The design and sensitivity analysis of experiments

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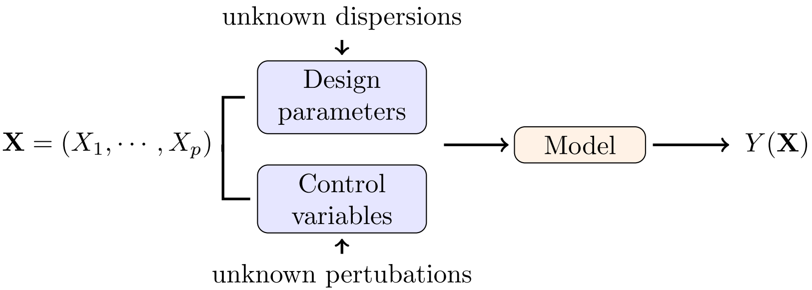
The design of experiments

The general context



Hypotheses

- The components of $\mathbf{X}$ are independent
- Each $\mathbf{X}_i$ is distributed into $[0, 1]$

The design of experiments

What is the design of experiments ?

- Set the experimentation/simulation points in the inputs space
- Select the combinations of input values that will provide the most informative inputs-output relationship

What is the design of experiments for ?

- Explore the model with a limited number of inputs
- Identify outputs of interest
- Provide an optimized design for sensitivity analysis

Designs families

1. Factorial designs
   - Settings
     - Turn quantitative inputs $\mathbf{X}$ into factors with levels $\{0, 1\}$
     - To a simple form of model $Y(\mathbf{X})$, there corresponds an optimized design (with the smallest number of points)
   - Example
     - The One at A Time (OAT) design
     - The full factorial design
     - The fractional factorial design
2. Numerical designs of experiments
   - Settings
     - More general than factorial designs
     - Space filling designs for computer experiments
   - Example
     - The Latin Hypercube sampling (LHS)
     - The Quasi Monte Carlo

The One at A Time (OAT) design

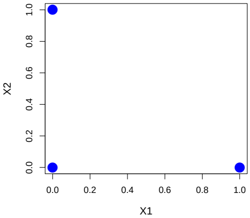
The linear model

$$Y(\mathbf{X}) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \varepsilon$$

The optimal design for this model is the OAT design, $X_i \in \{0, 1\}$

Example with $p = 2$

X_1	X_2
0	0
1	0
0	1



$$N = p + 1 \text{ simulations}$$

Drawbacks

- Do not detect interactions, discontinuities
- In high dimension, the inputs space is partially covered

The full factorial design

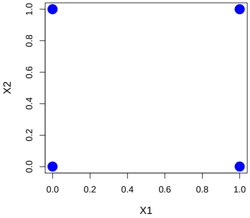
The linear model with interactions

$$Y(X) = \beta_0 + \beta_1 X_1 + \beta_p X_p + \sum_{i<j} \beta_{i,j} X_i X_j + \cdots + \beta_{1,\dots,p} X_1 \cdots X_p + \varepsilon$$

The optimal design is the full factorial design

Example with $p = 2$

X_1	X_2	$X_1 X_2$
0	0	1
1	0	0
0	1	0
1	1	1



$$N = 2^p \text{ simulations}$$

Drawbacks

- If p large, very expensive : $p = 10$, $N = 1024$ simulations !

The fractional factorial design

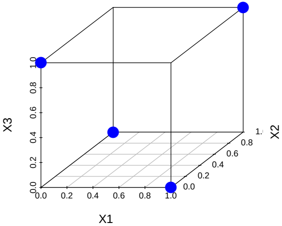
Linear model with partial interactions

$$Y(X) = \beta_0 + \beta_1 X_1 + \beta_p X_p + \sum_{i<j} \beta_{i,j} X_i X_j + \cdots + \varepsilon$$

- Choice of aliasing effects $\Rightarrow$ define the degree q of resolution
- Reduce the number of experiments to 2^{p-q}

Example with $p = 3$ and $q = 1$

X_1	X_2	$X_3 \equiv X_1 X_2$
0	0	1
1	0	0
0	1	0
1	1	1



$N = 2^{3-1}$ simulations

The fractional factorial design

Resolution

- Resolution 3 : Main effects may be aliased with two interaction effects
- Resolution 4 : Two interaction effects can be aliased
- Resolution 5 : Main effects are aliased with n-interaction effects, $n \geq 4$

	p							
	3	4	5	6	7	8	9	10
$N = 2^{p-q}$ / $N = 2^p$	8	16	32	64	128	256	512	1024
4	III							
8		IV	III	III	III			
16			V	IV	IV	IV	III	III
32				V	IV	IV	IV	IV
64					VII	V	IV	IV
128						VIII	VI	V
256							IX	VI
512								X

