Introduction to Global Sensibility Analysis

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Part I

Overview

inputs	$\longrightarrow$	model	$\longrightarrow$	output

$$\left.\begin{array}{c} X_1 \\ \cdot \\ \cdot \\ \cdot \\ X_d \end{array}\right\} \quad \_\_\_ \ \mathcal{M} \ \_\_\_ \quad Y = \mathcal{M}(X_1, \dots, X_d)$$

Experimental design: planification, sampling $\longleftrightarrow$ **Sensitivity analysis**: sensitivity indices' inference

Introduction

Background :

$$\mathcal{M} : \left\{ \begin{array}{ccc} \mathbb{R}^d & \to & \mathbb{R} \\ \mathbf{x} & \mapsto & y = \mathcal{M}(x_1, \ldots, x_d) \end{array} \right.$$

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.

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Sensitivity analysis may help identifying inappropriate models.

Introduction

Various approaches for quantitative sensitivity :

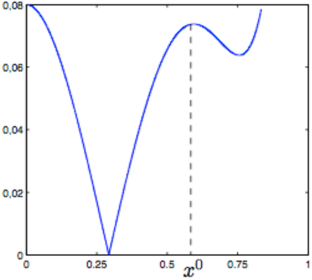
Local approaches :

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

First order sensitivity index for input i : $\left(\frac{\partial \mathcal{M}}{\partial x_i}\right)_{\mathbf{x^0}}$.

Pros : Low computational cost even for large d

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



Introduction

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.

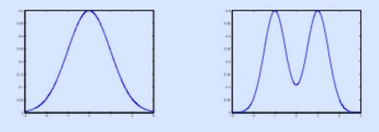


Figure: law (left) unimodal , (right) bimodal

Introduction

We vary inputs w.r.t. their probability distribution.

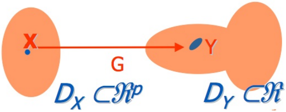


Figure: Local versus Global ($G := \mathcal{M}$)

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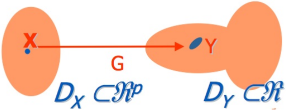
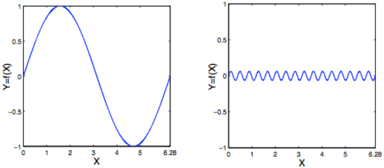


Figure: Local versus Global ($G := \mathcal{M}$), illustration.

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

Avantages : particularly interesting if adjoint available

Cons :
(1) does not discriminate enc



Introduction

(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.

However, let us provide, as an introduction, a first outlook to screening most usual methods.

A quick overlook on screening methods

Main objective : to screen among a large amount of inputs which ones are non influential on the quantity of interest (QoI).

Advantages : moderate computational cost.

Drawbacks : partial information, no hierarchisation.

A OAT screening method : Morris, 1991

OAT One At a Time we vary the factors one by one.
The screening method proposed by Morris is a global OAT approach.

Model $Y = \mathcal{M}(\mathbf{X})$, $\mathbf{X} = (X_1, \ldots, X_d)$ *with the* X_i*s independent uniform random variables on* $[0, 1]$.

More details on the method :

- input discretization on a grid with p values $\left\{0, \frac{1}{p-1}, \ldots, 1\right\}$.
- Δ a multiple of $1/(p-1)$, fixed once for all.
- $\Omega := \left\{0, \frac{1}{p-1}, \ldots, 1\right\}^d$.
- $\Omega_i^\Delta := \{x \in \Omega \text{ such that } (x_1, \ldots, x_{i-1}, x_i + \Delta, x_{i+1}, \ldots, x_d) \in \Omega\}$.

Definition

Elementary effect of X_i computed at $\mathbf{x} \in \Omega_i^\Delta$,

$$d_i(\mathbf{x}) = \frac{1}{\Delta}\left\{\mathcal{M}(x_1, \ldots, x_{i-1}, x_i + \Delta, x_{i+1}, \ldots, x_d) - \mathcal{M}(\mathbf{x})\right\} .$$

There are $p^{d-1}(p - \Delta(p-1))$ elementary effects to compute.

