.

Given a **set of players** $D = \{1, \dots, d\}$, who produces a **quantity** $v(D)$, how can one allocate shares of $v(D)$ among the d players ?

The **“cake cutting process”** is often described through **axioms** (i.e., desired properties), and results in an **allocation**.

Formally, a cooperative game is denoted (D, v) where D is a **set of players**, and $v : \mathcal{P}(D) \to \mathbb{R}$ is a **value function**, mapping every possible subset of players to a real value.

Cooperative game theory and GSA

In the **global sensitivity analysis** (GSA) framework, an **analogy** can be made between players and input variables. Originally, the **chosen value function**, for a subset of variables $A \in \mathcal{P}(D)$, is (Owen 2014):

$$v(A) = S_A^{\text{clos}} = \frac{\mathbb{V}\left(\mathbb{E}[G(X)|X_A]\right)}{\mathbb{V}(G(X))} \tag{3}$$

S_A^{clos} can be interpreted as a **measure of the output's variability due to the subset of inputs** X_A. Since $S_D^{\text{clos}} = 1$, the cooperative game (D, S^{clos}) aims at allocating **percentages of the output's variance to each input variables** in D.

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Which allocation to choose ?

Shapley values

The **Shapley values** is a **particular instance** of an **allocation**. They can be interpreted as

> "[...] *an a priori assessment of the situation, based on either ignorance or disregard of the social organization of the players."* - L. S. Shapley (2016)

They can be seen as a **uniform prior on the underlying bargaining process**, i.e., every player receives an **equal part of the coalitional surplus**:

$$\text{Shap}_i\Big((D,v)\Big) = \sum_{A\subset D: i\in A} \frac{\sum_{B\subseteq A}(-1)^{|A|-|B|}v(B)}{|A|}.$$

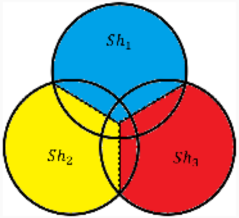
They are the unique allocation satisfying:

1. **(Efficiency)** $\sum_{j=1}^{d}\phi_j = v(D)$;
2. **(Symmetry)** If $v(A\cup\{i\}) = v(A\cup\{j\})$ for all $A\in\mathcal{P}(D)$, then $\phi_i = \phi_j$;
3. **(Null player)** If $v(A\cup\{i\}) = v(A)$ for all $A\in\mathcal{P}(D)$, then $\phi_i = 0$;
4. **(Additivity)** If (D,v) and (D,v') have Shapley Values ϕ and ϕ' respectively, then the game with cost function $(D, v+v')$ has Shapley values $\phi_j + \phi'_j$ for $j\in\{1,\dots,d\}$;

They can also be uniquely characterized by **other sets of axioms**.

Shapley effects

In the GSA context, this means that the originally considered "interaction effects" (S_A, $|A| \geq 2$) are **equally shared between the interacting inputs**.



The **Shapley effects** (Owen 2014) can be written as:

$$\text{Sh}_i = \text{Shap}_i\left((D, S^{\text{clos}})\right) = \sum_{A \subseteq D : i \in A} \frac{S_A}{|A|}$$

Back to the example :

$$G(X) = X_1 + X_2 X_3,$$

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

The three inputs have Shapley effects:

$$\text{Sh}_1 = 0.5 - 2\rho^2/12$$
$$\text{Sh}_2 = 0.25 + \rho^2/12$$
$$\text{Sh}_3 = 0.25 + \rho^2/12$$

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

Shapley's joke

The averaging property of the Shapley effects can be useful in order to quantify **input influence** (i.e., **model exploration**).

However, they can fail at quantifying **input importance** (i.e., **factor fixing/prioritization**):

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

lead to the following Shapley effects:

$$\text{Sh}_1 = 0.5 - \rho^2/4, \quad \text{Sh}_2 = 0.5, \quad \text{Sh}_3 = \rho^2/4.$$

An **exogenous variable** can have a **non-zero** Shapley effect.

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Is there another allocation that circumvents this phenomenon?