Drawbacks

- Determine which effects are aliasing

Factorial designs

To sum up

- Factorial designs are optimal for analytical polynomial models
- Fractional designs imply aliasing and degree of resolution
- Many other designs exit for polynomial/surface of response

Advantages

- Once the model is well defined, an optimal design can be easily built
- The number of experiments is minimized with respect to the complexity of the model
- The inputs-output relationship can be easily interpreted

Drawbacks

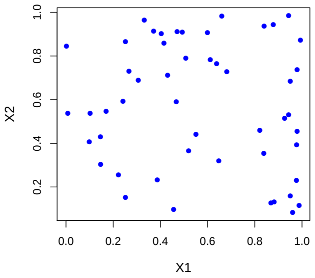
- All experiments have to be made
- Very oriented by the choice of the model
- Not suited to complex models

Numerical designs

Why a numerical design ?

- No assumption on the form of the model $Y(x)$
- General designs well suited to a large number of models
- Fill in "regularly and correctly" the inputs space by a number N of points

The Monte Carlo design



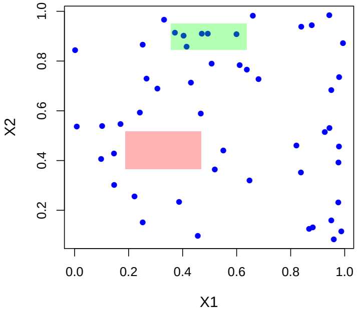
Does this "regurlarly and correctly" fill in the space ?

Numerical designs

What does "regularly and correctly" mean ?

- **Correctly :** The inputs space is entirely covered
- **Regularly :** No subspaces are over/under covered : No points to be too closed together

The Monte Carlo design



Does this "regurlarly and correctly" fill in the space ?

Not correctly

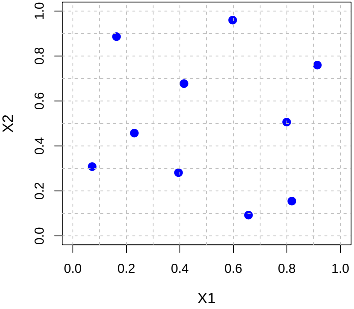
Not regularly

The Latin Hypercube Sampling (LHS)

The principle

- Divide each axis $[0,1]$ into N equally spaced intervals $[0, 1/N), \cdots, [(N-1)/N, 1]$
- Select randomly N points s.t. each appears exactly once in each row and each column of this grid

The LHS design



Optimization criteria

- Measure of closeness of the points in the N-points set $\mathcal{D}$. For example,

$$\max_{\mathcal{D}} \min_{\mathbf{x}^1, \mathbf{x}^2 \in \mathcal{D}} d(\mathbf{x}^1, \mathbf{x}^2),$$

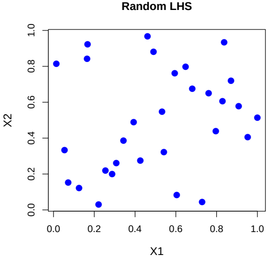
  Usually, $d(x, y) = \sqrt{\sum_j (x_j - y_j)^2}$
  - Low cost
  - Very efficient for small p only
- Low discrepancy sequence : proportion of points falling into an arbitrary set $\mathcal{B}$ close to proportional to the measure of $\mathcal{B}$

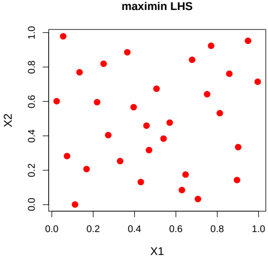
$$D_N(\mathcal{P}) = \sup_{\mathcal{B}} \left| \frac{A(\mathcal{B}; \mathcal{P})}{N} - \lambda(\mathcal{B}) \right|$$

- Sobol, Halton, Faure, . . . , sequences
- Fast convergence of the mean estimate
- Very complex to build

