

Shapley Effects for Sensitivity Analysis with Dependent Inputs

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Introduction

In this talk, we consider

$$f: \begin{cases} \mathcal{X} = \mathcal{X}_1 \times \dots \times \mathcal{X}_d & \rightarrow \mathcal{Y} \\ \mathbf{x} = (x_1, \dots, x_d) & \mapsto y = f(\mathbf{x}) \end{cases}$$

with

- f : mathematical or numerical model,
- \mathbf{x} : uncertain input parameters,
- y : output.

We model the uncertainty on the input parameters by a probability distribution P on \mathcal{X} and get

$$Y = f(X_1, \dots, X_d)$$

with the vector $\mathbf{X} = (X_1, \dots, X_d)$ distributed as P .



Introduction

Independent framework: $P(d\mathbf{x}) = P_1(dx_1) \dots P_d(dx_d)$

Why is the independent framework not always the right one?

Let us consider the following example: an agro-climatic model for the water status management of vineyard. Joint study with INRA and iTK (Montpellier, FRANCE).



Introduction

Project objective: control of grape/wine quality. SA as decision support.

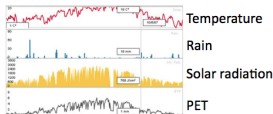
INPUTS

- Vine-plot

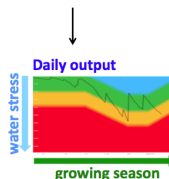
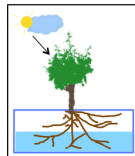
→ 22 scalar parameters: soil texture, rooting depth, vegetation size, row orientation, ...

- Weather data during the growing season

→ 4 correlated (daily) functional inputs



Water budget



Introduction

The soil texture was initially described by 3 scalar parameters: the percentages of argil, sand and silt.

These parameters are not independent as

$$\% \text{ argil} + \% \text{ sand} + \% \text{ silt} = 100\% .$$

In the study, this set of parameters has been replaced by a unique parameter **aSoil** describing the influence of the soil texture on its evaporation capacity.

Daily precipitations, solar radiation, mean air temperature and potential evapotranspiration are temporal correlated inputs.

We chose to use kind of **scenario approach**: it consists in grouping the 4 temporal inputs into a single input factor, defining a **weather scenario**.



Variance based sensitivity analysis, independent framework

Independent framework: $P(d\mathbf{x}) = P_1(dx_1) \dots P_d(dx_d)$

For sake of clarity, we consider

$$f: \begin{cases} \mathbb{R}^d & \rightarrow \mathbb{R} \\ \mathbf{x} = (x_1, \dots, x_d) & \mapsto y = f(\mathbf{x}) \end{cases}$$

Does the output Y vary more or less when fixing one of its input parameters?

$V[Y|X_i = x_i]$, how to choose x_i ?



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$V[Y|X_i = x_i]$, how to choose x_i ? $\rightarrow E[V(Y|X_i)]$



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$V[Y|X_i = x_i]$, how to choose x_i ? $\rightarrow E[V(Y|X_i)]$

The more this quantity is small, the more fixing X_i reduces the variance of Y : the input X_i is influential.



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Does the output Y vary more or less when fixing one of its **input parameters**?

$V[Y|X_i = x_i]$, how to choose x_i ? $\rightarrow E[V(Y|X_i)]$

The more this quantity is small, the more fixing X_i reduces the variance of Y : the input X_i is influential.

$$\xrightarrow[i=1, \dots, d]{\text{1st order Sobol' indices}} 0 \leq S_i = \frac{V[E(Y|X_i)]}{V[Y]} = 1 - \frac{E[V(Y|X_i)]}{V[Y]} \leq 1$$



Variance based sensitivity analysis, independent framework

For sake of clarity, we consider $f : [0, 1]^d \rightarrow \mathbb{R}$. Then, if $\int_{[0,1]^d} f^2(\mathbf{x})d(\mathbf{x}) < +\infty$, f admits a unique decomposition

$$f_0 + \sum_{i=1}^d f_i(x_i) + \sum_{1 \leq i < j \leq d} f_{i,j}(x_i, x_j) + \dots + f_{1,\dots,d}(x_1, \dots, x_d)$$

under the constraints

- ▶ f_0 constant,
- ▶ $\forall 1 \leq s \leq d, \forall 1 \leq i_1 < \dots < i_s \leq d, \forall 1 \leq p \leq s$

$$\int_0^1 f_{i_1, \dots, i_s}(x_{i_1}, \dots, x_{i_s}) dx_{i_p} = 0$$



Variance based sensitivity analysis, independent framework

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$$\int_0^1 f_{i_1, \dots, i_s}(x_{i_1}, \dots, x_{i_s}) dx_{i_p} = 0$$

