Introduction to Global Sensibility Analysis

Model exploration for approximation of complex, high-dimensional problems

MSIAM
Overview

\[ X_1 \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot X_d \]

\[ Y = \mathcal{M}(X_1, \ldots, X_d) \]

Experimental design:
planification, sampling

Sensitivity analysis:
sensitivity indices’ inference
Introduction

Background:

\[ M : \left\{ \begin{array}{c}
\mathbb{R}^d \rightarrow \mathbb{R} \\
\mathbf{x} \mapsto y = M(x_1, \ldots, x_d)
\end{array} \right. \]

Goal: find how model outputs vary with inputs changes.

Different strategies:
- Qualitative analysis: non-linear behaviors? possible interactions?
  ex. : screening .
- Quantitative analysis: factorial hierarchisation, statistical tests
  \( H_0 \) "negligible input"
  ex. : sensitivity Sobol’ indices

Sensitivity analysis may help identifying inappropriate models.
Introduction

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\[ \mathcal{M} : \begin{cases} \mathbb{R}^d & \rightarrow & \mathbb{R} \\ x & \mapsto & y = \mathcal{M}(x_1, \ldots, x_d) \end{cases} \]

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Sensitivity analysis may help identifying inappropriate models.
Various approaches for quantitative sensitivity:

Local approaches:

\[ M(x) \approx M(x^0) + \sum_{i=1}^{d} \left( \frac{\partial M}{\partial x_i} \right)_{x^0} (x_i - x_i^0) \] (Taylor approximation).

First order sensitivity index for input i:

\[ \left( \frac{\partial M}{\partial x_i} \right)_{x^0} \]

Pros: Low computational cost even for large d

Cons: local approaches, not well-suited for highly nonlinear models
**Global approaches:**

From expert knowledge or observations, we attribute a probability law to the **inputs** vector.

ex.: If independent inputs, then only margins are needed.

*Figure:* law (left) unimodal , (right) bimodal
We vary inputs w.r.t. their probability distribution.

**Figure:** Local versus Global \((G := \mathcal{M})\)
We vary input w.r.t. their probability law

"Globalized" local approaches: e.g. (1) $\mathbb{E}_X \left[ \left. \frac{\partial M}{\partial x_i} \right|_X \right]$, ou (2) $\mathbb{E}_X \left[ \left( \left. \frac{\partial M}{\partial x_i} \right|_X \right)^2 \right]$.  

Avantages: particularly interesting if adjoint available  

Cons:  
(1) does not discriminate enc
(2) is known as Derivative-based Global Sensitivity Measures, see Sobol’ & Gresham (1995), Sobol’ & Kucherenko (2009).

This index is more adapted for screening than for hierarchization (e.g. Lamboni et al., 2013).

This lecture targets global approaches that allow to efficiently rank input factors.
Sensitivity measures, definition, estimation

I- Measures based on linear regressions

II- Functional variance analysis

III- Sobol indices inference
  - Monte Carlo techniques,
  - Spectral techniques

IV- Distributional indices

V- Further topics
I- Measures based on linear regressions

\[ Y = \mathcal{M}(X_1, \ldots, X_d) \]

- Linear correlation

\[ \rho_i = \rho(X_i, Y) = \frac{\text{Cov}(X_i, Y)}{\sqrt{\text{Var}(X_i)} \sqrt{\text{Var}(Y)}} \]

- Partial correlation

\[ PCC_i = PCC(X_i, Y) = \rho \left( Y - \hat{Y}^{-(i)}, X_i - \hat{X}_i^{-(i)} \right) \]

Remarks:
- if \( Y = \sum_{i=1}^{d} \beta_i X_i \), and if inputs are independent, \( \sum_{i=1}^{d} \rho^2 (X_i, Y) = 1 \);
- if inputs are correlated, the PCC are more suitable.
I- Measures based on linear regressions

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\begin{itemize}
  \item **Linear correlation**
  \[ \rho_i = \rho(X_i, Y) = \frac{\text{Cov}(X_i, Y)}{\sqrt{\text{Var}(X_i)}} \sqrt{\frac{\text{Var}(Y)}} \]
  \item **Partial correlation**
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\end{itemize}

**Remarks:**
- if \( Y = \sum_{i=1}^{d} \beta_i X_i \), and if inputs are independent, \( \sum_{i=1}^{d} \rho^2(X_i, Y) = 1; \)
- if inputs are correlated, the PCC are more suitable.
I- Measures based on linear regressions

Assessment of linear model?