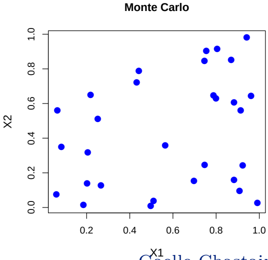
Optimization criteria

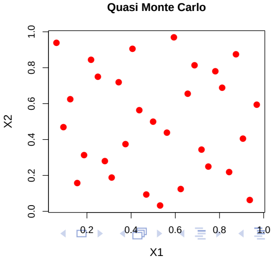
Maximin standard





Low discrepancy sequence





Numerical designs

To sum up

- Numerical designs are more adapted to complex models/computer experiments
- Are space filling designs

Advantages

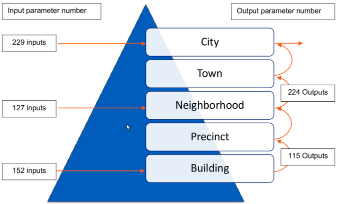
- Well suited for non linear models
- Cover a large variation domain
- The experiments are deterministic and the number can be increased if necessary

Drawbacks

- Define the best criteria to be optimized
- Can fail in high dimension

Sensitivity analysis methods

Industrial case study : The simulation of sustainable cities

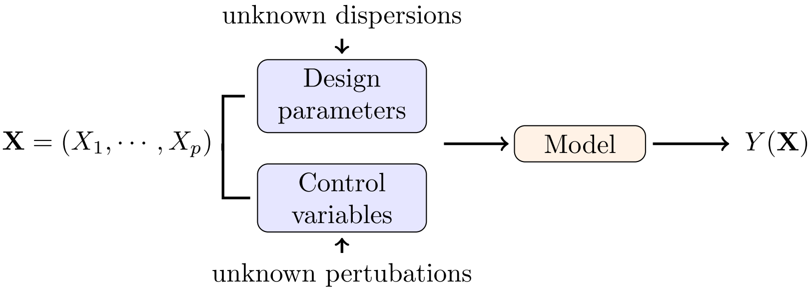


- Quantity of interest : Total annual thermal production, and treated waste
- 55 Input parameters : temperature, building features, waste, use of natural ressources,. . .

Why a sensitivity analysis ?

- The model is too time-consuming/complex because it depends on many input parameters
- Inputs are subject to different sources of variability ⇒ poor confidence in the response

The general context



Hypotheses

- The components of $\mathbf{X}$ are independent
- $\mathbf{X}$ are uniformely distributed $\mathcal{U}[0,1]^p$
- $Y \in L^2(\mathbb{R})$ i.e.

$$\int Y^2(\mathbf{x}) f_Y(\mathbf{x}) d\mathbf{x} = \mathbb{E}[Y^2(\mathbf{X})] < +\infty$$

The sensitivity analysis

What is sensitivity analysis ?

Identify the X_i's that most contribute to the variability of $Y(\mathbf{X})$

- Which one is the most/least influent ?
- What is the weight of the each contribution ?

What is sensitivity analysis for ?

- Understand/check if a model is a good approximation of the physical system/process
- Increase the confidence into the model
- Reduce the number of input parameters
- Determine if parameters interact with each other

Families of sensitivity methods

1. Screening methods
   - Morris algorithm
2. Local methods
   - Quadratic summation method
3. Global methods
   - The Sobol index

Screening methods

Goal

- Well suited to an important number of inputs and an expensive code
- Aim to determine a few influential factors and a majority of non influential ones $\Rightarrow$ reduce the model dimension
- These are qualitative methods to rank (groups of) parameters in order of importance

The general idea

- Based on the discretization of the inputs space called levels
- Linked to the field of designs of experiments

The Morris method

Preliminary

- Set a regular grid Ω of $[0,1]^p$ into Q levels :
  $\Omega = \left\{0, \frac{1}{Q-1}, \frac{2}{Q-1}, \cdots, 1\right\}^p$
- Choose a perturbation $\Delta \in [0,1]$ and $\Delta \propto \frac{1}{Q-1}$

The path

For $\mathbf{x}^* \in \Omega$ randomly chosen, One at A Time (OAT) design :

1. First point $P_0^* = Y(\mathbf{x}^*)$
2. Select a component, say x_i^*, disturbed by Δ

$$P_1^* = Y(x_1^*, \cdots, x_i^* \pm \Delta, x_{i+1}^*, \cdots, x_p^*)$$

3. Select $j \neq i$, and compute

$$P_2^* = Y(x_1^*, \cdots, x_i^* \pm \Delta, \cdots, x_j^* \pm \Delta, \cdots, x_p^*)$$