Consequences:

- * $f_0 = \int_{[0,1]^d} f(\mathbf{x})d\mathbf{x}$,
- * $\forall \mathbf{u} \subset \{1, \dots, d\}, \int_{[0,1]^d} f_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}})d\mathbf{x} = 0$,
- * $\forall \mathbf{u} \neq \mathbf{v} \subset \{1, \dots, d\}, \int_{[0,1]^d} f_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}})f_{\mathbf{v}}(\mathbf{x}_{\mathbf{v}})d\mathbf{x} = 0$.



Variance based sensitivity analysis, independent framework

We deduce from the constraints

- ▶ $f_i(x_i) = \int_{[0,1]^{d-1}} f(x) \prod_{p \neq i} dx_p - f_0$
- ▶ $i \neq j$
 $f_{i,j}(x_i, x_j) = \int_{[0,1]^{d-2}} f(x) \prod_{p \neq i,j} dx_p - f_0 - f_i(x_i) - f_j(x_j)$
- ▶ ...



Variance based sensitivity analysis, independent framework

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- ▶ ...

Or equivalently, for $\mathbf{X} \sim \mathcal{U}([0, 1]^d)$,

$$Y = f(\mathbf{X}) = f_0 + \sum_{i=1}^d f_i(X_i) + \sum_{1 \leq i < j \leq d} f_{i,j}(X_i, X_j) + \dots + f_{1,\dots,d}(X_1, \dots, X_d)$$

with

- ▶ $f_i(x_i) = E[Y|X_i = x_i] - E[Y]$,
- ▶ $i \neq j$, $f_{i,j}(x_i, x_j) =$
 $E[Y|X_i, X_j = x_i, x_j] - E[Y|X_i = x_i] - E[Y|X_j = x_j] + E[Y]$,
- ▶ ...



Variance based sensitivity analysis, independent framework

Variance decomposition:

$$V[Y] = \sum_{i=1}^d V[f_i(X_i)] + \dots + V[f_{1,\dots,d}(X_1, \dots, X_d)]$$

Sobol' indices:

$$\forall i = 1, \dots, d \quad S_i = \frac{V[f_i(X_i)]}{V[Y]} = \frac{V[\mathbb{E}[Y|X_i]]}{V[Y]}$$

$$\forall i \neq j \quad S_{i,j} = \frac{V[f_{i,j}(X_i, X_j)]}{V[Y]} = \frac{V[\mathbb{E}[Y|X_i, X_j]] - V[\mathbb{E}[Y|X_i]] - V[\mathbb{E}[Y|X_j]]}{V[Y]}$$

...

We have

$$1 = \sum_{i=1}^d S_i + \sum_{i \neq j} S_{i,j} + \dots + S_{1,\dots,d}$$

Factors Prioritization (FP): which factor should one try to determine first in order to have the largest expected reduction in the variance of the model output? \rightarrow first order Sobol' indices do the job.



Variance based sensitivity analysis, independent framework

Total Sobol' indices:

$$i = 1, \dots, d \quad S_i^{\text{tot}} = \sum_{\mathbf{u} \subset \{1, \dots, d\}, \mathbf{u} \cap \{i\} \neq \emptyset} S_{\mathbf{u}}$$

Factors Fixing (FF): which input factors can be fixed, anywhere in their range of variation, without sensibly affecting a specific output of interest? \rightarrow total Sobol' indices do the job.

We have:

$$S_i^{\text{tot}} = \frac{E[V[Y|\mathbf{X}_{-i}]]}{V[Y]} = 1 - \frac{V[E[Y|\mathbf{X}_{-i}]]}{V[Y]}$$

with $\mathbf{X}_{-i} = (X_1, \dots, X_{i-1}, X_{i+1}, \dots, X_d)$.