Proportional marginal values

The **proportional values** are another example of an allocation, which can be interpreted as

> "[...] *splitting the coalitional surplus so each player gains in equal proportion to that which could be obtained by each alone."* - B. Feldman (1999)

They can be seen as a **proportional redistribution**, i.e., every player receives a **part of the coalitional surplus proportional to their marginal contribution over all coalitions**. The formulation is defined recursively:

$$\text{PMV}_i\Big((D, v)\Big) = \frac{P(D, w)}{P(D \setminus \{i\}, w)}$$

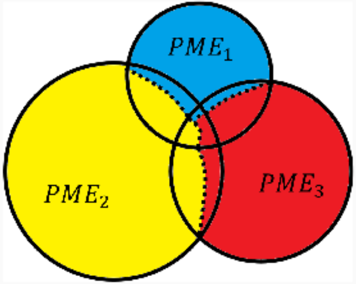
$$\text{with } w(A) = v(D) - v(D \setminus A), \quad P(A, w) = w(A) \left(\sum_{j \in A} \frac{1}{P(A \setminus \{j\}, w)} \right)^{-1}, \text{ and } P(\emptyset, w) = 1$$

They are the unique allocation $\phi((D, v))$ satisfying (Ortmann 2000):

1. **(Efficiency)** $\sum_{j=1}^{d} \phi_j = v(D)$;
2. **(Ratio preservation)** $\forall A \subseteq D, \frac{\phi_i(A,v)}{\phi_i(A \setminus \{j\}, v)} = \frac{\phi_j(A,v)}{\phi_j(A \setminus \{i\}, v)}$

Proportional marginal effects

In the GSA context, this means that the originally considered "interaction effects" (S_A, $|A| \geq 2$) are **shared between the interacting inputs proportionally to their individual effect**.



The **proportional marginal effects** can be written as:

$$PME_i = PMV_i\Big((D, S^{\text{clos}})\Big)$$

Back to the example :

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

The three inputs have proportional marginal effects:

$$\text{PME}_1 = \frac{2-\rho^2}{4-\rho^2}, \quad \text{PME}_2 = \frac{1}{4-\rho^2}$$

$$\text{PME}_3 = \frac{1}{4-\rho^2}$$

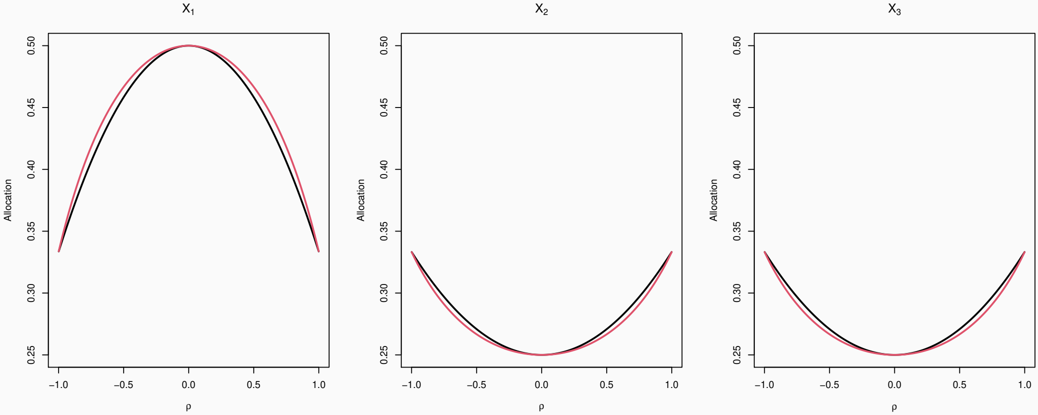

Figure 1: Comparison between the **Shapley effects** and the **proportional marginal effects**, with respect to ρ.

Exclusion equivalency property of the PME

The **Shapley values** allow for a **zero allocation** only if a player i is a **null player**:

$$\forall A \subset D \setminus \{i\}, v(A \cup \{i\}) - v(A) = 0,$$

meaning that adding i to **any coalition** does not increase the coalition's production.

The **proportional values**, in the other hand, fixes a player i allocation to zero if it is in every coalition $A \in \mathcal{P}(D)$ such that:

$$v(D) - v(D \setminus A) = 0, \text{ and } |A| = \max_{B \subseteq D} \{|B| : v(D) - v(D \setminus B) = 0\}$$

meaning that i is in all the **biggest coalitions** with **zero marginal contribution**.

Moreover, if X_i is a spurious variable (i.e., not in the model $G(.)$), then automatically $PME_i = 0$.