4. Repeat 3 until $x_1, \cdots, x_p$ successively vary $\Rightarrow P = \{P_0^*, \cdots, P_p^*\}$

The OAT design

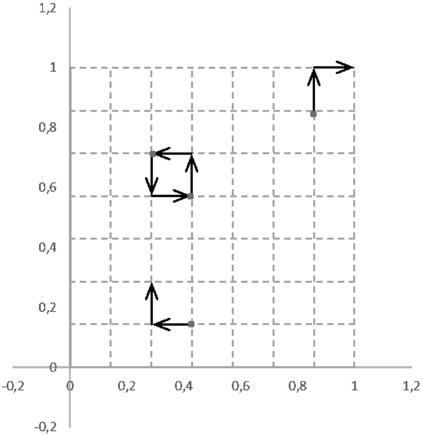


Figure: Examples of 4 paths in two dimensions. The support $[0, 1]$ is discretized into $Q = 8$ levels ; The perturbation is $\Delta = \frac{1}{7}$

The Morris algorithm

Repeat the previous procedure r times, so that there is $P^1, \cdots, P^r$ paths

Elementary effect of X_i

For a path P^k

$$d_i^k = \frac{|Y(\cdots, x_i^1 \pm \Delta, \cdots) - Y(\cdots, x_i^1, \cdots)|}{\Delta}$$

The mean effect of X_i

$$\mu_i = \frac{1}{r} \sum_{k=1}^{r} d_i^k$$

The variation effect of X_i

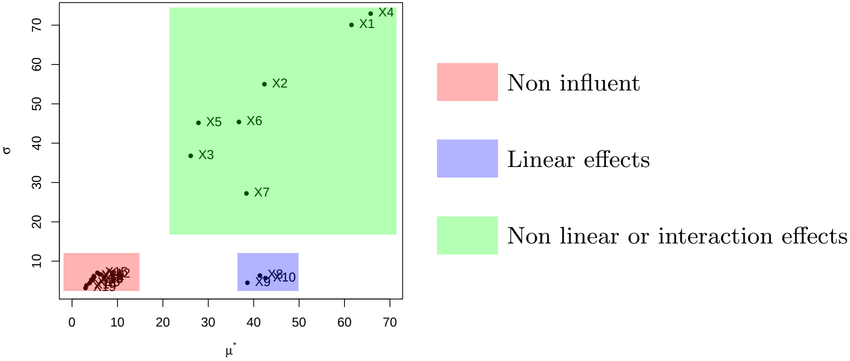
$$\sigma_i = \sqrt{\frac{1}{r-1} \sum_{k=1}^{r} (d_i^k - \mu_i)^2}$$

The cost

Requires $r(p+1)$ simulations

The Morris algorithm

Graphical representation of (μ_i, σ_i), for all $i \in \{1, \cdots, p\}$
Example on the Morris function ($p = 20$)



The Morris algorithm

To sum up

- Construct a OAT design and conpute the elementary effects from r paths
- If $(\mu_i, \sigma_i) \simeq 0$, the parameters are non influent
- If the variation effect $\sigma_i \simeq 0$ but $\mu_i \neq 0$, the parameters have linear effects

Advantages

- Intuitive and easy to use
- Only $r(p+1)$ simulations required
- Does not require any assumptions of the model's regularity

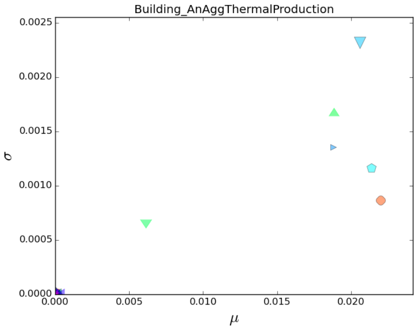
Drawbacks

- Qualitative method to detect the least influent parameters only
- Not able to split non linear effects from the interact ones

The simulation of sustainable cities

- Output : Total annual thermal production
- 55 Inputs : temperature, building features, waste, use of natural ressources,...

The screening results



Selected parameters : electricity demand, surface,luminaire.