**Toy example**: \( Y = 2X_1 + 3X_2^2 + 5, X_i \sim \mathcal{U}([0, 1]), i = 1, 2, X_1 \perp \perp X_2. \)

We can approximate this model by a linear model:
\[
Y = \beta_1 X_1 + \beta_2 X_2 + \beta_0 + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2).
\]

Learning sample : \( y_k = \mathcal{M}(x_{1,k}, \ldots, x_{d,k}), k = 1, \ldots, 100 \)
\[
\Rightarrow \quad \hat{y} = \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_0 = 2.06x_1 + 3.15x_2 + 4.34.
\]

Which measure to assess the fit of this model?
I- Measures based on linear regressions

★ Coefficient $R^2$

$$R^2 = \frac{SCE}{SCT} = \frac{\sum_{k=1}^{m} (\hat{y}_k - \bar{y})^2}{\sum_{k=1}^{m} (y_k - \bar{y})^2},$$

$$\hat{y}_k = \sum_{i=1}^{d} \hat{\beta}_i x_{i,k}, \quad \bar{y} = \frac{1}{m} \sum_{k=1}^{m} y_k.$$

★ Prediction error, e.g. cross-validation:

$$\frac{1}{m} \sum_{k=1}^{m} \left( \frac{\hat{y}_{k}^{\text{-(k)}} - y_k}{\bar{y}} \right)^2,$$

$$\hat{y}_{k}^{\text{-(k)}} = \sum_{i=1}^{d} \hat{\beta}_i^{\text{-(k)}} x_{i,k}, \quad \hat{\beta}_i^{\text{-(k)}} \text{ inferred from}$$

$$(y_j, x_j), \quad j = 1, \ldots, k-1, k+1, \ldots, m.$$
I- Measures based on linear regressions

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★ Prediction error, e.g. cross-validation:

$$1 \cdot \frac{\sum_{k=1}^{m} (\hat{y}_k^{-(k)} - y_k)^2}{m \cdot \frac{1}{m} \sum_{k=1}^{m} (y_k - \bar{y})^2},$$

$$\hat{y}_k^{-(k)} = \sum_{i=1}^{d} \hat{\beta}_i^{-(k)} x_{i,k}, \; \hat{\beta}_i^{-(k)} \text{ inferred from}$$

$$(y_j, x_j), \; j = 1, \ldots, k-1, k+1, \ldots, m.$$
If the relationship input/output is no more linear but simply monotonic, we work with ranks.

\[ y_k, x_{i,k}, \ k = 1, \ldots, m, \ i = 1, \ldots, d \]

\[ r_{i,k} \text{ rank of } x_{i,k} \text{ in } (x_{i,1}, \ldots, x_{i,m}), \ r_k \text{ rank of } y_k \text{ in } (y_1, \ldots, y_m) \]

- \[ \rho_i^S = \frac{\sum_{k=1}^{m} (r_{i,k} - \bar{r}_i)(r_k - \bar{r})}{\sqrt{\sum_{k=1}^{m} (r_{i,k} - \bar{r}_i)^2} \sqrt{\sum_{k=1}^{m} (r_k - \bar{r})^2}} \]

- idem for pcc_i
II- Functional variance analysis

ANOVA basics

$Y$ quantity of interest, $X_1$ (resp. $X_2$) qualitative factor with $I$ (resp. $J$) levels.

**model**: $Y_{ij} = \mu + \alpha_i + \beta_j + \gamma_{ij} + \varepsilon_{ij}$, $\varepsilon_{ij}$ i.i.d. $\mathcal{N}(0, \sigma^2)$.

**Identifiability constraints**: $\sum_{i=1}^{I} \alpha_i = 0$, $\sum_{j=1}^{J} \beta_j = 0$, $\sum_{i=1}^{I} \gamma_{ij} = 0$, $\sum_{j=1}^{J} \gamma_{ij} = 0$.