Shapley's joke

Recall the previous example:

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

In this case, one has the following allocations:

Shapley effects:

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Proportional marginal effects:

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Proportional marginal effects:

$$\text{PME}_1 = 0.5$$
$$\text{PME}_2 = 0.5$$
$$\text{PME}_3 = 0$$

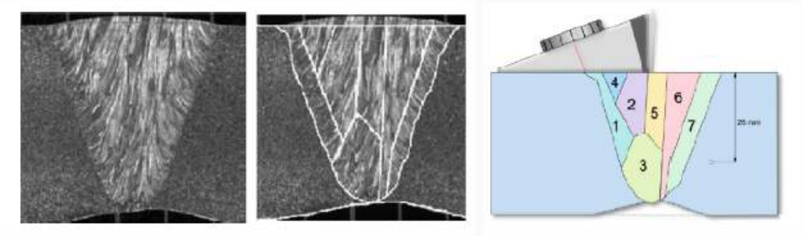
The proportional marginal effects allow to detect **exogenous inputs** in a **correlated setting**.

Ultrasonic control of a weld

Non-destructive control of a weld defect, using the *ATHENA2D* numerical code (Iooss and Prieur 2019).

- 11 input variables:
    - 4 elastic coefficients related to the welding material ;
    - 7 columnar grain orientation relative to the 7 different zones.
- Output : wave amplitude after the weld defect ultrasonic inspection.

The inputs are assumed to be **Gaussian**, and **the 7 columnar grain orientation** are **highly correlated**.



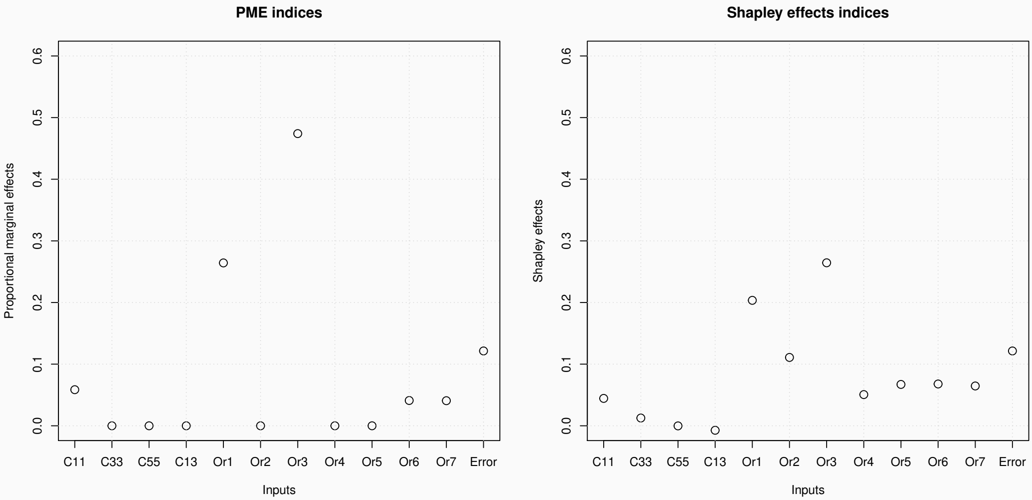


Figure 2: PME (left) and Shapley effects (right) for the ultrasonic control of a weld.

The indices have been computed on a 10^3 i.i.d. sample using a K-NN approach with $K = 5$ (Broto, Bachoc, and Depecker 2020).

Conclusion

GSA indices inspired from cooperative game theory are **not absolute**, and their use need to be **contextualized** by the chosen **allocation process**.

Some allocations allow for a **better understanding of the modeled phenomena** (e.g., Shapley effects), while others prioritize **factor prioritization** (e.g., proportional marginal effects).

Other promising allocation results can allow for better insights on the modeled phenomena such as **weighted Shapley values** (Kalai and Samet 1987).

Robust and **fast estimation** of such indices, in particular on a **unique i.i.d. sample** (i.e., data-driven), remain one of the main challenge in regards of these methods.

Broto, B, F Bachoc, and M Depecker. 2020. "Variance Reduction for Estimation of Shapley Effects and Adaptation to Unknown Input Distribution" [in en]. *SIAM/ASA Journal on Uncertainty Quantification* 8, no. 2 (January): 693–716. ISSN: 2166-2525, accessed December 2, 2020. https://doi.org/10.1137/18M1234631. https://epubs.siam.org/doi/10.1137/18M1234631.

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Sobol, I M. 1990. "On sensitivity estimation for nonlinear mathematical models" [in Russian]. *Mathematical Modelling and Computational Experiments* 2 (1): 112–118.

Thank you for your attention!

Any question?