Steps :

- one draws uniformly a r-sample in Ω_i^Δ : $\mathbf{x}^1, \ldots, \mathbf{x}^r$;
- one computes $d_i(\mathbf{x}^j)$, $j = 1, \ldots, r$, $i = 1, \ldots, d$;
- one computes

$$\left\{ \begin{array}{lcl} \mu_i & = & \frac{1}{r} \sum_{j=1} d_i(\mathbf{x}^j) \\ \sigma_i^2 & = & \frac{1}{r} \sum_{j=1}^{r} (d_i(\mathbf{x}^j) - \mu_i)^2 . \end{array} \right.$$

	σ_i^2 low	σ_i^2 high
$\lvert\mu_i\rvert$ low	non influential	nonlinearities and/or interactions
$\lvert\mu_i\rvert$ high	influential	nonlinearities and/or interactions

The efficiency of the method "number of elementary effects computed / number of model runs" is equal to $1/2$.

Morris (1991) presents an adaptation with an efficiency equal to $d/(d+1)$, with d the input space dimension.

A toy example

Advection-reaction-diffusion equation with Dirichlet boundary condition :

$$\begin{cases} \dfrac{\partial u}{\partial t} = -r.u - a\dfrac{\partial u}{\partial x} + \lambda \dfrac{\partial^2 u}{\partial x^2} + f \quad x \in [0, L],\ t \in [0, T] \\ u(x = 0, t) = \Psi_1(t) \quad t \in [0, T] \\ u(x = L, t) = \Psi_2(t) \quad t \in [0, T] \\ u(x, t = 0) = g(x) \quad x \in (0, L)\,. \end{cases}$$

A : energy norm of the solution at time $t = T$.

Sensitivity of A with respect to (a, r, λ)? Uncertain input parameters are modeled as $a, r \sim \mathcal{U}([0.4, 0.6])$, $\lambda \sim \mathcal{U}([0.04, 0.06])$.

Scheme : 2-stemps Adams-Moulton, sample size equals 2^{13}.

Sensitivity measures based on variance : $S_a = 0.0188$, $S_\lambda = 0.7299$, $S_r = 0.2488$, $S_a + S_\lambda + S_r = 0.988$.

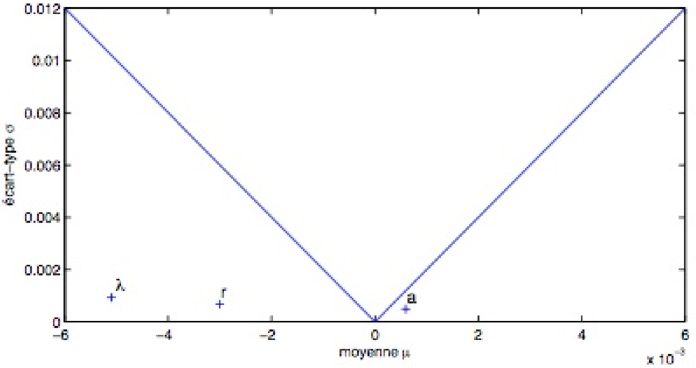


Figure: Morris with $p = 50$, $\Delta = 25/49$.

see Jupyter notebook of Part I on local or global OAT sensitivities

Lecture outline

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

$$Y = \mathcal{M}(X_1, \dots, X_d)$$

- Linear correlation

$$\rho_i = \rho\,(X_i, Y) = \frac{\mathrm{Cov}(X_i, Y)}{\sqrt{\mathrm{Var}(X_i)}\sqrt{\mathrm{Var}(Y)}}$$

- Partial correlation

$$PCC_i = PCC\,(X_i, Y) = \rho\left(Y - \widehat{Y}^{-(i)}, X_i - \widehat{X_i}^{-(i)}\right)$$

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 , PCCs are more suitable.