Effect inference:

Complete and balanced design with $r > 1$ replica $\rightarrow y_{ijk}$, $k = 1, \ldots, r$

$$
\hat{\mu} = \bar{y}, \quad \hat{\alpha}_i = \bar{y}_{i..} - \bar{y}, \quad \hat{\beta}_j = \bar{y}_{.j} - \bar{y}, \quad \hat{\gamma}_{ij} = \bar{y}_{ij} - \bar{y}_{i..} - \bar{y}_{.j} + \bar{y},
$$

with usual notation

$$
\bar{y} = \frac{1}{lJr} \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{r} y_{ijk},
$$

$$
\bar{y}_{i..} = \frac{1}{Jr} \sum_{j=1}^{J} \sum_{k=1}^{r} y_{ijk}, \quad \bar{y}_{.j} = \frac{1}{lr} \sum_{i=1}^{I} \sum_{k=1}^{r} y_{ijk}, \quad \bar{y}_{ij} = \frac{1}{r} \sum_{k=1}^{r} y_{ijk}.
$$
II- Functional variance analysis

In the previous model, we define:

- the forecasts $\hat{y}_{ijk} = \bar{y}_{ij}$,
- the residuals $\hat{e}_{ijk} = y_{ijk} - \hat{y}_{ijk} = y_{ijk} - \bar{y}_{ij}$.

Variance decomposition:

\[
SCT = SCM + SCR
\]

where

\[
SCT = \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{r} (y_{..} - \bar{y})^2, \quad SCM = \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{r} (y_{.j} - \bar{y})^2, \quad SCX_1 = \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{r} (y_{ij} - \bar{y}_{ij} - \bar{y}_{..} + \bar{y})^2, \quad SCX_2 = \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{r} (\hat{y}_{ijk} - y_{ijk})^2 = \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{r} (\bar{y}_{ij} - y_{ijk})^2.
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- the forecasts $\hat{y}_{ijk} = \bar{y}_{ij}.$
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Variance decomposition:

$$SCM = SCX_1 + SCX_2 + SCX_1X_2 \quad \text{with}$$

$$SCX_1 = \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{r} (\bar{y}_{i..} - \bar{y})^2,$$

$$SCX_2 = \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{r} (\bar{y}_{.j.} - \bar{y})^2,$$

$$SCX_1X_2 = \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{r} (\bar{y}_{i..} - \bar{y}_{i.} - \bar{y}_{.j.} + \bar{y})^2,$$

$$SCR = \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{r} (\hat{y}_{ijk} - y_{ijk})^2 = \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{r} (\bar{y}_{ij} - y_{ijk})^2.$$
Hypothesis testing: many possible tests
ex. : $H_0$ : additive model versus $H_1$ : complete model

Test statistic :

$$T = \frac{SCX_1 X_2 / (IJ - I - J + 1)}{SCR / (IJr - IJ)} \sim F(IJ - I - J + 1, IJr - IJ).$$

ANOVA assumptions :

- the factors only impact the mean of the quantitative variable $Y$, but not its variance;
- All other variations are Gaussian and independent
II- Functional variance analysis

Functional framework: (Antoniadis, 1984)

\[ Y(s, t) = M(s, t) + \varepsilon(s, t), \quad (s, t) \in S \times T \]

with

- \( \varepsilon(s, t) \) zero-mean Gaussian process with covariance \( K(s, t) \),
- \( S \) and \( T \) two metric compacts spaces

More general setup: (Hoeffding, 1948; Sobol', 1993)

\[ Y = M(X_1, \ldots, X_d), \quad (X_1, \ldots, X_d) \sim P_{X_1,\ldots,X_d}. \]

In the following, we assume:

i) the \( X_i \) are independent;

ii) \( \forall i = 1, \ldots, d, \ X_i \sim U([0, 1]). \)
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Assumption ii) is not restrictif: with the inverse technique, $Y = \mathcal{M}(X_1, \ldots, X_d)$ can be written as

$$Y = \mathcal{M}(F_{X_1}^{-1}(U_1), \ldots, F_{X_d}^{-1}(U_d)) = \widetilde{\mathcal{M}}(U_1, \ldots, U_d)$$

with $U_i, i = 1, \ldots, d$ independent and for all $i$, $U_i \sim \mathcal{U}([0, 1])$, $F_{X_i}^{-1}$ inverse of the cumulative distribution function of $X_i$.

The complex case of correlated inputs will be mentioned at the end of this lecture.
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Towards Sobol sensitivity indices

Is the output $Y$ more or less variable when input are fixed?

