COOPERATIVE GAME THEORY AND GLOBAL SENSITIVITY ANALYSIS

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September, 14th 2021

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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**.
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.

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 $A \in \{1, \ldots, d\}$, are defined as:

$$S_A = \sum_{B \subseteq A} (-1)^{|A| - |B|} \frac{\mathbb{V}(\mathbb{E}[G(X) | X_B])}{\mathbb{V}(G(X))},$$

and allow for

$$\sum_{C \subseteq \{1, \ldots, d\}} S_C = 1. \quad (1)$$

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):

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

(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** \((\rho \neq 0)\)

\[ S_1 = 0.5, \quad S_2 = 0, \quad S_3 = \rho^2/2, \]
\[ S_{\{1,2\}} = \rho^2/2, \quad S_{\{1,3\}} = -\rho^2/2, \quad S_{\{2,3\}} = 0.5, \]
\[ S_{\{1,2,3\}} = -\rho^2/2 \]
Let's take an example (Iooss and Prieur 2019):

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

Given a set of players \( D = \{1, \ldots, d\} \), 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.
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):

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

$S_A^{\text{clos}}$ 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 $(D, S^{\text{clos}})$ aims at allocating percentages of the output’s variance to each input variables in $D$. 
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):

$$v(A) = S^\text{clos}_A = \frac{\mathbb{V}(\mathbb{E}[G(X)|X_A])}{\mathbb{V}(G(X))}$$  \hspace{1cm} (3)

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

**Which allocation to choose?**
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:

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

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 \( \phi \) and \( \phi' \) respectively, then the game with cost function \((D, v + v')\) has Shapley values \( \phi_j + \phi'_j \) for \( j \in \{1, \ldots, d\} \);

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:

\[
S_{hi} = \text{Shap}_i \left( (D, S^{\text{clos}}) \right) - \sum_{A \subseteq D : i \notin A} \frac{S_A}{|A|}
\]

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

Back to the example:

\[
G(X) = X_1 \times X_2 X_3,
\]

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

The three inputs have Shapley effects:

\[
S_{h1} = 0.5 - 2\rho^2 / 12
\]
\[
S_{h2} = 0.25 + \rho^2 / 12
\]
\[
S_{h3} = 0.25 + \rho^2 / 12
\]
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:

\[
Sh_1 = 0.5 - \frac{\rho^2}{4}, \quad Sh_2 = 0.5, \quad Sh_3 = \frac{\rho^2}{4}.
\]

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

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lead to the following Shapley effects:

\[ Sh_1 = 0.5 - \rho^2/4, \quad Sh_2 = 0.5, \quad Sh_3 = \rho^2/4. \]

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

Is there another allocation that circumvents this phenomenon?
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:

\[
PMV_i((D, v)) = \frac{P(D, w)}{P(D \setminus \{i\}, w)}
\]

with \( w(A) = v(D) - v(D \setminus A) \), \( P(A, w) = w(A) \left( \sum_{j \in A} \frac{1}{P(A \setminus \{j\}, w)} \right)^{-1} \), 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:

\[
PME_i = PMV_i\left((D, S^{clos})\right)
\]

Back to the example:

\[
G(X) = X_1 \times X_2 X_3,
\]

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

The three inputs have proportional marginal effects:

\[
PME_1 = \frac{2 - \rho^2}{4 - \rho^2}; \quad PME_2 = \frac{1}{4 - \rho^2}
\]

\[
PME_3 = \frac{1}{4 - \rho^2}
\]
Figure 1: Comparison between the Shapley effects and the proportional marginal effects, with respect to $\rho$. 
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 $A \in P(D)$ 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 $PME_i = 0$. 
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:**

- \( \text{Sh}_1 = 0.5 - \rho^2 / 4 \)
- \( \text{Sh}_2 = 0.5 \)
- \( \text{Sh}_3 = \rho^2 / 4 \)

**Proportional marginal effects:**

- \( \text{PME}_1 = 0.5 \)
- \( \text{PME}_2 = 0.5 \)
- \( \text{PME}_3 = 0 \)
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:**

\[
\begin{align*}
Sh_1 &= 0.5 - \frac{\rho^2}{4} \\
Sh_2 &= 0.5 \\
Sh_3 &= \frac{\rho^2}{4}
\end{align*}
\]

**Proportional marginal effects:**

\[
\begin{align*}
PME_1 &= 0.5 \\
PME_2 &= 0.5 \\
PME_3 &= 0
\end{align*}
\]

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 (Looss 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).
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.


Thank you for your attention!

Any question?
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:

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

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

with:

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

and since, by monotony assumption, one has that:

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

$L(r)$ will take relatively high values for order of increasing values.
Dual of a game as a backward procedure

Backward selection procedure

Full Model: \( X_N = (X_1, X_2, X_3) \)

Permutations of \( \{1,2,3\} \):

- (1,2,3)
- (1,3,2)
- (2,1,3)
- (2,3,1)
- (3,1,2)
- (3,2,1)
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:

$$v_p(S) = \begin{cases} v(S) & \text{if } v(S) > 0 \\ \epsilon_p \rightarrow 0 & \text{if } v(S) = 0. \end{cases} \quad (4)$$

Then one can define the extended proportional values as:

$$\forall i \in N, \quad \tilde{\phi}_i^P(v) = \lim_{p \rightarrow \infty} \phi_i^P(v_p) \quad (5)$$
Extension of the proportional values

Theorem

... 

- If there exists a null coalition of cardinality \( n - 1 \):

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

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

\[
\lim_{p \to \infty} \phi_i^{Pv}(v_p) = \begin{cases} 
\sum_{r \in \mathcal{R}(N\setminus i)} \frac{\prod_{m=k_r+1}^{n-1} v(S^r_m)^{-1}}{k_r=k_M(N)} & \text{if } \exists S \subseteq N \setminus i \text{ s.t } |S| = k_M(N), \ v(S) = 0 \\
\sum_{r \in \mathcal{R}(N)} \frac{\prod_{m=k_r+1}^{n} v(S^r_m)^{-1}}{k_r=k_M(N)} & \text{otherwise.}
\end{cases}
\]

where \( \forall S \subseteq N, v_S : \mathcal{P}(N \setminus S) \to \mathbb{R}^+ \) is defined by: \( \forall T \subset N \setminus S, v_S(T) = v(S \cup T) \).
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 \(f : (\mathbb{R}, \mathcal{B}(\mathbb{R}))^{n-1} \rightarrow (\mathbb{R}, \mathcal{B}(\mathbb{R}))\) such that \(Y = f(X_{N\setminus\{i\}})\), then:

\[ \text{PME}_i = 0. \]
### Ultrasonic weld control: empirical dependence structure

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*Heatmap values range from -1 to 1.*
$Y = X_1 + X_2 + \beta_3 X_3$, $(X_1, X_2, X_3)$ centered Gaussian vector, and $\text{Cov}(X_2, X_3) = \rho$.

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