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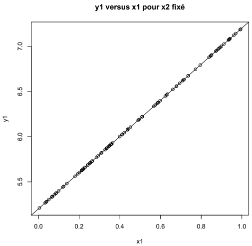
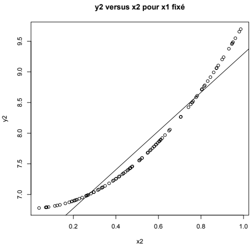
I- Measures based on linear regressions

Assessment of linear model?

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





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

Learning sample : $y_k = \mathcal{M}(x_{1,k}, \ldots, x_{d,k})$, $k = 1, \ldots, 100$

$\Rightarrow \quad \hat{y} = \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_0 = 2.06x1 + 3.15x2 + 4.34.$

Which measure to assess the fit of this model?

I- Measures based on linear regressions

⋆ Coefficient R^2

$$R^2 = \frac{SCE}{SCT} = \frac{\sum_{k=1}^m \left(\widehat{y}_k - \overline{y}\right)^2}{\sum_{k=1}^m \left(y_k - \overline{y}\right)^2},$$

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

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

$$\frac{1}{m}\frac{\sum_{k=1}^m \left(\widehat{y}_k^{-(k)} - y_k\right)^2}{\frac{1}{m}\sum_{k=1}^m \left(y_k - \overline{y}\right)^2},$$

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

$$(y_j, \mathbf{x}_j),\ j = 1, \ldots, k-1, k+1, \ldots, m.$$

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I- Measures based on linear regressions

If the relationship input/output is no more linear but simply monotonic, we work with ranks.

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

$r_{i,k}$ rank of $x_{i,k}$ in $(x_{i,1}, \ldots, x_{i,m})$, r_k rank of y_k 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 : $Y_{ij} = \mu + \alpha_i + \beta_j + \gamma_{i,j} + \varepsilon_{ij}, \quad \varepsilon_{ij}$ i.i.d. $\mathcal{N}(0, \sigma^2)$.

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

Inference :

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

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

with usual notation $\quad \overline{y} = \frac{1}{IJr} \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{r} y_{ijk}$,

$$\overline{y}_{i..} = \frac{1}{Jr} \sum_{j=1}^{J} \sum_{k=1}^{r} y_{ijk}, \quad \overline{y}_{.j.} = \frac{1}{Ir} \sum_{i=1}^{I} \sum_{k=1}^{r} y_{ijk}, \quad \overline{y}_{ij.} = \frac{1}{r} \sum_{k=1}^{r} y_{ijk}.$$

II- Functional variance analysis

In the previous model, we define :

- the forecasts $\hat{y}_{ijk} = \overline{y}_{ij\cdot}$,
- the residuals $\hat{\varepsilon}_{ijk} = y_{ijk} - \hat{y}_{ijk} = y_{ijk} - \overline{y}_{ij\cdot}$.

Variance decomposition :

$$\begin{array}{ccccc} SCT & = & SCM & + & SCR \\ \text{total variance} & = & \text{variance explained by the model} & + & \text{residual variance} \end{array}$$

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

$$SCX_1 = \sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{r}\hat{\alpha}_i^2, \qquad SCX_2 = \sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{r}\hat{\beta}_j^2,$$

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II- Functional variance analysis

Hypothesis testing: many possible tests

ex. : H_0 : additive model versus H_1 : complete model

Test statistic :

$$T = \frac{SCX_1X_2/(IJ - I - J + 1)}{SCR/(IJr - IJ)} \underset{H_0}{\sim} F(IJ - I - J + 1, IJr - IJ).$$

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)

$$Y(s,t) = \mathcal{M}(s,t) + \varepsilon(s,t)\ , \quad (s,t) \in S \times T$$

with

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

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

$Y = \mathcal{M}(X_1, \ldots, X_d)$, $(X_1, \ldots, X_d) \sim P_{X_1,\ldots,X_d}$.