$\text{Var}(Y|X_i = x_i)$, how to choose $x_i$? $\Rightarrow E[\text{Var}(Y|X_i)]$

the smaller this quantity, (i.e. fixing $X_i$), the smaller is the variance of $Y$ when fixing the $i$th input: variable $X_i$ has a strong impact.

**Theorem (Total variance)**

$$\text{Var}(Y) = \text{Var}[E(Y|X_i)] + E[\text{Var}(Y|X_i)].$$

**Definition (First order Sobol’ Index)**

$$0 \leq S_i = \frac{V[E(Y|X_i)]}{\text{Var}(Y)} \leq 1$$

ex. : linear output $Y = \sum_{i=1}^{d} \beta_i X_i$, we get $S_i = \frac{\beta_i^2 \text{Var}(X_i)}{\text{Var}(Y)} = \rho_i^2$. 
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$$\text{Var} \left( Y \mid X_i = x_i \right), \text{how to choose } x_i? \Rightarrow E \left[ \text{Var} \left( Y \mid X_i \right) \right]$$

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II- Functional variance analysis

**Toy case:**

\[ Y = X_1^2 + X_2 \quad X_i \sim U([0, 1]) \quad X_1 \perp \perp X_2 \]

\[
\begin{align*}
\mathbb{E}(Y|X_1) &= X_1^2 + \mathbb{E}(X_2) \Rightarrow \text{Var}[\mathbb{E}(Y|X_1)] = \text{Var}(X_1^2) = \frac{4}{45} \\
\mathbb{E}(Y|X_2) &= \mathbb{E}(X_1^2) + X_2 \Rightarrow \text{Var}[\mathbb{E}(Y|X_2)] = \text{Var}(X_2) = \frac{1}{12} \\
\text{Var}(Y) &= \text{Var}(X_1^2) + \text{Var}(X_2) = \frac{31}{180} \\
S_1 &= \frac{16}{31} \approx 0.516, \quad S_2 = \frac{15}{31} \approx 0.484 \\
S_1 + S_2 &= 1, \text{ additive model}
\]
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\[ \mathbb{E}(Y|X_2) = \mathbb{E}(X_2^2) + X_2 \Rightarrow \text{Var}[\mathbb{E}(Y|X_2)] = \text{Var}(X_2) = \frac{1}{12} \]

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\[ \mathbb{E}(Y|X_1) = X_1^2 + \mathbb{E}(X_2) \Rightarrow \text{Var}\left[\mathbb{E}(Y|X_1)\right] = \text{Var}(X_1^2) = \frac{4}{45} \]

\[ \mathbb{E}(Y|X_2) = \mathbb{E}(X_1^2) + X_2 \Rightarrow \text{Var}\left[\mathbb{E}(Y|X_2)\right] = \text{Var}(X_2) = \frac{1}{12} \]

\[ \text{Var}(Y) = \text{Var}(X_1^2) + \text{Var}(X_2) = \frac{31}{180} \]

\[ S_1 = \frac{16}{31} \approx 0.516, \quad S_2 = \frac{15}{31} \approx 0.484 \]

\[ S_1 + S_2 = 1, \text{ additive model} \]
II- Functional variance analysis

Toy case:

\[ Y = X_1^2 + X_2 \quad X_i \sim U([0, 1]) \quad X_1 \perp \perp X_2 \]

\[ \mathbb{E}(Y|X_1) = X_1^2 + \mathbb{E}(X_2) \Rightarrow \text{Var}[\mathbb{E}(Y|X_1)] = \text{Var}(X_1^2) = \frac{4}{45} \]

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\[ S_1 = \frac{16}{31} \approx 0.516, \quad S_2 = \frac{15}{31} \approx 0.484 \]

\[ S_1 + S_2 = 1, \text{ additive model} \]
More generally,

**Theorem (Hoeffding decomposition)**

\[ \mathcal{M} : [0,1]^d \to \mathbb{R}, \int_{[0,1]^d} \mathcal{M}^2(x)dx < \infty \]

\[ \mathcal{M} \text{ has an unique decomposition} \]

\[ \mathcal{M}_0 + \sum_{i=1}^d \mathcal{M}_i(x_i) + \sum_{1 \leq i < j \leq d} \mathcal{M}_{i,j}(x_i, x_j) + \ldots + \mathcal{M}_{1,\ldots,d}(x_1, \ldots, x_d) \]

under the constraint

- \( \mathcal{M}_0 \) constant,
- \( \forall 1 \leq s \leq d, \forall 1 \leq i_1 < \ldots < i_s \leq d, \forall 1 \leq p \leq s \)

\[ \int_0^1 \mathcal{M}_{i_1,\ldots,i_s}(x_{i_1}, \ldots, x_{i_s})dx_{i_p} = 0 \]
II- Functional variance analysis

Consequences: $M_0 = \int_{[0,1]^d} M(x) dx$ and the terms of the decomposition are orthogonal.