Variance based sensitivity analysis, general framework

We consider

$$f: \begin{cases} \mathbb{R}^d & \rightarrow \mathbb{R} \\ \mathbf{x} = (x_1, \dots, x_d) & \mapsto y = f(\mathbf{x}) \end{cases}$$

$P(d\mathbf{x})$ not necessarily equal to $P_1(dx_1) \dots P_d(dx_d)$.

Let, $\forall i = 1, \dots, d$, $F_{X_i}(\cdot) = P(X_i \leq \cdot)$ and

$$\forall \mathbf{x} = (x_1, \dots, x_d) \in \mathbb{R}^d, F_{\mathbf{X}}(\mathbf{x}) = P(X_1 \leq x_1, \dots, X_d \leq x_d).$$

Sklar's Theorem $F_{\mathbf{X}}(\mathbf{x}) = C(F_{X_1}(x_1), \dots, F_{X_d}(x_d))$.

If the F_{X_i} are continuous, then the copula C is unique.



Variance based sensitivity analysis, general framework

We can still define Sobol' indices as:

$$\forall i = 1, \dots, d \quad S_i = \frac{V[\mathbb{E}[Y|X_i]]}{V[Y]}$$

$$\forall i \neq j \quad S_{i,j} = \frac{V[\mathbb{E}[Y|X_i, X_j]] - V[\mathbb{E}[Y|X_i]] - V[\mathbb{E}[Y|X_j]]}{V[Y]}$$

...

We do not have anymore $1 = \sum_{i=1}^d S_i + \sum_{i \neq j} S_{i,j} + \dots + S_{1, \dots, d}$

We do not have anymore

$$\sum_{\mathbf{u} \subset \{1, \dots, d\}, \mathbf{u} \cap \{i\} \neq \emptyset} S_{\mathbf{u}} = \frac{E[V[Y|\mathbf{X}_{-i}]]}{V[Y]}$$

FP and FF are not easy tasks anymore.



An alternative, the Shapley effects

Shapley paradigm

Let team $\mathbf{u} \subseteq \{1, 2, \dots, d\}$ create value $\text{val}(\mathbf{u})$. Let $\mathbf{u} \mapsto \text{val}(\mathbf{u})$, with $\text{val}(\emptyset) = 0$, be the **characteristic function** of the game. The total value of the game is $\text{val}(\{1, 2, \dots, d\})$. We attribute ϕ_i of this to $i \in \{1, 2, \dots, d\}$.

Shapley axioms

- ▶ **Efficiency** $\sum_{i=1}^d \phi_i = \text{val}(\{1, \dots, d\})$.
- ▶ **Dummy** $[\forall \mathbf{u}, \text{val}(\mathbf{u} \cup \{i\}) = \text{val}(\mathbf{u})] \Rightarrow \phi_i = 0$.
- ▶ **Symmetry**
 $[\forall \mathbf{u}$ such that $\mathbf{u} \cap \{i, j\} = \emptyset, \text{val}(\mathbf{u} \cup \{i\}) = \text{val}(\mathbf{u} \cup \{j\})]$
 $\Rightarrow \phi_i = \phi_j$.
- ▶ **Additivity** If games with characteristic functions val, val' correspond to ϕ_i, ϕ'_i , then the game with characteristic function $\text{val} + \text{val}'$ corresponds to $\phi_i + \phi'_i$.

[Shapley, 1953] shows there is a unique solution to these axioms.



An alternative, the Shapley effects

The solution is:

$$\phi_i = \frac{1}{d} \sum_{\mathbf{u} \subseteq -\{i\}} \binom{d-1}{|\mathbf{u}|}^{-1} (\text{val}(\mathbf{u} + i) - \text{val}(\mathbf{u}))$$

Let variables x_1, x_2, \dots, x_d be team members trying to explain f . The value of any subset \mathbf{u} is how much can be explained by $\mathbf{x}_{\mathbf{u}}$.

The **Shapley effects** [Owen, 2014] are the ϕ_i s corresponding to the value function $\mathbf{u} \mapsto \sum_{\mathbf{v} \subseteq \mathbf{u}} S_{\mathbf{v}} = \frac{V[E[Y|\mathbf{X}_{\mathbf{u}}]]}{V[Y]}$.