Random model representations

Let $\mathcal{R}(D)$ be the set of all $d!$ permutations (orderings) of D, let $r = (r_1, \ldots, r_d)$, and denote $r(i)$ the position of the player i in a permutation r (i.e., $r_{r(i)} = i$). Then:

$$Shap_i((D,v)) = \sum_{r \in \mathcal{R}(D)} \frac{1}{d!}(v(r_1, .., r_{r(i)}) - v(r_1, .., r_{r(i)-1}))$$

$$PV((D,v))_i = \sum_{r \in \mathcal{R}(D)} p(r)(v(r_1, .., r_{r(i)}) - v(r_1, .., r_{r(i)-1}))$$

with:

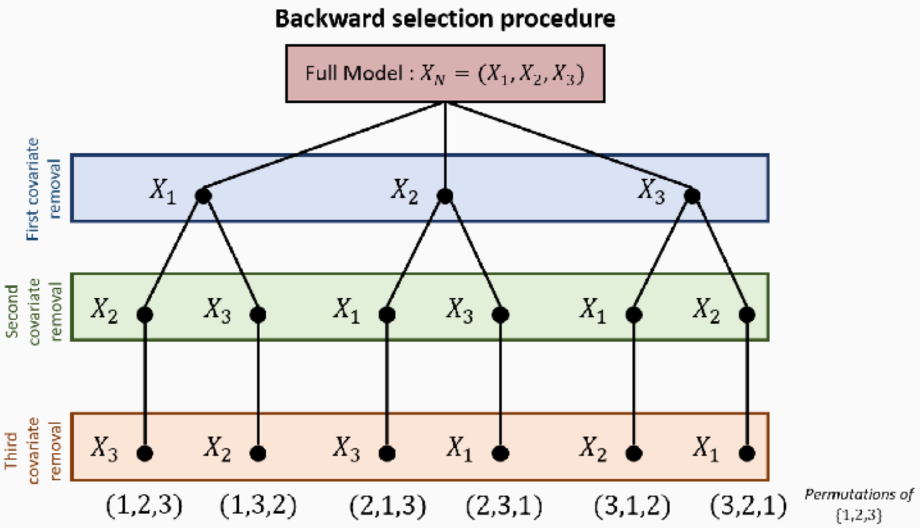
$$p(r) = \frac{L(r)}{\sum_{m \in \mathcal{R}(D)} L(m)}, \quad L(r) = \frac{1}{v(\{r_1\})v(\{r_1, r_2\})...v(D)}$$

and since, by monotony assumption, one has that:

$$v(\{r_1\}) \leq v(\{r_1, r_2\}) \leq .. \leq v(\{r_1, r_2, .., r_n\}), \quad \forall r \in \mathcal{R}(N)$$

$L(r)$ will take relatively high values for order of increasing values.

Dual of a game as a backward procedure



Extension of the proportional values

The proportional values (Feldman 1999) are originally defined on strictly positive games (i.e., $v(A) > 0$), which has then been extended to *some* non-strictly positive games (Feldman 2007). The following results (Margot Hérin) allow to extend the proportional values to *any* non-strictly positive games:

Theorem (Continuity in zero of the proportional values)

Let (N, v) be a monotonic cooperative game. Consider the associated sequence of cost functions (v_p) defined by:

$$\forall p \in \mathbb{N},\ \forall S \subset N, \quad v_p(S) = \begin{cases} v(S) & \text{if } v(S) > 0 \\ \epsilon_p \xrightarrow[p \to \infty]{} 0 & \text{if } v(S) = 0. \end{cases} \tag{4}$$

Then one can define the extended proportional values as:

$$\forall i \in N, \quad \tilde{\phi}_i^{Pv}(v) = \lim_{p \to \infty} \phi_i^{Pv}(v_p) \tag{5}$$

...

Extension of the proportional values

Theorem

...

- *If there exists a null coalition of cardinality $n-1$:*

$$\lim_{p\to\infty} \phi_i^{Pv}(v_p) = \begin{cases} \frac{v(N)}{|\{j\in N | v(N_{-j})=0\}|} & \text{if } \exists S \subseteq N_{-i} \text{ s.t } |S| = k_M(N),\ v(S)=0 \text{ i.e., } v(N_{-i})=0 \\ 0 & \text{otherwise.} \end{cases}$$