The computation of each term in the decomposition writes:

- $M_i(x_i) = \int_{[0,1]^{d-1}} M(x) \prod_{p \neq i} dx_p - M_0$
- $i \neq j$
  $M_{i,j}(x_i, x_j) = \int_{[0,1]^{d-2}} M(x) \prod_{p \neq i,j} dx_p - M_0 - M_i(x_i) - M_j(x_j)$
- $\ldots$

$\Rightarrow$ computation of multiple integrals.
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$\Rightarrow$ computation of multiple integrals.
II- Functional variance analysis

Variance decomposition: $X_1, \ldots, X_d$ i.i.d. $\sim \mathcal{U}([0, 1])$

$$Y = \mathcal{M}(X) = \mathcal{M}_0 + \sum_{i=1}^{d} \mathcal{M}_i(X_i) + \ldots + \mathcal{M}_{1,\ldots,d}(X_1, \ldots, X_d)$$

- $\mathcal{M}_0 = \mathbb{E}(Y)$,
- $\mathcal{M}_i(X_i) = \mathbb{E}(Y|X_i) - \mathbb{E}(Y)$,
- $i \neq j \quad \mathcal{M}_{i,j}(X_i, X_j) = \mathbb{E}(Y|X_i, X_j) - \mathbb{E}(Y|X_i) - \mathbb{E}(Y|X_j) + \mathbb{E}(Y)$,
- \ldots

$$\text{Var}(Y) = \sum_{i=1}^{d} \text{Var}(\mathcal{M}_i(X_i)) + \ldots + \text{Var}(\mathcal{M}_{1,\ldots,d}(X_1, \ldots, X_d))$$
II- Functional variance analysis

Variance decomposition : \( X_1, \ldots, X_d \) i.i.d. \( \sim U([0, 1]) \)

\[ Y = M(X) = M_0 + \sum_{i=1}^{d} M_i(X_i) + \ldots + M_{1,\ldots,d}(X_1, \ldots, X_d) \]

- \( M_0 = \mathbb{E}(Y) \),
- \( M_i(X_i) = \mathbb{E}(Y|X_i) - \mathbb{E}(Y) \),
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- \ldots

\[ \text{Var}(Y) = \sum_{i=1}^{d} \text{Var}(M_i(X_i)) + \ldots + \text{Var}(M_{1,\ldots,d}(X_1, \ldots, X_d)) \]
II- Functional variance analysis

Definition (Sobol’ indices)

\[ \forall i = 1, \ldots, d \quad S_i = \frac{\text{Var}(M_i(X_i))}{\text{Var}(Y)} = \frac{\text{Var}[\mathbb{E}(Y|X_i)]}{\text{Var}(Y)} \]

\[ \forall i \neq j \quad S_{i,j} = \frac{\text{Var}(M_{i,j}(X_i,X_j))}{\text{Var}(Y)} = \frac{\text{Var}[\mathbb{E}(Y|X_i,X_j)] - \text{Var}[\mathbb{E}(Y|X_i)] - \text{Var}[\mathbb{E}(Y|X_j)]}{\text{Var}(Y)} \]

\[ \ldots \]

\[ 1 = \sum_{i=1}^{d} S_i + \sum_{i \neq j} S_{i,j} + \ldots + S_{1,\ldots,d} \]

Definition (Total indices)

\[ i = 1, \ldots, d \quad S_{T_i} = \sum_{u \subset \{1,\ldots,d\}, u \neq \emptyset, i \in u} S_u \]
II- Functional variance analysis

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\[ \forall i = 1, \ldots, d \quad S_i = \frac{\text{Var}(M_i(X_i))}{\text{Var}(Y)} = \frac{\text{Var}[E(Y|X_i)]}{\text{Var}(Y)} \]

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Sobol’ indices:

Definition (Total indices)