In the following, we assume :

i) the X_i are independent ;

ii) $\forall\, i = 1, \ldots, d$, $X_i \sim \mathcal{U}([0,1])$.

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

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 and in the lecture on Shapley effects.

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II- Functional variance analysis

Towards Sobol sensitivity indices

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

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

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

Theorem (Total variance)

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

Definition (First order Sobol' Index)

$i = 1, \ldots, d$

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

ex. : linear output $Y = \sum_{i=1}^{d} \beta_i X_i$, we get $S_i = \frac{\beta_i^2 \mathrm{Var}(X_i)}{\mathrm{Var}(Y)} = \rho_i^2$.

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II- Functional variance analysis

Towards Sobol sensitivity indices

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

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

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

Theorem (Total variance)

$\mathrm{Var}(Y) = \mathrm{Var}\left[\mathbb{E}\left(Y|X_i\right)\right] + \mathbb{E}\left[\mathrm{Var}\left(Y|X_i\right)\right].$

Definition (First order Sobol' Index)

$i = 1, \ldots, d$

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II- Functional variance analysis

Toy case:

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

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

$$\mathbb{E}(Y|X_2) = \mathbb{E}(X_1^2) + X_2 \Rightarrow \mathrm{Var}[\mathbb{E}(Y|X_2)] = \mathrm{Var}(X_2) = \tfrac{1}{12}$$

$$\mathrm{Var}(Y) = \mathrm{Var}(X_1^2) + \mathrm{Var}(X_2) = \tfrac{31}{180}$$

$$S_1 = \frac{16}{31} \approx 0,516\,, \quad S_2 = \frac{15}{31} \approx 0,484$$

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More generally,

Theorem (Hoeffding decomposition)

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

$\mathcal{M}$ 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 : $\mathcal{M}_0 = \int_{[0,1]^d} \mathcal{M}(x)dx$ and the terms of the decomposition are orthogonal.

The computation of each term in the decomposition writes:

- $\mathcal{M}_i(x_i) = \int_{[0,1]^{d-1}} \mathcal{M}(x) \Pi_{p \neq i} dx_p - \mathcal{M}_0$
- $i \neq j$
  $\mathcal{M}_{i,j}(x_i, x_j) = \int_{[0,1]^{d-2}} \mathcal{M}(x) \Pi_{p \neq i,j} dx_p - \mathcal{M}_0 - \mathcal{M}_i(x_i) - \mathcal{M}_j(x_j)$
- $\ldots$

$\Rightarrow$ computation of multiple integrals.

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II- Functional variance analysis

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

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

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

$$\forall\, i = 1, \ldots, d \;\; S_i = \frac{\mathrm{Var}(\mathcal{M}_i(X_i))}{\mathrm{Var}(Y)} = \frac{\mathrm{Var}[\mathbb{E}(Y|X_i)]}{\mathrm{Var}(Y)}$$

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$$\ldots$$

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

Definition (Total indices)

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

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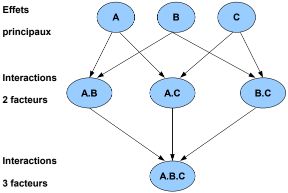
$X_{(-i)} = (X_1, \dots, X_{i-1}, X_{i+1}, \dots, X_d)$

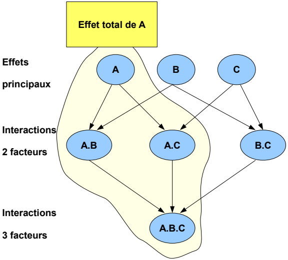
Using the theorem of the total variance,

$$S_{T_i} = \frac{\mathbb{E}\left[\mathrm{Var}\left(Y|X_{(-i)}\right)\right]}{\mathrm{Var}(Y)} = 1 - \frac{\mathrm{Var}\left[\mathbb{E}\left(Y|X_{(-i)}\right)\right]}{\mathrm{Var}(Y)} \ .$$

