

Importance measures with dependent inputs: linear and non-linear cases

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Plan

1. The linear case

- Uncertainty quantification context in neutronic

- Basics of multivariate linear regression

- Multicolinearity illustration with a two-input regression model

- Variance-based Importance Measures : LMG and Johnson

- Sensitivity analysis in a neutronic study

2. The non-linear case

- Cooperative game theory

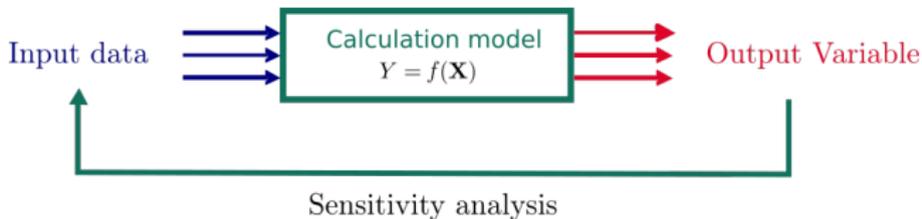
- Shapley effects

- Proportional marginal effects

- Application to an optical filter model

3. Conclusion

Uncertainty quantification context in neutronic



Calculation model :

$$\vec{\Omega} \cdot \vec{\nabla} \psi(\vec{r}, E, \vec{\Omega}) + \Sigma_t(\vec{r}, E) \psi(\vec{r}, E, \vec{\Omega}) = \int_0^\infty dE' \int_{4\pi} d^2\vec{\Omega}' \Sigma_s(\vec{r}, E' \rightarrow E, \vec{\Omega}, \vec{\Omega}') \psi(\vec{r}, E', \vec{\Omega}') + \mathbf{Q}(\vec{r}, E, \vec{\Omega})$$

Interest variable :

- ▶ ψ the neutron flux.

Input variables :

- ▶ ~ 2000 variables : **large size and correlations.**

Approached model :

- ▶ **Linear regression model**

The linear case : Context of our presentation

[Article in press in the journal SESMO \[Clo+25\]](#)



An overview of variance-based importance measures in the linear regression context: comparative analyses and numerical tests

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Basics of multivariate linear regression

Framework and notations

Experimental design

- ▶ n observations (\mathbb{R} -valued) of an **explained** random variable Y and of d **explanatory** random variables $\mathbf{X} = (X_1, \dots, X_d)$:

$$(\mathbf{X}^n, \mathbf{y}^n) = \left(x_1^{(i)}, \dots, x_d^{(i)}, y^{(i)} \right)_{i=1, \dots, n},$$

Assumption. *without any loss of generality*

$$\mathbb{E}[X_j] = 0 \text{ for } j = 1, \dots, d \text{ and } \mathbb{E}[Y] = 0$$

Basics of multivariate linear regression

Framework and notations

Multivariate linear regression model

$$Y = \mathbf{X}\beta + \varepsilon.$$

- ▶ where $\beta = (\beta_1, \dots, \beta_d)^\top \in \mathbb{R}^d$ is the vector of coefficients,
- ▶ ε is a random error assumed to be Gaussian and centered.

Assumption. $\varepsilon \sim \mathcal{N}(0, \sigma_\varepsilon^2)$ and $\mathbb{E}[\varepsilon | \mathbf{X}] = 0$.

- ▶ For each observation $i = 1, \dots, n$, $y^{(i)} = \mathbf{x}^{(i)}\beta + \varepsilon^{(i)}$ where for all $i = 1, \dots, n$, the $\varepsilon^{(i)}$ s are independent and identically distributed with the same law as ε . Therefore, determine :

$$\mathbb{E} \left[Y | \mathbf{X} = \left(x_1^{(i)}, \dots, x_d^{(i)} \right) \right] = \mathbf{x}^{(i)}\beta.$$

Basics of multivariate linear regression

Framework and notations

Estimating model coefficients β

Hypothesis. The sample size is large enough ($n \gg d$), and the matrix $\mathbf{X}^{n\top} \mathbf{X}^n$ is positive-definite.

- ▶ The unbiased maximum likelihood estimator (Ordinary Least Squares [Chr90]) :

$$\hat{\beta} = (\mathbf{X}^{n\top} \mathbf{X}^n)^{-1} \mathbf{X}^{n\top} \mathbf{y}^n.$$

Coefficient of determination

- ▶ Quantify the **output variability captured** by the linear regression model :

$$R^2 = R_{Y(X)}^2 := 1 - \frac{\mathbb{E}[\mathbb{V}(Y|X)]}{\mathbb{V}(Y)} = \frac{\mathbb{V}(\mathbb{E}[Y|X])}{\mathbb{V}(Y)}.$$

The R^2 decomposition

The Variance-based importance measures (VIM) describe the impact of input data on **output dispersion** and are equivalent to partition R^2 among the d inputs

Criteria for R^2 decomposition

Four basic desirability criteria can be sought after for a VIM (according to Grothendieck [Grö07]) :

- ▶ (C_1) *Proper decomposition* : the sum of all shares should be equal to the total variance ;
- ▶ (C_2) *Non-negativity* : all shares should be nonnegative ;
- ▶ (C_3) *Exclusion* : if $\beta_j = 0$, then the share of X_j should be zero ;
- ▶ (C_4) *Inclusion* : if $\beta_j \neq 0$, then the share of X_j should be nonzero.

An additional criterion that is sometimes mentioned in the literature, but more related to regularization-based techniques [ZH05 ; Wal19] :

- ▶ (C_5) *Grouping* : shares tend to equate for highly correlated inputs.

Multicolinearity illustration

Two-input regression model

An illustrative example :

Two-input regression model

Consider the linear regression model (for $d = 2$) of the output Y with X_1 and X_2 .