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i = 1, \ldots, d \quad S_{T_i} = \sum_{\mathbf{u} \subset \{1, \ldots, d\}, \mathbf{u} \neq \emptyset, i \in \mathbf{u}} S_{\mathbf{u}}.
\]

\[
X_{(-i)} = (X_1, \ldots, X_{i-1}, X_{i+1}, \ldots, X_d)
\]

Using the theorem of the total variance,

\[
S_{T_i} = \frac{\mathbb{E} \left[ \text{Var} \left( Y | X_{(-i)} \right) \right]}{\text{Var}(Y)} = 1 - \frac{\text{Var} \left[ \mathbb{E} \left( Y | X_{(-i)} \right) \right]}{\text{Var}(Y)}.
\]
II- Functional variance analysis

Indices with factor:

Effets principaux

Interactions 2 facteurs

Interactions 3 facteurs

Effet total de A
II- Functional variance analysis

Indices with groupe of factors:
Fact: Analytical expressions of Sobol’ indices, with integrals in high dimensional spaces, are rarely available.

Two inferential approaches

1) Monte-Carlo type (hypothesis $L^2$ with the model);
2) spectral techniques (additional hypotheses of regularity).

If the model is too costly to assess, we fit a metamodel before applying these techniques.

ex.: parametric and non-parametric regressions, Gaussian metamodel (see practical session), . . .
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III- Sobol indices inference

Monte-Carlo type Approaches: (Sobol’ 93, Saltelli 02, Mauntz, . . .)

Idea: $X'_{(-i)}$ indep. copy of $X_{(-i)}$, $Y = M(X_i, X_{(-i)})$, $Y^i = M(X_i, X'_{(-i)})$

We have $S_i = \frac{\text{Cov}(Y, Y^i)}{\text{Var}(Y)}$, the idea is based on empirical formulas.

Two independent samples A and B (Monte-Carlo, LHS)

$$A = \begin{pmatrix} x_{1,1}^A & \cdots & x_{d,1}^A \\ \vdots & \ddots & \vdots \\ x_{1,n}^A & \cdots & x_{d,n}^A \end{pmatrix} \quad B = \begin{pmatrix} x_{1,1}^B & \cdots & x_{d,1}^B \\ \vdots & \ddots & \vdots \\ x_{1,n}^B & \cdots & x_{d,n}^B \end{pmatrix}$$

From A and of B, we create d sampling matrices $C_i$, $i = 1, \ldots, d.$

$$C_i = \begin{pmatrix} x_{1,1}^A & \cdots & x_{i,1}^B & \cdots & x_{d,1}^A \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ x_{1,n}^A & \cdots & x_{i,n}^B & \cdots & x_{d,n}^A \end{pmatrix}$$
We compute \((2 + d) \times n\) the model \(\mathcal{M}\):

\[
y^A = \begin{pmatrix}
y_1^A \\
\vdots \\
y_n^A
\end{pmatrix} \quad y^B = \begin{pmatrix}
y_1^B \\
\vdots \\
y_n^B
\end{pmatrix} \quad \forall 1 \leq i \leq d \quad y_{ci} = \begin{pmatrix}
y_1^c_i \\
\vdots \\
y_n^c_i
\end{pmatrix}
\]
III- Sobol’ indices inference

\texttt{sobолEff()} \ (\textit{Janon et al.}, 2012 & 2013)

- \( \hat{V}_i = \frac{1}{n} \sum_{k=1}^{n} y_k^B y_k^C_i - \left( \frac{1}{n} \sum_{k=1}^{n} \frac{y_k^B+y_k^C_i}{2} \right)^2 \) numerator of the first-order index

- \( \hat{V} = \frac{1}{n} \sum_{k=1}^{n} \left( \frac{(y_k^B)^2+(y_k^C_i)^2}{2} \right) - \left( \frac{1}{n} \sum_{k=1}^{n} \frac{y_k^B+y_k^C_i}{2} \right)^2 \) denominator

asymptotic or bootstrap confidence intervals (see practical session)
asymptotic efficiency of the estimator

Remark :
We can also replace the MC ou LHS samplings with QMC (hyp. of regular variations).
III- Sobol indices inference

The $g$-function of Sobol' : 

$$f(x) = f_1(x_1) \times f_2(x_2)$$

with

$$f_i(x_i) = \frac{|4x_i - 2| + a_i}{1 + a_i},$$

$a_1 = 9$, $a_2 = 1$.