If we define the value function as $\mathbf{u} \mapsto \frac{E[V[Y|\mathbf{X}_{\mathbf{u}}]]}{V[Y]}$ instead of $\mathbf{u} \mapsto \frac{V[E[Y|\mathbf{X}_{\mathbf{u}}]]}{V[Y]}$, we also get the **Shapley effects**.



An alternative, the Shapley effects

Independent framework: $\forall i = 1, \dots, d, \phi_i = \sum_{u: i \in u} \frac{1}{|u|} S_u$

We also have: $\forall i = 1, \dots, d, 0 \leq S_i \leq \phi_i \leq S_i^{\text{tot}} \leq 1$ and $\sum_{i=1}^d \phi_i = 1$.



An alternative, the Shapley effects

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We also have: $\forall i = 1, \dots, d, 0 \leq S_i \leq \phi_i \leq S_i^{\text{tot}} \leq 1$ and $\sum_{i=1}^d \phi_i = 1$.

Dependent framework:

In this framework, it is usual to define first order and total Sobol' indices as

$$S_i = \frac{V[E[Y|\mathbf{X}_i]]}{V[Y]}$$

$$S_i^{\text{tot}} = \frac{E[V[Y|\mathbf{X}_{-i}]]}{V[Y]}$$

We still have $0 \leq \phi_i \leq 1$ and $\sum_{i=1}^d \phi_i = 1$

We do not necessarily have $S_i \leq \phi_i \leq S_i^{\text{tot}}$



Some properties

- ▶ **Property 1** Let $Y = f(\mathbf{X}) = f(X_1, \dots, X_d)$, with $X_1 = h(X_2)$ and $X_2 = h^{-1}(X_1)$ with probability one. Then $\phi_1 = \phi_2$.

- ▶ **Property 2** Let $Y = f(\mathbf{X})$ and for $i = 1, \dots, d$, $X_i = \tau_i^{-1}(Z_i)$. We define $g(\mathbf{Z}) = f(\tau_1^{-1}(Z_1), \dots, \tau_d^{-1}(Z_d))$.
Let ϕ'_i be the Shapley importance of Z_i as a predictor of $Y' = g(\mathbf{Z})$. Then, for all $i = 1, \dots, d$, $\phi'_i = \phi_i$.



A few analytical examples

[Owen and Prieur, 2017, Iooss and Prieur, 2017]

Gaussian framework, affine model, $d = 2$

We consider $\mathbf{X} \sim \mathcal{N}_2(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ and $Y = \beta_0 + \boldsymbol{\beta}^T \mathbf{X}$, 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 $\sigma^2 = V[Y] = \beta_1^2\sigma_1^2 + 2\rho\beta_1\beta_2\sigma_1\sigma_2 + \beta_2^2\sigma_2^2$ and

$$\sigma^2 Sh_1 = \beta_1^2\sigma_1^2\left(1 - \frac{\rho^2}{2}\right) + \rho\beta_1\beta_2\sigma_1\sigma_2 + \beta_2^2\sigma_2^2\frac{\rho^2}{2},$$

$$\sigma^2 Sh_2 = \beta_2^2\sigma_2^2\left(1 - \frac{\rho^2}{2}\right) + \rho\beta_1\beta_2\sigma_1\sigma_2 + \beta_1^2\sigma_1^2\frac{\rho^2}{2}.$$



A few analytical examples

Farlie-Gumbel-Morgenstern copula, uniform marginals, affine model, $d = 2$

We consider $Y = \beta_0 + \beta^T \mathbf{X}$, with

- ▶ marginal distributions $X_i \sim \mathcal{U}([0, 1]^2)$ for $i = 1, 2$,
- ▶ joint probability density function
 $c_\theta(x_1, x_2) = 1 + \theta(1 - 2x_1)(1 - 2x_2)$, $-1 \leq \theta \leq 1$.

We then have

- ▶ $\sigma_i^2 = V[X_i] = 1/12$,
- ▶ $\rho = \text{cor}(X_1, X_2) = \frac{\theta}{3}$.