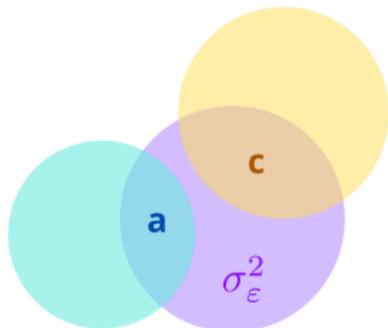
$$b_1 := \beta_1 \sigma_1, \quad b_2 := \beta_2 \sigma_2, \quad \text{and } r := r_{X_1, X_2}.$$

The coefficient of determination is :

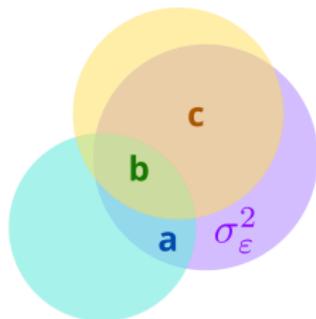
$$R^2 = \frac{b_1^2 + 2b_1 b_2 r + b_2^2}{b_1^2 + 2b_1 b_2 r + b_2^2 + \sigma_\varepsilon^2}.$$

Metrics to deal with multicollinearity

Venn diagrams illustrating the challenges of the multicollinearity framework :



(a) $r = 0, b = 0$



(b) $r \neq 0, b \neq 0$

- ▶ Three circles :
 - ▶ the variance of Y ; the variance of X_1 ; the variance of X_2 .
- ▶ Two overlapping area - the **additional explanatory power** :
 - ▶ of X_1 on the regression model $Y(X)$: $a = b_1^2(1 - r^2)$,
 - ▶ of X_2 on the regression model $Y(X)$: $c = b_2^2(1 - r^2)$.
- ▶ The area b : $b = b_1^2 r^2 + 2b_1 b_2 r + b_2^2 r^2$.

Variance-based Importance Measures

LMG

Shapley Values in regression model :

- ▶ inspired from the cooperative game [Sha53],
- ▶ measure the **average marginal contribution** of each variable X_j to all possible combinations of variables in a regression model :

$$\psi_j = \frac{1}{d!} \sum_{\pi \in \mathcal{S}_D} \Delta_{\pi}(X_j)$$

where :

- ▶ \mathcal{S}_D is the set of all permutations of $D = \{1, \dots, d\}$,
- ▶ $\Delta_{\pi}(X_j) = c(v \cup j) - c(v)$ the **marginal performance difference** of the model between the permutation π with and without X_j ,
- ▶ v the list of indices preceding j in the order π .

Variance-based Importance Measures

LMG

Owen[Owe14] proposes to set the function c such as :

$$c(v) = \frac{\mathbb{V}(\mathbb{E}[Y|\mathbf{X}_v])}{\mathbb{V}(Y)}$$

In the linear regression context, Lindeman-Merenda-Gold indices [LMG80] :

- ▶ LMG _{j} average the additional explanatory power of X_j in each subset $\mathbf{X}_{v \cup \{j\}}$ defined for all the permutations of $D = \{1, \dots, d\}$:

$$\text{LMG}_j = \frac{1}{d!} \sum_{\pi \in \mathcal{S}_D} r_{Y, (X_j | \mathbf{X}_\pi)}^2$$

where

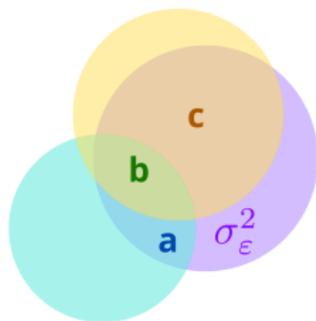
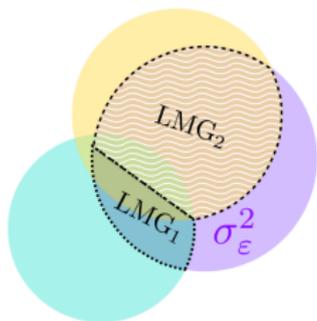
- ▶ the squared SPCC $r_{Y, (X_j | \mathbf{X}_\pi)}^2 = R_{Y(\mathbf{X}_{v \cup \{j\}})}^2 - R_{Y(\mathbf{X}_v)}^2$
- ▶ gives the **additional explanatory power** of X_j in the model $Y(\mathbf{X}_{v \cup \{j\}})$.

Variance-based Importance Measures

LMG

$$\begin{aligned} \text{LMG}_1 &= \frac{b_1^2 + b_1 b_2 r + \frac{r^2}{2}(b_2^2 - b_1^2)}{b_1^2 + 2b_1 b_2 r + b_2^2 + \sigma_\varepsilon^2} \\ &= \frac{a + b/2}{a + b + c + \sigma_\varepsilon^2} \end{aligned}$$

$$\begin{aligned} \text{LMG}_2 &= \frac{b_2^2 + b_1 b_2 r + \frac{r^2}{2}(b_1^2 - b_2^2)}{b_2^2 + 2b_1 b_2 r + b_1^2 + \sigma_\varepsilon^2} \\ &= \frac{c + b/2}{a + b + c + \sigma_\varepsilon^2} \end{aligned}$$



LMG redistributes b equally between the portions attributed to X_1 and X_2 .

Variance-based Importance Measures

LMG

With correlated inputs : $r \neq 0$

$$\text{LMG}_1 = \frac{b_1^2 + b_1 b_2 r + \frac{r^2}{2}(b_2^2 - b_1^2)}{b_1^2 + 2b_1 b_2 r + b_2^2 + \sigma_\varepsilon^2} \quad \text{LMG}_2 = \frac{b_2^2 + b_1 b_2 r + \frac{r^2}{2}(b_1^2 - b_2^2)}{b_2^2 + 2b_1 b_2 r + b_1^2 + \sigma_\varepsilon^2}$$

\mathcal{C}_1	Proper decomposition	$\sum_j \text{IM}_j = R^2$	YES
\mathcal{C}_2	Non-negativity	for all j , $\text{IM}_j \geq 0$	YES
\mathcal{C}_3	Exclusion	if $\beta_j = 0$, $\text{IM}_j = 0$	NO if $r \neq 0$
\mathcal{C}_4	Inclusion	if $\beta_j \neq 0$, $\text{IM}_j \neq 0$	YES
\mathcal{C}_5	Grouping	shares equate for high correlations	YES
			$\text{LMG}_1 = \text{LMG}_2$, if $r = 1$

Variance-based Importance Measures

Johnson indices

Drawback of LMG :

- ▶ its **exponential complexity** : one needs to perform $2^d - 1$ different linear regressions.