- *if $k_M(N) < n-1$, i.e., if there exists no null coalition of cardinality $n-1$:*

$$\lim_{p\to\infty} \phi_i^{Pv}(v_p) = \begin{cases} \dfrac{\sum\limits_{\substack{r\in\mathcal{R}(N_{-i})\\ k_r=k_M(N)}} \prod\limits_{m=k_r+1}^{n-1} v(S_m^r)^{-1}}{\sum\limits_{\substack{r\in\mathcal{R}(N)\\ k_r=k_M(N)}} \prod\limits_{m=k_r+1}^{n} v(S_m^r)^{-1}} & \text{if } \exists S \subseteq N_{-i} \text{ s.t } |S| = k_M(N),\ v(S)=0 \\ 0 & \text{otherwise.} \end{cases}$$

where $\forall S \subseteq N$, $v_S : \mathcal{P}(N\backslash S) \to \mathbb{R}^+$ *is defined by:* $\forall T \subset N\backslash S$, $v_S(T) = v(S \cup T)$.

Consequences of the extension

Corollary

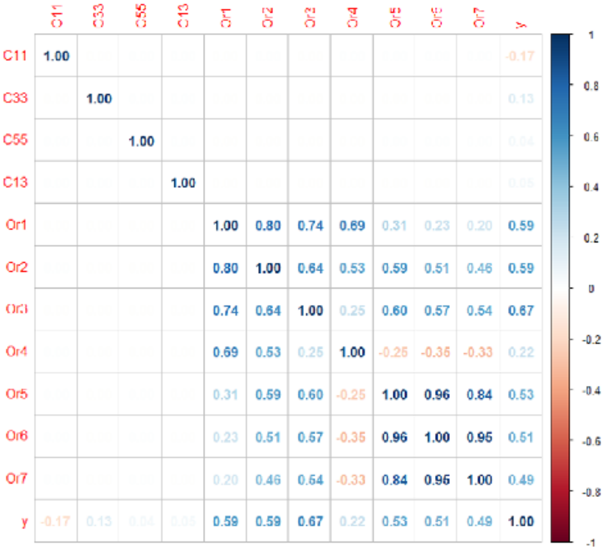
Let (N, v) be a non null monotonic cooperative game. A player gets null proportional value if and only if it is included in all the null coalitions of maximal cardinality. Equivalently, a player gets a strictly positive proportional value if and only if one can find a null coalition of maximum cardinality which do not include him.

Corollary

If $i \in N$ is a variable that is not in the model $G(.)$, i.e., such that one can find a measurable function $f : (\mathbb{R}, \mathcal{B}(\mathbb{R}))^{n-1} \to (\mathbb{R}, \mathcal{B}(\mathbb{R}))$ such that $Y = f(X_{N\setminus\{i\}})$, then:

$$PME_i = 0.$$

Ultrasonic weld control : empirical dependence structure



Shapley Effects vs. PME: Linear models

$Y = X_1 + X_2 + \beta_3 X_3$, (X_1, X_2, X_3) centered Gaussian vector, and $\text{Cov}(X_2, X_3) = \rho$.

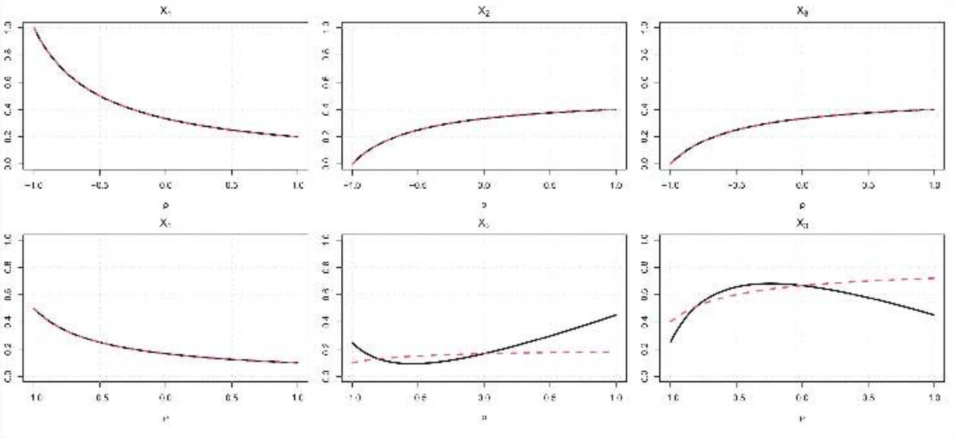


Figure 3: Sh and PME indices with respect to ρ, when $\beta_3 = 1$ (top row), and $\beta_3 = 2$ (bottom row).