We also have

- ▶ $\sigma^2 = V[Y] = \frac{\beta_1^2 + \beta_2^2}{12} + \beta_1\beta_2\frac{\theta}{18} = \beta_1^2\sigma_1^2 + 2\rho\beta_1\beta_2\sigma_1\sigma_2 + \beta_2^2\sigma_2^2$.



A few analytical examples

We get once more

$$\sigma^2 Sh_1 = \beta_1^2 \sigma_1^2 \left(1 - \frac{\rho^2}{2}\right) + \rho \beta_1 \beta_2 \sigma_1 \sigma_2 + \beta_2^2 \sigma_2^2 \frac{\rho^2}{2},$$

$$\sigma^2 Sh_2 = \beta_2^2 \sigma_2^2 \left(1 - \frac{\rho^2}{2}\right) + \rho \beta_1 \beta_2 \sigma_1 \sigma_2 + \beta_1^2 \sigma_1^2 \frac{\rho^2}{2}.$$

That is

$$Sh_1 = \frac{1}{2} \left(1 + \left(1 - \frac{\theta^2}{9} \right) \frac{\beta_1^2 - \beta_2^2}{12\sigma^2} \right),$$

$$Sh_2 = \frac{1}{2} \left(1 + \left(1 - \frac{\theta^2}{9} \right) \frac{\beta_2^2 - \beta_1^2}{12\sigma^2} \right),$$

$$\text{with } \sigma^2 = \frac{\beta_1^2 + \beta_2^2}{12} + \beta_1 \beta_2 \frac{\theta}{18}.$$



A few analytical examples

Gaussian framework, exponential model, $d = 2$

Let $f(\mathbf{X}) = \exp(\mathbf{X}^T \boldsymbol{\beta})$ for $\mathbf{X}, \boldsymbol{\beta} \in \mathbb{R}^2$ and $\mathbf{X} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$, for $\boldsymbol{\Sigma} = \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}$. Then

$$Sh_1 = \frac{1}{2} \left(1 + \frac{e^{(\beta_1 + \beta_2 \rho)^2} - e^{(\beta_2 + \beta_1 \rho)^2}}{e^{\beta_1^2 + \beta_2^2 + 2\rho\beta_1\beta_2} - 1} \right)$$

$$Sh_2 = \frac{1}{2} \left(1 + \frac{e^{(\beta_2 + \beta_1 \rho)^2} - e^{(\beta_1 + \beta_2 \rho)^2}}{e^{\beta_1^2 + \beta_2^2 + 2\rho\beta_1\beta_2} - 1} \right)$$

From [Property 2](#), we can extend the result to unnormalized X_1 and X_2 .



A few analytical examples

General bivariate framework

We consider $Y = f(\mathbf{X})$ with finite variance $\sigma^2 > 0$. We have

$$Sh_1 = \frac{1}{2} \left(1 + \frac{V[E[Y|X_1]] - V[E[Y|X_2]]}{\sigma^2} \right),$$

$$Sh_2 = \frac{1}{2} \left(1 + \frac{V[E[Y|X_2]] - V[E[Y|X_1]]}{\sigma^2} \right).$$



A few analytical examples

Gaussian framework, model with a second order interaction, $d = 3$

We consider $Y = X_1 + X_2X_3$ with $\mathbf{X} \sim \mathcal{N}_2(\mathbf{0}, \Sigma)$ and

$$\Sigma = \begin{pmatrix} \sigma_1^2 & 0 & \rho\sigma_1\sigma_3 \\ 0 & \sigma_2^2 & 0 \\ \rho\sigma_1\sigma_3 & 0 & \sigma_3^2 \end{pmatrix}, \rho \in [-1, 1], \sigma_i > 0.$$

We have $\sigma^2 = V[Y] = \sigma_1^2 + \sigma_2^2\sigma_3^2$ and

- ▶ $\sigma^2 Sh_1 = \sigma_1^2(1 - \frac{\rho^2}{2}) + \frac{\sigma_2^2\sigma_3^2}{6}\rho^2$
- ▶ $\sigma^2 Sh_2 = \frac{\sigma_2^2\sigma_3^2}{6}(3 + \rho^2)$
- ▶ $\sigma^2 Sh_3 = \frac{\rho^2\sigma_1^2}{2} + \frac{\sigma_2^2\sigma_3^2}{6}(3 - 2\rho^2)$



A few analytical examples

General model with a block-additive structure, $d = 3$

We consider $Y = g(X_1, X_2) + h(X_3)$. We assume that all the three inputs have a finite variance and that X_3 is independent from (X_1, X_2) .