The Johnson indices [Joh66 ; Joh00] :

- ▶ $\mathbf{X}^n \in \mathbb{R}^{n \times d}$ is **transformed in an orthogonal matrix** $\mathbf{Z}^n \in \mathbb{R}^{n \times d}$ in the least square sense. It consists in finding \mathbf{Z}^n and $\mathbf{W} \in \mathbb{R}^{d \times d}$ such as :

$$\left\{ \begin{array}{l} \mathbf{X}^n = \mathbf{Z}^n \mathbf{W} \\ (\mathbf{Z}^n)^\top \mathbf{Z}^n = \mathbf{I} \\ \mathbf{Z}^n = \arg \min_{\mathbf{\Pi}^n} \text{Tr} (\mathbf{X}^n - \mathbf{\Pi}^n)^\top (\mathbf{X}^n - \mathbf{\Pi}^n) \end{array} \right.$$

Variance-based Importance Measures

Johnson indices

The Johnson indices [Joh66 ; Joh00] :

- ▶ Johnson shows that the solution is to define $\mathbf{P}^n \in \mathbb{R}^{n \times d}$ and $\mathbf{Q} \in \mathbb{R}^{d \times d}$ thanks to the **singular value decomposition** of \mathbf{X}^n :

$$\mathbf{X}^n = \mathbf{P}^n \mathbf{\Delta} \mathbf{Q}^T.$$

- ▶ and compute the **orthogonal matrix** \mathbf{Z}^n and the **weight matrix** W thanks to the following equations :

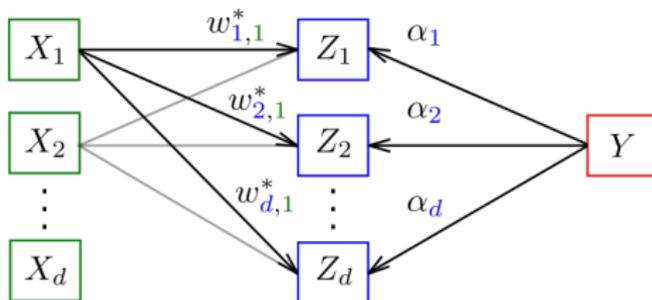
$$\mathbf{Z}^n = \mathbf{P}^n \mathbf{Q}^T \text{ and } W = \mathbf{Q} \mathbf{\Delta} \mathbf{Q}^T.$$

Variance-based Importance Measures

Johnson indices

The **Johnson index** associated with the input X_j is finally expressed as :

$$J_j = \sum_{i=1}^d \alpha_i^{*2} w_{ij}^{*2}.$$



- ▶ A first least square regression of \mathbf{y}^n on \mathbf{Z}^n gives the vector of the standardized regression coefficient α^* of the model $Y(Z)$.
- ▶ The d linear combinations between \mathbf{X}^n and \mathbf{Z}^n gives the *weights* W^* allowing to come back to the initial observations \mathbf{X}^n .

Variance-based Importance Measures

Johnson indices

With a linear relation hypothesis between Y and \mathbf{X} :

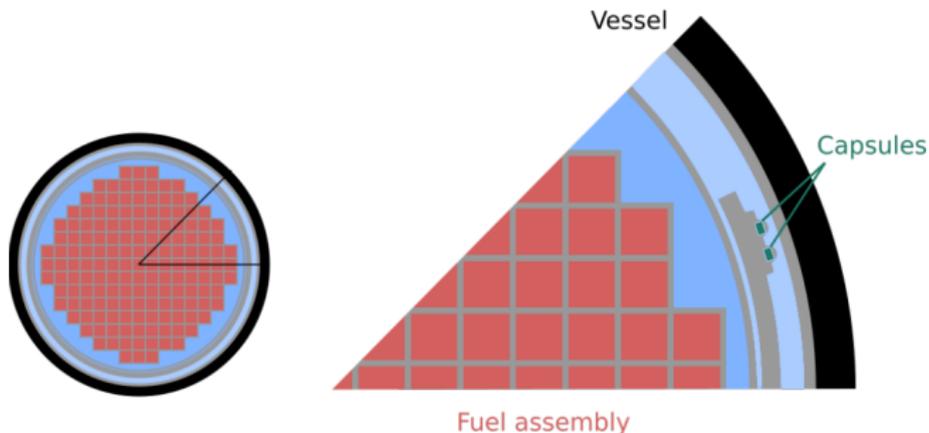
- ▶ The Johnson indices are equal to the LMG indices in the case of a two-input model.

$$J_1 = \text{LMG}_1 = \frac{b_1^2 + b_1 b_2 r + \frac{r^2}{2}(b_2^2 - b_1^2)}{b_1^2 + 2b_1 b_2 r + b_2^2 + \sigma_\varepsilon^2} \quad J_2 = \text{LMG}_2 = \frac{b_2^2 + b_1 b_2 r + \frac{r^2}{2}(b_1^2 - b_2^2)}{b_2^2 + 2b_1 b_2 r + b_1^2 + \sigma_\varepsilon^2}$$

- ▶ They give empirically similar results for a higher-dimensional input data ($d \geq 3$).

