Sensitivity Analysis - Exercises
EMSE, Major "Data Science"

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In the following, we assume that $X_1, \dots, X_d$ are *independent* random variables with probability measures $\nu_1, \dots, \nu_d$. We denote:

- $X = (X_1, \dots, X_d)$;
- $\nu = \nu_1 \otimes \dots \otimes \nu_d$ the probability measure of X;
- $\Delta = \Delta_1 \times \dots \times \Delta_d$, the integration domain;
- $m_i^{(1)} = E(X_i)$, $m_i^{(2)} = E(X_i^2)$: the first and second order moments.

1 Additive functions - 1st order polynomials & SRCs.

Consider an additive function:

$$f(x) = \beta_0 + f_1(x_1) + \dots + f_d(x_d),$$

where the $f_i(X_i)$'s are *centered* (with respect to the measure μ_i) and square-integrable.

1. What should be the ANOVA decomposition of f? Prove it and compute all Sobol indices.
2. Deduce from 1 the ANOVA decomposition of a first order polynomial:

   $$f(x) = \beta_0 + \beta_1 x_1 + \dots + \beta_d x_d$$

   and all Sobol indices. The results can be expressed in function of the $m_i^{(1)}$'s.
3. Deduce that the Sobol indices of a 1st order polynomial are equal to the squared SRCs.

2 Models with product interactions

Consider a 2-dimensional function of the form:

$$f(x) = \beta_0 + f_1(x_1) + f_2(x_2) + \lambda g_1(x_1) g_2(x_2)$$

where the $f_i(X_i)$'s and $g_i(X_i)$'s are *centered* and square-integrable.

1. What should be the ANOVA decomposition of f? Prove it and compute all Sobol indices.
2. Deduce from 1 the ANOVA decomposition of a first order polynomial with interactions:

   $$f(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2$$

   as well as the Sobol indices in the following cases:

   (a) $X_1$and X_2 are centered;

   (b) In general: Express the results in function of the $m_i^{(1)}$'s.
3. Same question with a second order polynomial with interactions. Then express the results also with the $m_i^{(2)}$'s.

3 A 3-dimensional test-function

The ***Ishigami*** function is defined over $\Delta := [-\pi; \pi]^3$ by:

$$f(x) = \sin(x_1) + A\sin^2(x_2) + Bx_3^4\sin(x_1)$$

with A = 7 and B = 0.1.

1. Visualize the function, by cutting it at different levels of x_2.
2. Compute the ANOVA decomposition and Sobol indices when μ is uniform over Δ.
3. Estimate the main effects by using simulations of the inputs. Plot them on the same figure and compare with the theoretical ones. Same question with the 2-dimensional projection over (x_1, x_3) and the second order interaction $f_{1,3}(x_1, x_3)$.

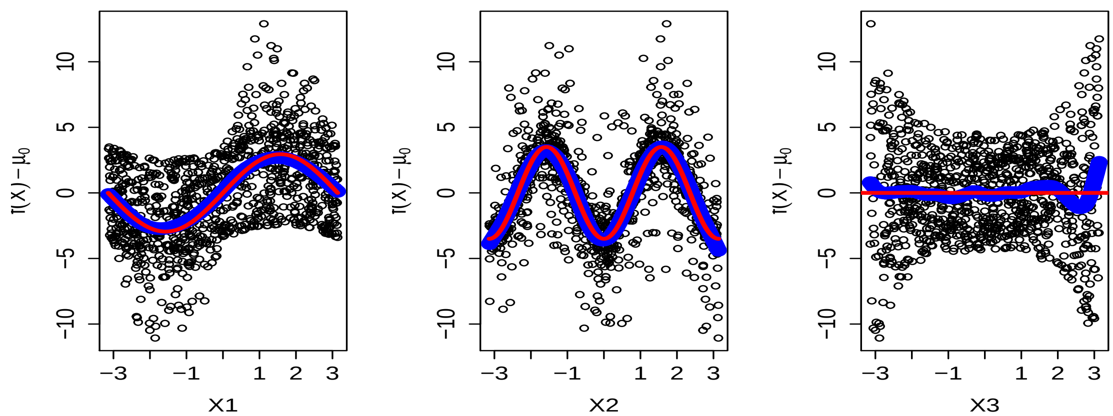

Figure 1: Main effects of Ishigami function: Theoretical (straight line) and estimated (bold line)

4 1-mean separable functions

Consider a separable (or "tensor-product") function of the form:

$$f(x) = \prod_{i=1}^{d}(1 + f_i(x_i))$$

where the $f_i(X_i)$'s are *centered* and square-integrable.