II- Functional variance analysis

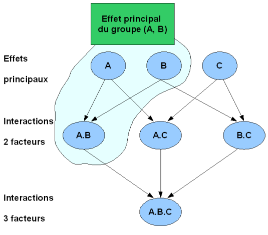
Indices with factor:

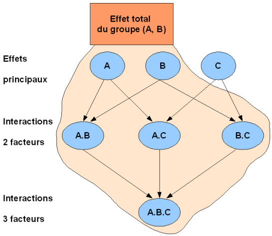




II- Functional variance analysis

Indices with groupe of factors:





III- Sobol' indices inference

Fact : Analytical expressions of Sobol' indices, with integrals in high dimensional spaces, are rarely available.

Two inferential approaches

1) Monte-Carlo type (hypothesis $\mathbb{L}^2$ 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. . .

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III- Sobol indices inference

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

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

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

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

$$A = \begin{pmatrix} x^A_{1,1} & \cdots & x^A_{d,1} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ x^A_{1,n} & \cdots & x^A_{d,n} \end{pmatrix} \qquad B = \begin{pmatrix} x^B_{1,1} & \cdots & x^B_{d,1} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ x^B_{1,n} & \cdots & x^B_{d,n} \end{pmatrix}$$

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

$$C_i = \begin{pmatrix} x^A_{1,1} & \cdots & x^B_{i,1} & \cdots & x^A_{d,1} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ x^A_{1,n} & \cdots & x^B_{i,n} & \cdots & x^A_{d,n} \end{pmatrix}$$

III- Sobol indices inference

We compute $(1+d) \times n$ the model $\mathcal{M}$:

$$y^B = \begin{pmatrix} y_1^B \\ \cdot \\ \cdot \\ \cdot \\ y_n^B \end{pmatrix} \quad \text{and} \quad \forall\, 1 \leq i \leq d \quad y^{C_i} = \begin{pmatrix} y_1^{C_i} \\ \cdot \\ \cdot \\ \cdot \\ y_n^{C_i} \end{pmatrix}$$

III- Sobol' indices inference

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

asymptotic or bootstrap confidence intervals (see practical session)

asymptotic efficiency of the estimator

Remark :

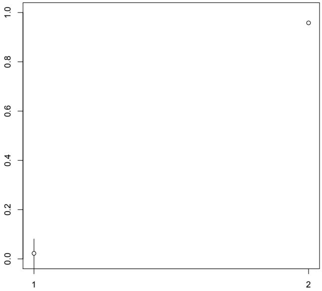
We can also replace the MC or LHS samplings with QMC (hyp. of regular variations).

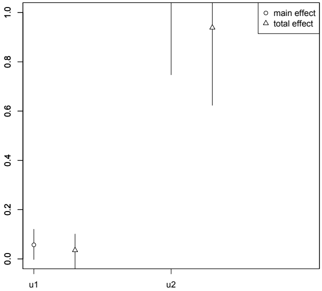
III- Sobol indices inference

The g-function of Sobol' : $f(x) = f_1(x_1) * f_2(x_2)$ with $f_i(x_i) = \frac{|4x_i - 2| + a_i}{1 + a_i}$, $a_1 = 9$, $a_2 = 1$.