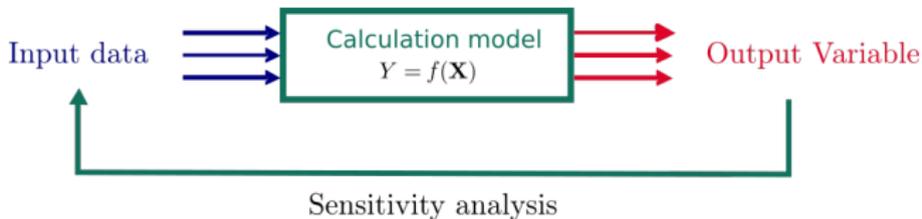
Sensitivity analysis in a neutronic study

Assessment of the neutron irradiation contributing to the aging of the reactor vessel
[Clo19]



- ▶ The neutron flux is calculated to be compared with the measured flux.
- ▶ The calculation gives a prediction of the neutron flux received by the vessel, which is not measured.

Sensitivity analysis in a neutronic study



Calculation model :

$$\vec{\Omega} \cdot \vec{\nabla} \psi(\vec{r}, E, \vec{\Omega}) + \Sigma_t(\vec{r}, E) \psi(\vec{r}, E, \vec{\Omega}) = \int_0^\infty dE' \int_{4\pi} d^2\vec{\Omega}' \Sigma_s(\vec{r}, E' \rightarrow E, \vec{\Omega}, \vec{\Omega}') \psi(\vec{r}, E', \vec{\Omega}') + \mathbf{Q}(\vec{r}, E, \vec{\Omega})$$

Interest variable :

- ▶ ψ the neutron flux.

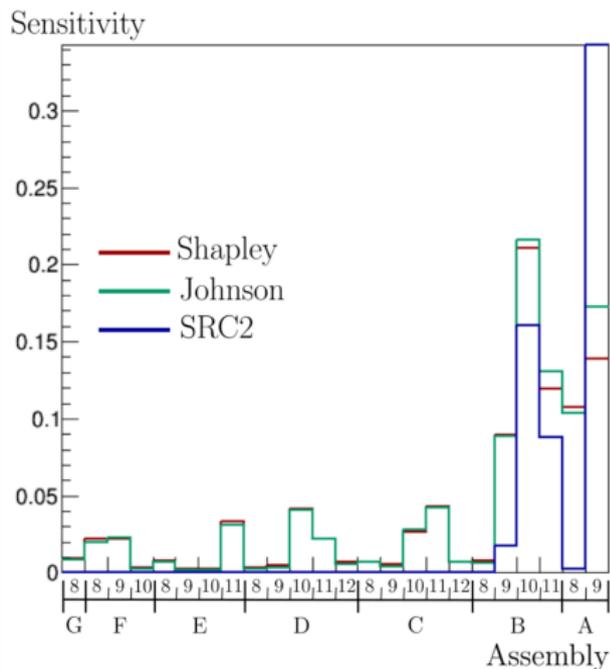
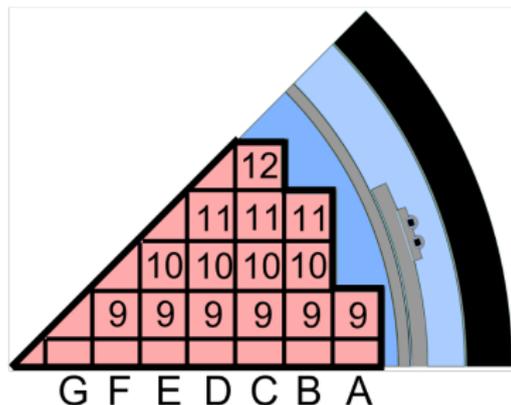
Input variables :

- ▶ the **power of 25 assemblies**

Approached model :

- ▶ Linear regression model

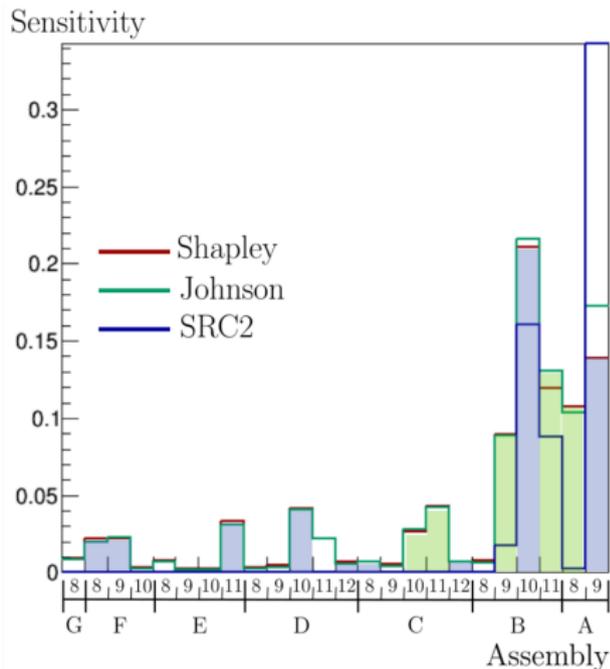
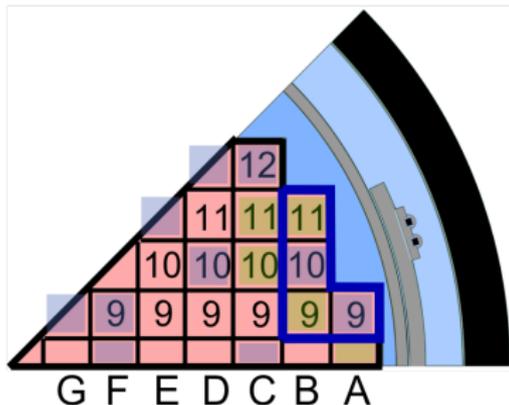
Sensitivity analysis in a neutronic study



- ▶ The SRC² indices (blue) of the assemblies **A9**, **B10**, **B11** are the highest.
- ▶ The SRC² indices only explain 75% of the output variance.