1. What is the ANOVA decomposition of f? Compute all Sobol indices.
2. Considering the uniform measure over $[0, 1]^d$, deduce from 1 the ANOVA decomposition and the Sobol indices of the famous ***g-Sobol*** function:

$$f(x) = \prod_{i=1}^{d} \frac{|4x_i - 2| + a_i}{1 + a_i}$$

   where the a_i's are non-negative real numbers.

3. Let $d = 2$, and $a_1 = 1, a_2 = 5$. Perform simulations of the inputs (denote them X^{*k}, $k = 1, \ldots, N\}$, and estimate the main effects. Draw them on the same figure, and compare with the theoretical ones.

5 Closed and total indices. Pick-and-freeze formulas (Sobol)

In this exercise, we consider a function f such that $f(X)$ is in $L^2(\nu)$, and denote by $\sigma^2 = \mathrm{var}(f(X))$ the overall variance, $D_I = \mathrm{var}(E[f(X)|X_I])$, and $S_I = D_I/\sigma^2$ the Sobol indices.

1. Prove that the un-normalized Sobol index of X_1 is given by:

$$D_1 = \mathbf{cov}(f(X_1, X_{-1}), f(X_1, Z_{-1})),$$

   where Z_{-1} is an independent copy of X_{-1} (same distribution and independent of the X_i's). *Hint: Conditionaly to X_1, what can you say of $f(X_1, X_{-1})$ and $f(X_1, Z_{-1})$?*

2. Deduce that:

$$D_1 = \int_{\Delta\times\Delta_{-1}} f(x_1, x_2, \ldots, x_d) f(x_1, z_2, \ldots, z_d) d\nu(x) d\nu_{-1}(z_{-1}) - (\mu_0)^2$$

   Explain how to compute numerically D_1 and S_1. Justify the word "pick-and-freeze".

3. Generalize to "***closed indices***" $D_I^C := \sum_{J\subseteq I} D_J$ for a subset I.

4. Explain how Sobol indices are obtained from closed indices: For instance, express $D_{1,2}$ as a linear combination of closed indices.

5. Prove the pick-and-freeze formula for "***total indices***", $D_i^T = \sum_{J\supseteq\{i\}} D_J$:

$$D_1^T = \frac{1}{2}\mathbf{var}(f(X_1, X_{-1}) - f(Z_1, X_{-1})),$$

   or equivalently:

$$D_1^T = \frac{1}{2}\int_{\Delta\times\Delta_1} [f(x_1, x_2, \ldots, x_d) - f(z_1, x_2, \ldots, x_d)]^2 d\nu(x) d\nu_1(z_1)$$

   Hint: Prove first that $D_1^T = \sigma^2 - D_{-1}^C$.

6. Generalize to a subset I, with $D_I^T := \sum_{J\cap I\neq\emptyset} D_J$.

.../...

6 Computer lab

The aim of the lab is to perform a global SA of the 3-dimensional Ishigami (toy) function, directly on it, or on a Kriging metamodel.

1. Consider the Ishigami function of Exercise 3. Perform question 3.

2. Estimate the Sobol indices of Ishigami, with **R** package **sensitivity** (function `fast99`).

3. In this question we build a Kriging metamodel for Ishigami. We first consider a design size of $n = 30$.

   (a) Build a maximin Latin hypercube design X with **DiceDesign** (function `maximinESE_LHS`). Visualize the space-filling properties (compare visually with the uniform design serving as a initial design for `maximinESE_LHS`).

   (b) Compute the response y at X, and construct a Kriging model with **DiceKriging**. Look at the validation results.

4. Perform a sensitivity analysis on the Kriging metamodel. For that goal, use `sensitivity::fast99` function on the following wrapper:
   ```
   kriging.mean <- function(Xnew, m) {
   predict(m, Xnew, "UK", se.compute = FALSE, checkNames = FALSE)$mean
   }
   ```
   where `m` is the name of the metamodel object of question 3.b.

5. Compare the results of 2 and 4.

6. Redo questions 3-5 with $n = 60, 90$. Conclusion?