Local methods

Goal

- Deterministic method
- Provide the slope of Y in the parameter space at given values
- Allow a rapid preliminary exploration of the model

The intuitive idea

1. Locally disturb one parameter X_i at a time
2. Run the model with the perturbated X_i
3. Compare with the response without perturbation, i.e.

$$\frac{Y(X_i + \Delta_{X_i}) - Y(X_i)}{\Delta_{X_i}} \simeq \frac{\partial Y}{\partial X_i}$$

The quadratic summation method

The Taylor expansion

$$
\begin{aligned}
Y(\mathbf{X}) \quad = \quad & Y(\mu) + \sum_{i=1}^{p} \left.\frac{\partial Y}{\partial X_i}\right|_{\mathbf{X}=\mu} (X_i - \mu_i) \\
& + \frac{1}{2} \sum_{i=1}^{p} \sum_{j=1}^{p} \left.\frac{\partial^2 Y}{\partial X_i \partial X_j}\right|_{\mathbf{X}=\mu} (X_i - \mu_i) \cdot (X_j - \mu_j) + o(\|\mathbf{X} - \mu\|)
\end{aligned}
$$

Hypotheses

- The model is linear around μ
- μ_i is the nominal value of X_i
- $V(X_i)$, $V(Y)$ are the variances of X_i and Y

The quadratic summation method

The Taylor expansion becomes

$$Y(\mathbf{X}) = Y(\mu) + \sum_{i=1}^{p} \left.\frac{\partial Y}{\partial X_i}\right|_{\mathbf{X}=\mu} (X_i - \mu_i)$$

Then

$$V(Y) = \sum_{i=1}^{p} \left(\left.\frac{\partial Y}{\partial X_i}\right|_{\mathbf{X}=\mu} \right)^2 V(X_i)$$

Scaled sensitivity index

$$\boxed{\eta_i^2 = \left(\left.\frac{\partial Y}{\partial X_i}\right|_{\mathbf{X}=\mu} \right)^2 \frac{V(X_i)}{V(Y)} \in [0;1]}$$

Estimation method

- Monte Carlo estimation to compute $V(X_i)$ and $V(Y)$
- Automatic differentiation, finite differences to get the partial derivatives

Summary

To sum up

- Local variation of the inputs around a nominal value
- Estimation of partial derivatives

Advantages

- Useful information on the behavior of Y near the nominal values of parameters
- Rapid preliminary exploration of the model
- Could be well suited to the probability of failure

Drawbacks

- Can only be used when the model is linear or when the variation around a baseline is small
- Not well suited to measure the effects of various parameters on the output

The simulation of sustainable cities

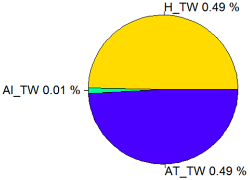
- Output : Total treated waste
- Inputs :
  1. ACT Households 1
     1. Population (H_pop)
     2. Total Treated Waste (H_TW)
  2. ACT Activities Industrials W1
     1. Population (AI_pop)
     2. Total Treated Waste (AI_TW)
  3. ACT Tertiary Activities W1
     1. Population (AT_pop)
     2. Total Treated Waste (AT_TW)

Taylor expansion around the mean

1-order	2-order
592,332	592,842

$\Rightarrow$ Linear model

Local sensitivity indices



Global methods

Goal

- Instead of local perturbation, global methods aim to consider the whole input space
- Able to quantify (and to rank) the sensitivity of each parameter on the model response
- Able to quantify the interactions among parameters

The general idea

- Based on the random distribution of inputs-output
- Generate a sample of observations from the inputs distribution

The Sobol index

Intuitive idea

- When X_i is fixed, how does the output Y behave ?

$$V(Y|X_i) \quad \text{and} \quad \mathbb{E}[V(Y|X_i)]$$

  X_i is influent if $\mathbb{E}[V(Y|X_i)]$ is small

- The total variance decomposition

$$V(Y) = \mathbb{E}[V(Y|X_i)] + V[\mathbb{E}(Y|X_i)]$$

- The first-order Sobol index

$$\boxed{S_i = \frac{V[\mathbb{E}(Y|X_i)]}{V(Y)} \in [0,1]}$$

  X_i is influent if S_i is close to 1.

The FANOVA

The functional decomposition ANOVA

$$Y(\mathbf{X}) = Y_0 + \sum_{i=1}^{p} Y_i(X_i) + \sum_{i<j=1}^{p} Y_{ij}(X_i, X_j) + \cdots + Y_{1\cdots p}(\mathbf{X}) \qquad (1)$$

The decomposition exists and is unique if

$$\mathbb{E}[Y_u(\mathbf{X}_u)Y_v(\mathbf{X}_v)] = 0, \ \forall u \neq v \subseteq \{1, \cdots, p\}$$

Applying the variance to (1),

$$V[Y(\mathbf{X})] = \sum_{i=1}^{p} V[Y_i(X_i)] + \sum_{i<j=1}^{p} V[Y_{ij}(X_i, X_j)] + \cdots + V[Y_{1\cdots p}(\mathbf{X})]$$