Sensitivity analysis in a neutronic study

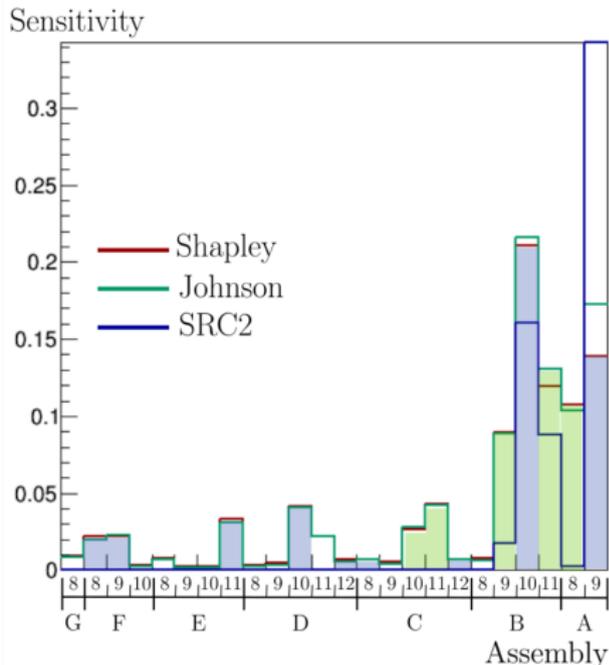
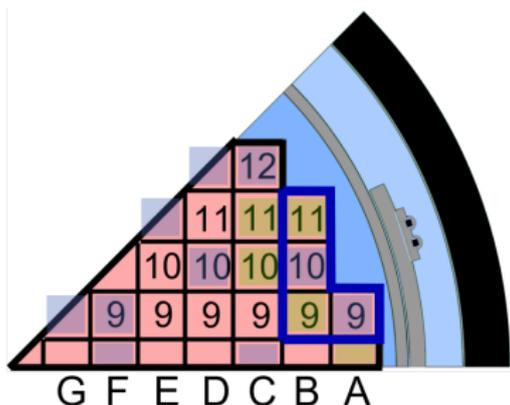
Assemblies where the power is directly measured



- The variables with a **stronger correlation** with A9, B10, B11 have a **higher Johnson/Shapley index** than the associated SRC² index.

Sensitivity analysis in a neutronic study

Assemblies where the power is directly measured



- ▶ The power map is based on calculation and measures. Some powers are measured and the value of the other variables are **reconstructed thanks to measured assemblies**.
- ▶ The variables positioned next to a **measured and influential power** in the model have a higher Johnson/Shapley index than that of SRC².

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The nonlinear case : Context of our presentation

[Article in SIAM/ASA JUQ \[Hér+24\]](#)

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Proportional Marginal Effects for Global Sensitivity Analysis*

Margot Herin[†], Marouane Il Idrissi^{†§¶}, Vincent Chabridon^{†§}, and Bertrand Iooss^{†§¶}

Pitch

Given **random inputs** X_1, \dots, X_d and a **random output** $G(X_1, \dots, X_d)$, how much each **input contribute** to $\mathbb{V}(G(X_1, \dots, X_d))$?

G is a **deterministic black-box model** :

- ▶ **Numerical model** (e.g., simulation codes)
- ▶ **Learned ML/DL models** (e.g., post-hoc interpretations).

The inputs X_1, \dots, X_d are **not necessarily mutually independent**. **Global sensitivity analysis (GSA)** provides an answer : the **Shapley effects** [Owe14; IP19].

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The inputs X_1, \dots, X_d are **not necessarily mutually independent**. **Global sensitivity analysis (GSA)** provides an answer : the **Shapley effects** [Owe14; IP19].

However, **exogenous inputs can be granted a non-zero contribution**.

Can we build **interpretable indices** that **circumvent this drawback**?

Solution : Use a **different allocation** than the Shapley values.

Cooperative game theory

Cooperative game theory

“Cooperative game theory = The art of cutting a cake”.



Formally, given :

A **set of players** $D = \{1, \dots, d\}$, and the subsequent **set of coalitions** $\mathcal{P}(D)$.

A **value function** $v : \mathcal{P}(D) \rightarrow \mathbb{R}$ quantifying the **value produced** by each **coalition**.

(D, v) defines a **cooperative game**.

Main question : How can we redistribute $v(D)$
among the players?

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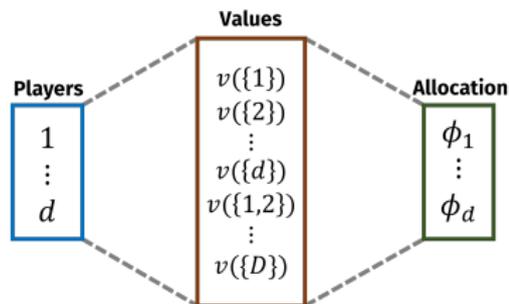
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among the players? **Answer** : By using

allocations!

Allocation : description of the “cake-cutting”
process.



Cooperative game theory

Random order allocations

Allocating “the **whole cake** and **nothing but the cake**” is ensured by two criteria :

Efficiency : $\sum_{i=1}^d \phi_i = v(D)$ (The whole cake).

Nonnegativity : $\forall i \in D, \phi_i \geq 0$ (Nothing but the cake).

Cooperative game theory

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Random order allocations (or the Weber set [Web88]) are a **class of allocations** that are **always efficient**. They can be written $\forall i \in D$, as :

$$\phi_i = \sum_{\pi \in \mathcal{S}_D} p(\pi) [v(C_{\pi(i)}(\pi)) - v(C_{\pi(i)-1}(\pi))].$$

where \mathcal{S}_D is the set of permutations of D and :

$C_{\pi(i)-1}(\pi)$ is the set of players **before** i in π .

$C_{\pi(i)}(\pi) = C_{\pi(i)-1}(\pi) \cup \{i\}$

$p(\pi)$ assigns a **probability to every permutation** $\pi \in \mathcal{S}_D$.