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

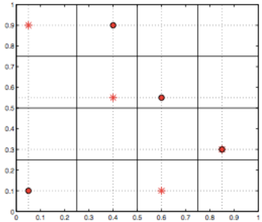
$n = 1000$, $b = 100$, IC(0.95) `sobolEff` (left), `sobol2007` (right)





III- Sobol' indices inference

Replicate latin hypercubes: (Tissot *et al.*)



Definition (Replicated Latin Hypercube Sampling)

$k = 1, \ldots, n$

$$\mathbf{x}_k = \left(\frac{\pi_1(k) - U_{1,\pi_1(k)}}{n}, \ldots, \frac{\pi_d(k) - U_{d,\pi_d(k)}}{n} \right)$$

$$\tilde{\mathbf{x}}_k = \left(\frac{\tilde{\pi}_1(k) - U_{1,\tilde{\pi}_1(k)}}{n}, \ldots, \frac{\tilde{\pi}_d(k) - U_{d,\tilde{\pi}_d(k)}}{n} \right)$$

We have two matrices B and $\widetilde{B}$ at our disposal

III- Sobol' indices inference

$$B = \begin{pmatrix} x_{1,1} & \dots & x_{d,1} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ x_{1,n} & \dots & x_{d,n} \end{pmatrix} \qquad \widetilde{B} = \begin{pmatrix} \tilde{x}_{1,1} & \dots & \tilde{x}_{d,1} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \tilde{x}_{1,n} & \dots & \tilde{x}_{d,n} \end{pmatrix}$$

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

permut. of lines :

$$\begin{cases} \widetilde{B} = (\tilde{x}_{k,l})_{1\leq k\leq n, 1\leq l\leq d} & \rightarrow \quad \widetilde{B}_i = (\tilde{x}^i_{k,l})_{1\leq k\leq n, 1\leq l\leq d} \\ L_k & \mapsto \quad L_{\tilde{\pi}_i^{-1}\circ\pi_i(k)}, \; k = 1, \dots, n \end{cases}$$

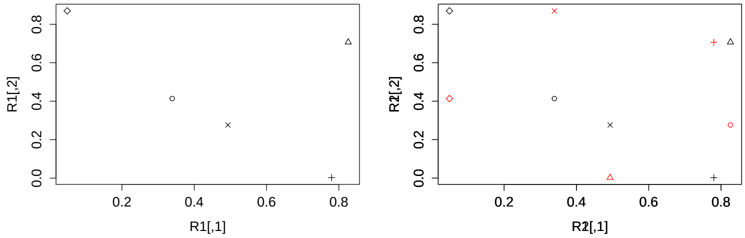
Then, $\tilde{x}^i_{k,i} = \tilde{x}_{\tilde{\pi}_i^{-1}\circ\pi_i(k),i} = x_{k,i}$, $k = 1, \dots, n$.

To estimate S_i, we replace C_i with $\widetilde{B}_i$ (same column number i).

III- Sobol' indices inference

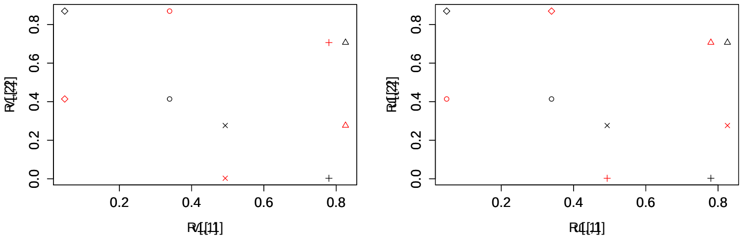
Caption:
point 1 $\circ$ point 2 $\triangle$ point 3 $+$ point 4 $\times$ point 5 $\diamond$

Design B (left), B and $\widetilde{B}$ (right, black and red)



III- Sobol' indices inference

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



Asymptotic confidence intervals with variance smaller than for MC.

Possible extension to indices of order two (via orthogonal arrays of strength 2).