$S_1 \approx 0.038$, $S_2 \approx 0.958$.

$n = 1000$, $b = 100$, IC(0.95) sobolEff (left), sobol2007 (right)
Replicate latin hypercubes: (Tissot et al.)

**Definition (Replicated Latin Hypercube Sampling)**

\[ k = 1, \ldots, n \]

\[ x_k = \left( \frac{\pi_1(k) - U_1, \pi_1(k)}{n}, \ldots, \frac{\pi_d(k) - U_d, \pi_d(k)}{n} \right) \]

\[ \tilde{x}_k = \left( \frac{\tilde{\pi}_1(k) - U_1, \tilde{\pi}_1(k)}{n}, \ldots, \frac{\tilde{\pi}_d(k) - U_d, \tilde{\pi}_d(k)}{n} \right) \]

We have two matrices \( B \) and \( \tilde{B} \) at our disposal.
III- Sobol’ indices inference

\[ B = \begin{pmatrix} x_{1,1} & \cdots & x_{d,1} \\ \vdots & \ddots & \vdots \\ x_{1,n} & \cdots & x_{d,n} \end{pmatrix} \quad \tilde{B} = \begin{pmatrix} \tilde{x}_{1,1} & \cdots & \tilde{x}_{d,1} \\ \vdots & \ddots & \vdots \\ \tilde{x}_{1,n} & \cdots & \tilde{x}_{d,n} \end{pmatrix} \]

We compute the model \( \mathcal{M} \) 2n times (on the n lines of \( B \) and the n lines of \( \tilde{B} \)).

permut. of lines :
\[
\left\{ \begin{array}{l}
\tilde{B} = (\tilde{x}_{k,l})_{1 \leq k \leq n, 1 \leq l \leq d} \quad \rightarrow \quad \tilde{B}_i = (\tilde{x}^i_{k,l})_{1 \leq k \leq n, 1 \leq l \leq d} \\
L_k \quad \mapsto \quad L_{\pi_i^{-1} \circ \tilde{\pi}_i(k)}, \ k = 1, \ldots, n
\end{array} \right.
\]

Then, \( \tilde{x}^i_{k,i} = \tilde{x}_{\pi_i^{-1} \circ \tilde{\pi}_i(k),i} = x_{k,i}, \ k = 1, \ldots, n. \)

To estimate \( S_i \), we replace \( C_i \) with \( \tilde{B}_i \) (same column number i).
III- Sobol’ indices inference

Caption:
point 1 ○ point 2 △ point 3 + point 4 × point 5 ◊

Design B (left), B and \( \tilde{B} \) (right, black and red)
III- Sobol’ indices inference

Design $\tilde{B}_1$ (left), $\tilde{B}_2$ (right)

Asymptotic confidence intervals with variance smaller than for MC.
Possible extension to indices of order two (via orthogonal arrays of
strength 2).
Asymptotic confidence intervals with variance smaller than for MC.
Possible extension to indices of order two (via orthogonal arrays of strength 2).
Spectral approaches: (case $d = 2$)

$$Y = \sum_{k=(k_1,k_2)\in\mathbb{Z}^2} c_k(M) \Phi_{1,k_1}(X_1) \Phi_{2,k_2}(X_2)$$

with, for all $i = 1, 2$, $(\Phi_{i,k})_{k\in\mathbb{Z}}$ is an orthonormal basis of $L^2([0, 1])$ and $\Phi_{i,0} \equiv 1$.

- $M_0 = c_0(M)$,
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- $M_2(X_2) = \sum_{k_2\in\mathbb{Z}^*} c_{0,k_2}(M) \Phi_{2,k_2}(X_2)$,
- $M_{1,2}(X_1, X_2) = \sum_{k_1\in\mathbb{Z}^*, k_2\in\mathbb{Z}^*} c_{k_1,k_2}(M) \Phi_{1,k_1}(X_1) \Phi_{2,k_2}(X_2)$.