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A choice of $p \implies$ An efficient allocation

Shapley effects

Shapley values

The **Shapley values** is a **random order allocation** with the choice :

$$p(\pi) = \frac{1}{d!}, \quad \forall \pi \in \mathcal{S}_D,$$

and 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 [Sha53]

They are a **uniform prior on the underlying redistribution process**, leading to an **egalitarian allocation principle**.

Shapley effects

Shapley effects

By **analogy between players and inputs**, [Owe14] proposed to study the game :

$$(D, S^T), \quad \text{where } \forall A \in \mathcal{P}(D), \quad S_A^T = \frac{\mathbb{E}[\mathbb{V}(G(X) \mid X_{\bar{A}})]}{\mathbb{V}(G(X))}.$$

The **Shapley effects** are the Shapley values of (D, S^T) [SNS16].

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Since S^T is monotonic and $S_D^T = 1$, the **Shapley effects are efficient and nonnegative** : **They can be interpreted as shares of variance allocated to each input.** They are a **suitable solution** for **importance quantification with dependent inputs.**

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However, **they do not detect exogenous inputs** :

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

$$Sh_1 = 0.5 - \rho^2/4, \quad Sh_2 = 0.5, \quad Sh_3 = \rho^2/4 > 0 \text{ if } \rho \neq 0.$$

Proportional marginal effects

Proportional values

Is it possible to find a suitable ρ , whose **indices detect exogenous inputs** ?

Proportional marginal effects

Proportional values

Is it possible to find a suitable p , whose **indices detect exogenous inputs** ?

Yes with the **proportional values** [Ort00], based on a **proportional allocation principle** for **positive games**. If $\forall A \in \mathcal{P}(D), v(A) > 0$, the choice of p is :

$$p(\pi) = \frac{L(\pi)}{\sum_{\sigma \in \mathcal{S}_D} L(\sigma)}, \quad L(\pi) = \left(\prod_{j \in D} v(C_j(\pi)) \right)^{-1} = \exp \left(- \sum_{j \in D} \log v(C_j(\pi)) \right)$$

Proportional marginal effects

Proportional values

Is it possible to find a suitable ρ , whose **indices detect exogenous inputs** ?

Yes with the **proportional values** [Ort00], based on a **proportional allocation principle** for **positive games**. If $\forall A \in \mathcal{P}(D), v(A) > 0$, the choice of ρ is :

$$\rho(\pi) = \frac{L(\pi)}{\sum_{\sigma \in \mathcal{S}_D} L(\sigma)}, \quad L(\pi) = \left(\prod_{j \in D} v(C_j(\pi)) \right)^{-1} = \exp \left(- \sum_{j \in D} \log v(C_j(\pi)) \right)$$

This is the unique allocation $\phi((D, v))$ satisfying efficiency and **ratio preservation** [Ort00] :

$$\forall A \in \mathcal{P}(D), \frac{\phi_i(A, v)}{\phi_i(A \setminus \{j\}, v)} = \frac{\phi_j(A, v)}{\phi_j(A \setminus \{i\}, v)}$$

“...each player gains in **equal proportion** to that which could be obtained by each alone” [Fel00]

Remark : Shapley's allocation satisfies efficiency and equal contribution property :

$$\forall A \in \mathcal{P}(D), \phi_i(A, v) - \phi_i(A \setminus \{j\}, v) = \phi_j(A, v) - \phi_j(A \setminus \{i\}, v)$$

A linear variance-based importance measure

The proportional marginal variance decomposition

The proportional marginal variance decomposition [Fel05] :

- ▶ use of sequential sum of squares, but differ from the LMG on the averaging process over the different orderings of inputs :

$$\text{PMVD}_j = \sum_{\pi \in \mathcal{S}_D} \frac{L(\pi)}{\sum_{\pi} L(\pi)} r_{Y, (X_j | \mathbf{X}_{\pi})}^2,$$

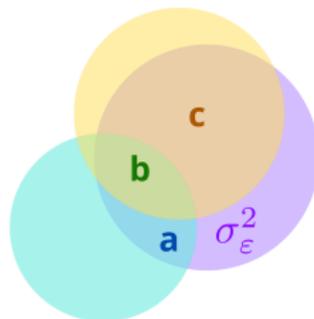
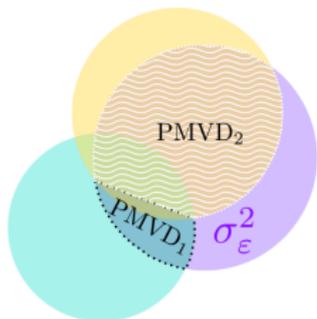
where :

$$L(\pi) = \prod_{i=1}^{d-1} \left[r_{Y, (\mathbf{X}_{\pi_{i+1}, \dots, \pi_d} | \mathbf{X}_{\pi_1, \dots, \pi_i})}^2 \right]^{-1}.$$

A linear variance-based importance measure

The proportional marginal variance decomposition

$$\text{PMVD}_1 = \frac{b_1^2 + b_1 b_2 r + \frac{r^2}{2}(b_2^2 - b_1^2)}{b_1^2 + 2b_1 b_2 r + b_2^2 + \sigma_\varepsilon^2} = \frac{a[1 + b/(a + c)]}{a + b + c + \sigma_\varepsilon^2}$$



Criterion fulfilled. (C_1 -Proper decomposition), (C_2 -Non-negativity), (C_3 -Exclusion), (C_4 -Inclusion)

Criterion not fulfilled. (C_5 -Grouping)

Proportional marginal effects

Proportional marginal effects

We extended the proportional values to **nonnegative value functions** [Hér+24].

The **proportional marginal effects (PME)** are the (extended) proportional values of the game (D, S^T) .

Proposition (Exogeneity detection [Hér+24]).

Let $E \in \mathcal{P}(D)$. If X_E is the largest set of exogenous inputs, then :

$$\forall i \in E, \quad PME_i = 0, \quad \forall j \in \bar{E}, \quad PME_j > 0.$$

They are **efficient** and **nonnegative** : interpretation as shares of the output variance.