The Sobol index

The Sobol index of a group of parameters $\mathbf{X}_u$

$$S_u = \frac{V[Y_u(\mathbf{X}_u)]}{V[Y(\mathbf{X})]}$$

Properties of the FANOVA

$$\begin{array}{lcl} Y_0 & = & \mathbb{E}[Y(\mathbf{X})] \\ Y_i(X_i) & = & \mathbb{E}[Y(\mathbf{X})|X_i] - Y_0 \\ Y_{ij}(X_i, X_j) & = & \mathbb{E}[Y(\mathbf{X})|X_i, X_j] - \mathbb{E}[Y(\mathbf{X})|X_i] - \mathbb{E}[Y(\mathbf{X})|X_j] + Y_0 \\ & & \vdots \end{array}$$

Finally, the first-order Sobol index of X_i is

$$\boxed{S_i = \frac{V[\mathbb{E}(Y(\mathbf{X})|X_i)]}{V[Y(\mathbf{X})]}}$$

The second-order Sobol index of the couple (X_i, X_j) is

$$\boxed{S_{ij} = \frac{V[\mathbb{E}(Y(\mathbf{X})|X_i, X_j)]}{V[Y(\mathbf{X})]} - S_i - S_j}$$

The Sobol index

Properties of the Sobol index

- $2^p - 1$ Sobol indices are constructed
- $S_i \in [0, 1]$. The closer to 1, the more influent is X_i
- If $\sum_{i=1}^{p} S_i = 1$, the model is additive
- The total index measures the total contribution of X_i

$$S_{T_i} = \sum_{u \ni i} S_u$$

Sobol index estimation

- Monte Carlo estimation
- Spectral decomposition (FAST)
- Meta-modeling if the model is too expensive (linear model, polynomial chaos)

The Monte Carlo estimation

Let

- $\mathbf{X} = (X_i, \mathbf{X}_{-i})$ and an independent copy $\mathbf{X}^* = (X_i, \mathbf{X}^*_{-i})$
- $Y = Y(\mathbf{X})$, $Y^* = Y(\mathbf{X}^*)$

Then

$$S_i = \frac{\mathrm{Cov}(Y, Y^*)}{V(Y)}$$

- Take two independant n-samples $(\mathbf{x}^l)_{l=1}^n$, $(\mathbf{x}^{*,l})_{l=1}^n$
- Set $y^l = y(\mathbf{x}^l)$ and $y^{*,l} = y(x_i^l, \mathbf{x}^{*,l}_{-i})$

The estimation of S_i is

$$\hat{S}_i = \frac{\sum_{l=1}^n (y^l - \bar{y}) \cdot (y^{*,l} - \bar{y^*})}{\sum_{l=1}^n (y^l - \bar{y})^2}, \quad \bar{y} = \frac{1}{n} \sum_{l=1}^n y^l, \ \bar{y^*} = \frac{1}{n} \sum_{l=1}^n y^{*,l}$$

The numerical cost is $n(p+1)$ for first order indices

Summary

To sum up

- Sensitivity indices based on variance decomposition
- S_u, for $|u| \geq 2$ quantifies the interaction of parameters $\mathbf{X}_u$
- The closer is S_u to 1, the more influent the group $\mathbf{X}_u$ is

Advantages

- Global sensitivity measure able to detect interactions
- Clear and unambiguous definition of sensitivity
- Many techniques have been developped to estimate Sobol indices

Drawbacks

- The estimation can be very expensive
- The FANOVA expansion is not true if input parameters are dependent

The simulation of sustainable cities

- Output : Total treated waste
- Inputs :
  1. ACT Households 1
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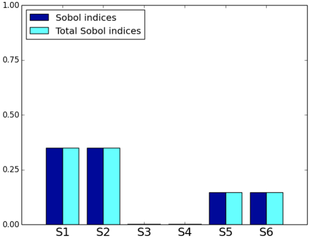
First-order Sobol indices



User's guide

The aim of the sensibility analysis is to...

	Screening	Local	Global method
Rank variables	x	x	x
Quantify sensitivity		x	x
Look at around a nominal value		x	
Explore the whole inputs space	x		x

What to do if the model is/has ...

	Expensive	Large p
Expensive	Sobol[2] + meta-modeling[4]	
Large p	Morris[1]	Morris[1] + Sobol

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