We then have

- ▶ $S_3 = Sh_3 = S_3^{\text{tot}}$
- ▶ for $i = 1, 2$,

$$[S_i \leq Sh_i] \Leftrightarrow [Sh_i \leq S_i^{\text{tot}}]$$

$$\Leftrightarrow \left[\frac{V[E[Y|X_1]] + V[E[Y|X_2]]}{2} \leq \frac{V[E[Y|X_1, X_2]]}{2} \right]$$



What about algorithms?

Algorithms to compute Shapley effects [Castro et al., 2009] are based on the value function $\mathbf{u} \mapsto \frac{E[V[Y|\mathbf{X}_u]]}{V[Y]}$. Note that

$$Sh_i = \frac{1}{d!} \sum_{\pi \in \Pi(\{1, \dots, d\})} (\text{val}(P_i(\pi) \cup \{i\})) - \text{val}(P_i(\pi)))$$

with $\Pi(\{1, \dots, d\})$ the set of all possible permutations of the inputs and for a permutation $\pi \in \Pi(\{1, \dots, d\})$, the set $P_i(\pi)$ is defined as the inputs that precede input i in π .

Exact permutation algo. (moderate d) all possible permutations are covered.

Random permutation algo. ($d \gg 1$) it randomly sample permutations of the inputs.



What about algorithms?

In [Song et al., 2016], $\text{val}(\mathbf{u}) \rightarrow \widehat{\text{val}}(\mathbf{u})$.

For each iteration of the loop on the inputs' permutations, a conditional variance expectation must be computed.

The cost C of these algorithms is the following:

$$C = N_v + m(d - 1)N_0N_i$$

with N_v the sample size for the variance computation, N_0 the outer loop size for the expectation, N_i the inner loop size for the conditional variance and m the number of permutations according to the selected method.

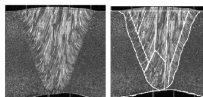
Bootstrap confidence intervals can be computed. A costly model can be replaced by a metamodel. [Iooss and Prieur, 2017, Benoumechiara and Elie-Dit-Cosaque, 2018]



An industrial application

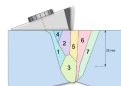
Industrial problem: **ultrasonic non-destructive control of a weld containing manufacturing defect**

The heterogeneous and anisotropic weld's structure is represented by a simplified model consisting of a partition of 7 equivalent homogeneous regions with a specific grain orientation.



Metallographic picture (left)

Description of the weld in 7 homogeneous domains (right)



Inspection configuration

Input parameters: 11 scalar inputs (4 elastic coefficients and 7 orientations).

Scalar output: the amplitude of the defect echoes resulting from an ultrasonic inspection.

An industrial application

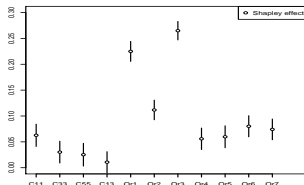
Probabilistic model: all the inputs are modeled by Gaussian distributions, there are dependences between the orientations.

$$(O_{r_1}, \dots, O_{r_7})^T \sim \mathcal{N}_7(\mu, \Sigma)$$

[Rupin et al., 2014, Moysan et al., 2003]

Shapley effects for the ultrasonic non-destructive control application. The vertical bars represent the **95%-confidence intervals** of each effect.

Algorithm's parameters: $m = 10^4$, $N_i = 3$, $N_0 = 1$, $N_v = 10^4$, total cost $C = 3 \times 10^5$ metamodel evaluations.



Conclusion, perspectives

Conclusion: Shapley effects present an alternative to allocate parts of variance in the dependent framework. There exist algorithms to estimate these indices.

Perspectives

- ▶ Can we propose goal-oriented Shapley effects?
- ▶ What are the theoretical finite sample properties of both algorithms?
- ▶ How can Shapley effects be related to gradient-based measures of sensitivity?
- ▶ ...



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