Proportional marginal effects

Estimation

Estimating the PME/Shapley effects \iff Estimating S_A^T for every $A \in \mathcal{P}(D)$.

It can be achieved :

Via **Monte Carlo sampling** [SNS16] : **no bias** but requires $O(d!(d-1))$ model evaluations and the simulation of any inputs' combinations conditionally to any other inputs' combinations !

Given-data (i.i.d. input-output sample) via :

- ▶ a **nearest-neighbor procedure** [BBD20] : no new model evaluation but provides **bias** and requires 2^d estimates.
- ▶ SHAFF : **no bias** but no error estimates at this stage.

These methods are time-consuming and do not scale with the number of inputs, but the estimates can be recycled to compute Shapley and PME at once.

Proportional marginal effects

Ishigami Model - Exogeneity detection

The (modified) Ishigami model is given by

$$G(X) = \sin(X_1) + 7 \sin^2(X_2) + 0.1X_3^4 \sin(X_1)$$

where

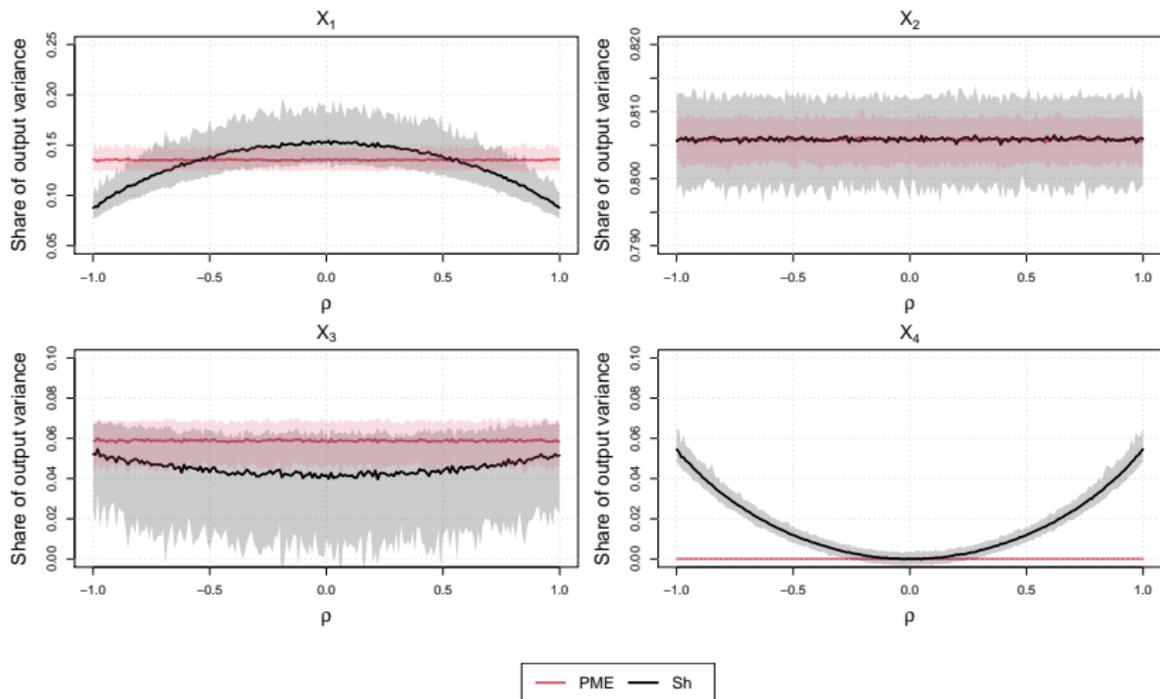
$$X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \end{pmatrix} \sim \mathcal{N} \left(\begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}, \begin{pmatrix} (\pi/3)^2 & 0 & 0 & \rho \\ 0 & (\pi/3)^2 & 0 & 0 \\ 0 & 0 & (\pi/3)^2 & 0 \\ \rho & 0 & 0 & (\pi/3)^2 \end{pmatrix} \right).$$

where X_4 is exogenous.

Estimation using Monte Carlo sampling, 200 repetitions.

Proportional marginal effects

Ishigami Model - Exogeneity detection



Application to an optical filter model

Feature selection

Quantification of the **transmittance performance** of an **optical filter** composed of 13 consecutive layers [Vas+10].

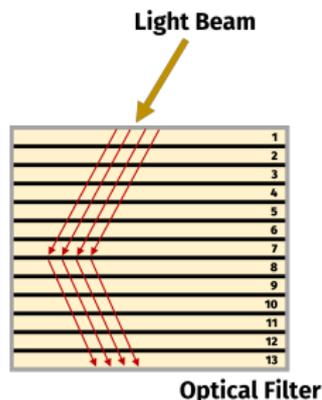
The inputs l_1, \dots, l_{13} represent the **refractive index error** of each filter ($\mathcal{U}([-0.05, 0.05])$)

These errors are (highly) correlated due to the manufacturing process (Gaussian copula, $\rho = 0.95$).

The black-box model computes the **transmittance error w.r.t. the “perfect filter”** over several wavelengths.