We have with Parseval identity:

- $\text{Var}(M_1(X_1)) = \sigma_1^2 = \sum_{k_1\in\mathbb{Z}^*} |c_{k_1,0}(M)|^2$, (idem for $\sigma_2^2$),
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ex. : orthogonal polynomials, wavelet basis, Fourier basis.
III- Sobol' indices inference

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ex.: orthogonal polynomials, wavelet basis, Fourier basis.
III- Sobol’ indices inference

Inference scheme:
If \( D \) is an experimental design with \([0, 1]^2\), we propose the quadrature formula:

\[
\hat{c}_{k_1, k_2}(M, D) = \frac{1}{\text{card}D} \sum_{x=(x_1,x_2) \in D} M(x) e^{-2i\pi(k_1 x_1 + k_2 x_2)}.
\]

We then infer each part of variance with a truncation:
- \( \hat{\sigma}^2_1(M, K_1, D) = \sum_{k_1 \in K_1} |\hat{c}_{k_1,0}(M, D)|^2 \), with \( K_1 \subset \mathbb{Z}^* \) of finite cardinal, (idem for \( \hat{\sigma}^2_2 \)),
- \( \hat{\sigma}^2_{1,2}(M, K_{1,2}, D) = \sum_{(k_1,k_2) \in K_{1,2}} |\hat{c}_{k_1,k_2}(M, D)|^2 \), with \( K_{1,2} \subset \mathbb{Z}^* \times \mathbb{Z}^* \) of finite cardinal.

We infer the total variance with
\( \hat{\sigma}^2(M, D) = \hat{c}_{0,0}(M^2, D) - \hat{c}_{0,0}(M, D)^2 \).

The estimators of Sobol’ indices can be written as:
\[
\hat{S}_i = \frac{\hat{\sigma}^2_i}{\hat{\sigma}^2}, \quad i = 1, 2, \quad S_{1,2} = \frac{\hat{\sigma}^2_{1,2}}{\hat{\sigma}^2}.
\]
Inference scheme:
If $D$ is an experimental design with $[0, 1]^2$, we propose the quadrature formula:

$$
\hat{c}_{k_1, k_2}(\mathcal{M}, D) = \frac{1}{\text{card} D} \sum_{x=(x_1, x_2) \in D} \mathcal{M}(x) e^{-2i\pi(k_1 x_1 + k_2 x_2)}.
$$

We then infer each part of variance with a truncation:

- $\hat{\sigma}^2_1(\mathcal{M}, K_1, D) = \sum_{k_1 \in K_1} |\hat{c}_{k_1, 0}(\mathcal{M}, D)|^2$, with $K_1 \subset \mathbb{Z}^*$ of finite cardinal, (idem for $\hat{\sigma}^2_2$),

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III- Sobol’ indices inference

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Classical designs:

(a) grille régulière

(b) sous-groupe fini

(c) grille creuse

(d) tableau orthogonal
The performance of previous estimators is linked to the decreasing speed of Fourier spectrum (regularity) of $\mathcal{M}$. The techniques FAST and RBD are two particular cases of such approaches (after model regularisation).

**FAST:** (Cukier et al., 78) *Fourier Amplitude Sensitivity Test*

- we fix $K_u$ an ensemble of a priori non negligible frequencies;
- we chose $D$ cyclic group (design (b)) in order to control the quadrature error.

**Remarks:**

- if $\mathcal{M}$ regular, we can obtain a speed of convergence $\gg \sqrt{n}$;
- for the total indices $\text{fast99()}$ (no confidence intervals in the function) Saltelli et al., 99.
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- we choose $D$ a orthogonal array of strength 1 (design (d)), randomized by a random permutation ($D(\pi)$);

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- these estimators are known to be biased;
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Conclusions about the inference:

The spectral approach is interesting in terms of cost, but it requires more hypotheses in terms of regularity.

The Monte Carlo approach with replicated latin hypercubes is not as costly as the naive Monte Carlo approach.

see exercise 4 in the practical session
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Borgonovo et al. ≥ 2007

\[ \delta_i = \frac{1}{2} \mathbb{E}_{X_i} \left( S_i(X_i) \right) \text{ with } S_i(X_i) = \int \left| f_Y(y) - f_{Y|X_i}(y) \right| \, dy. \]

Remark: extension to \( u \subset \{1, \ldots, d\} \)
WE CAN BUILD META MODELS WHEN THE INITIAL MODEL IS TOO COSTLY;

FUNCTIONALS INPUTS: MC APPROACHES CAN BE APPLIED;

VECTORIAL OUTPUT: APPROACHES COMPONENT BY COMPONENT, OR GENERALISED INDICES GSI (LAMONI ET AL.);

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we can build metamodels when the initial model is too costly;

functionals inputs: MC approaches can be applied;

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