III- Sobol' indices inference

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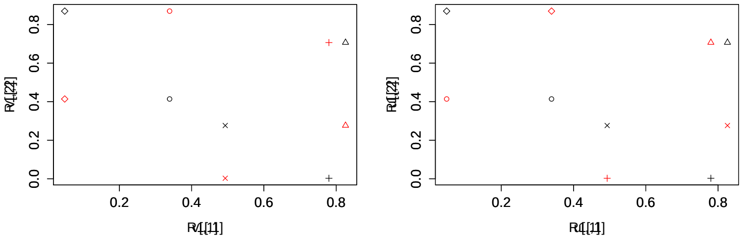

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III- Sobol' indices inference

Spectral approaches: (case $d = 2$)

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

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

$$\mathcal{M}_0 = c_0(\mathcal{M}),$$

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We have with Parseval identity:

- $\mathrm{Var}\left(\mathcal{M}_1(X_1)\right) = \sigma_1^2 = \sum_{k_1\in\mathbb{Z}^*} |c_{k_1,0}(\mathcal{M})|^2$, (idem for σ_2^2),
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ex. : orthogonal polynomials, wavelet basis, Fourier basis.

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If D is an experimental design with $[0,1]^2$, we propose the quadrature formula:

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The estimators of Sobol' indices can be written as:

$$\hat{S}_i = \frac{\hat{\sigma}_i^2}{\hat{\sigma}^2},\ i = 1,2, \quad S_{1,2} = \frac{\hat{\sigma}_{1,2}^2}{\hat{\sigma}^2} .$$

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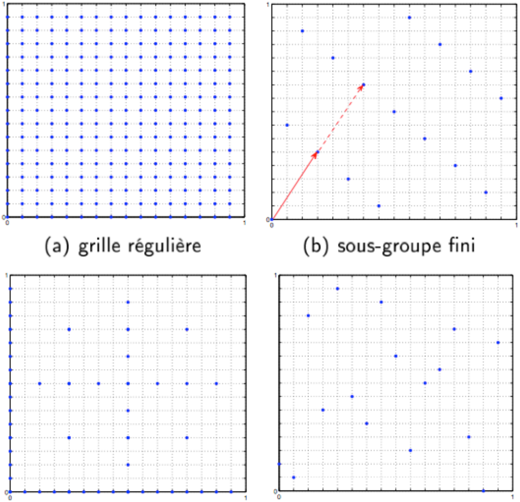
Classical designs:



(a) grille régulière
(b) sous-groupe fini
(c) grille creuse
(d) tableau orthogonal

III- Sobol' indices inference

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 $K_{\mathbf{u}}$ 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 $>> \sqrt{n}$;
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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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Conclusions about the inference :

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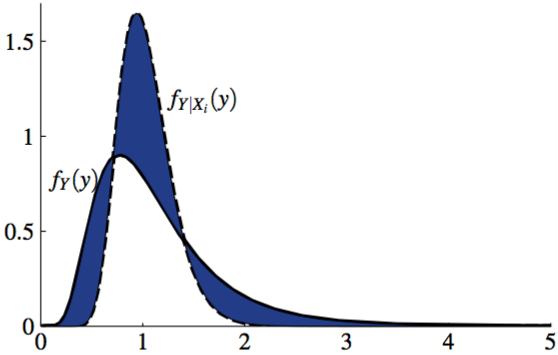
IV- Indices based on probability distribution

$\delta_i = \frac{1}{2}\mathbb{E}_{X_i}\left(S_i(X_i)\right)$ with $S_i(X_i) = \int \left| f_Y(y) - f_{Y|X_i}(y) \right| dy$, see Borgonovo *et al.* (2007)

Remark: extension to $\mathbf{u} \subset \{1, \ldots, d\}$. Recent results on



V- Further topics

- we can build metamodels when the initial model is too costly;
- functional inputs: MC approaches can be applied;
- vectorial output: approaches component by component, or aggregated indices (see Lamboni *et al*, 2011) ;
- functional output : we summarize the output by a vector (projection on an appropriate basis) or we make a movie (temporal output) or a map (spatial output) of indices;
- very interesting results providing kernel based ANOVA decomposition (see Da Veiga, 2021) ;
- correlated inputs: the decomposition is not unique, it is hard to decouple interactions and correlation effects $\Rightarrow$ we turn to Shapley effects (see Owen, 2014)

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