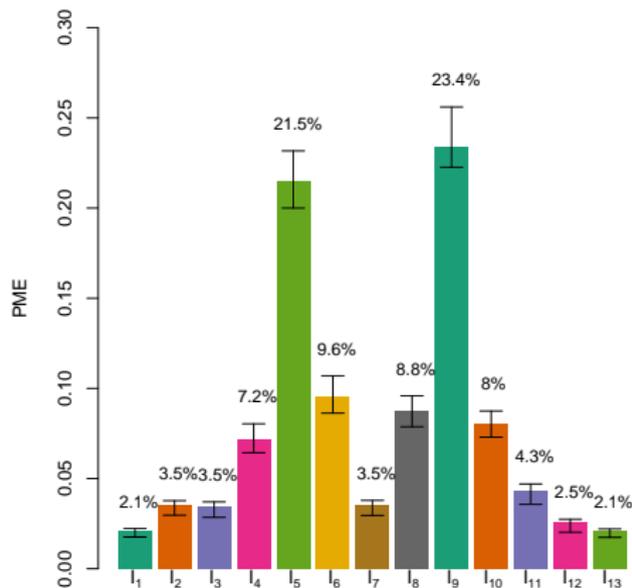
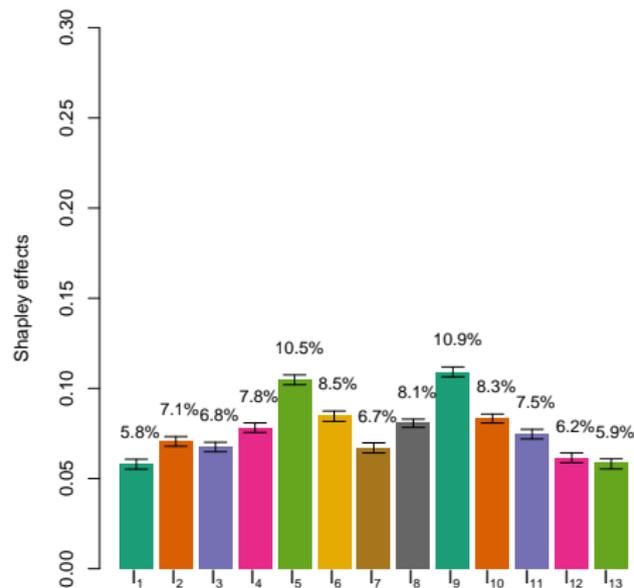
We only have access to an i.i.d. input-output sample ($n = 1000$).

The indices are computed using the nearest-neighbors approach (6 neighbors).



Application to an optical filter model

Feature selection



Remark : Due to the estimation bias, PME cannot be pushed to zero (as would be physically expected)

Application to an optical filter model

Feature selection

Scenario : We want to build a surrogate model (Gaussian process*) of this numerical model.

Using the whole dataset : $Q^2 = 99.48\%$.

Feature selection :

First threshold : 2.5% importance.

- ▶ **Shapley effects :** No features removed.
- ▶ **PME :** l_1 and l_3 are removed, $Q^2 = 99.14\%$.

Second threshold : 5% importance.

- ▶ **Shapley effects :** No features removed.
- ▶ **PME :** 7 inputs are removed, $Q^2 = 98.79\%$.

Conclusion : Useless inputs have been correctly identified (the strong reduction dimension only reduces to a negligible loss in Q^2)

* 5/2 Matérn covariance kernel, constant trend.

Plan

1. The linear case

- Uncertainty quantification context in neutronic

- Basics of multivariate linear regression

- Multicolinearity illustration with a two-input regression model

- Variance-based Importance Measures : LMG and Johnson

- Sensitivity analysis in a neutronic study

2. The non-linear case

- Cooperative game theory

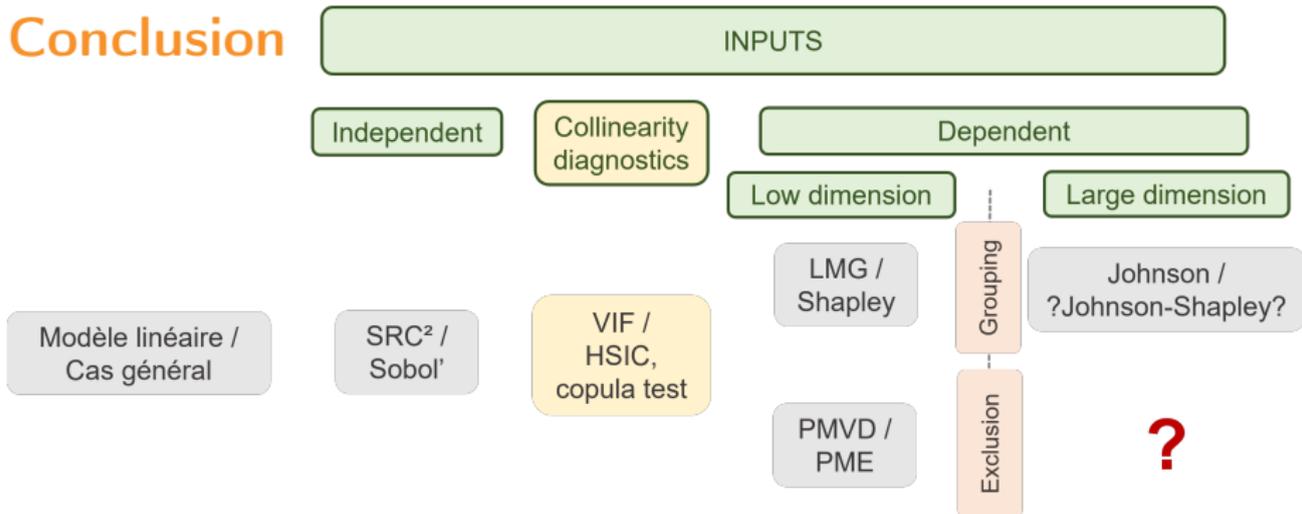
- Shapley effects

- Proportional marginal effects

- Application to an optical filter model

3. Conclusion

Conclusion



Cooperative game theory for GSA of non-linear models :

- ▶ **Random order allocations** : reduce the allocation problem to a choice of p .
- ▶ **Shapley** : Equalize importance & Shapley's joke/correlation distortion [VW23]
- PME** : Discriminative power & exogenous input detection

Software : R package *sensitivity* : LMG/Johnson/PMVD, Shapley/PME.

Perspectives :

- ▶ SHAFF-type estimation for solving the estimation cost issues
- ▶ High-dimensional linear model : Johnson-type approximation for PMVD
- ▶ Extension of Johnson indices to **nonlinear models** [IC23]

Merci de votre attention !

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