Sensitivity Analysis - INSA Toulouse - 2019-2020
Correction of the exercise on Polynomial Chaos

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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:

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

1 Polynomial chaos

Polynomial chaos are defined as a tensor basis of orthonormal polynomials. It is very famous in sensitivity analysis since, as we see now, the Sobol indices are easily computed by sum of squares.

For each probability distribution ν_i $(i = 1, \dots, d)$, we denote by

$$P_{i,0}(x_i) = 1, \quad P_{i,1}(x_i), \quad \dots \quad P_{i,\ell}(x_i), \quad \dots$$

a set of orthonormal polynomials in $L^2(\nu_i)$ (of degree $0, 1, 2, \dots, \ell, \dots$). Then the *polynomial chaos* indexed by the multi-index $\underline{\ell} = (\ell_1, \dots, \ell_d)$ is the tensor:

$$P_{\underline{\ell}}(x) = \prod_{i=1}^{d} P_{i,\ell_i}(x_i).$$

We denote by $\mathcal{I} = \mathbb{N}^d$ the set of all multi-indices.

1. For two multi-indices $\underline{\ell}, \underline{\ell'}$, compute $\langle P_{\underline{\ell}}, P_{\underline{\ell'}} \rangle = \mathbb{E}(P_{\underline{\ell}}(X) P_{\underline{\ell'}}(X))$. Deduce that polynomial chaos are orthonormal in $L^2(\nu)$. We admit that they form a Hilbert basis of $L^2(\nu)$.

   By independence of the input variables,

   $$\mathbb{E}(P_{\underline{\ell}}(X) P_{\underline{\ell'}}(X)) = \prod_{i=1}^{d} \mathbb{E}(P_{i,\ell_i}(X_i) P_{i,\ell'_i}(X_i)) = \prod_{i=1}^{d} \delta_{\ell_i, \ell'_i} = \delta_{\underline{\ell}, \underline{\ell'}}$$

2. Deduce the expression of f

   $$f(x) = \sum_{\underline{\ell} \in \mathcal{I}} c_{\underline{\ell}} P_{\underline{\ell}}(x)$$

   with $c_{\underline{\ell}} = \langle f, P_{\underline{\ell}} \rangle$. Express the total variance D in function of the $c_{\underline{\ell}}$'s.

The first formula is just the expansion in an orthonormal basis. By Pythagore's theorem (Parseval formula), we have

$$\mathbb{E}(f(X)^2) = \|f\|^2 = \sum_{\underline{\ell}\in\mathcal{I}} c_{\underline{\ell}}^2.$$

Moreover, $\mathbb{E}(f(X)) = \langle f, 1\rangle = \langle f, P_{\underline{0}}\rangle = c_{\underline{0}}$. *Finally,*

$$D = Var(f(X)) = \sum_{\underline{\ell}\in\mathcal{I}\setminus\underline{0}} c_{\underline{\ell}}^2$$

3. Compute $\mathbb{E}(P_{\underline{\ell}}(X)|X_1)$.

   (We give here a computational proof, in order to practice conditional expectation.)
   Notice that if $\ell_i \neq 0$, *then* P_{i,ℓ_i} *is orthogonal to* $P_{i,0} = 1$, *and hence* $\mathbb{E}(P_{i,\ell_i}) = 0$. *Thus,* $\mathbb{E}(P_{i,\ell_i}) = \delta_{\ell_i,0}$. *Now, by independence of the inputs,*

$$\begin{aligned}\mathbb{E}(P_{\underline{\ell}}(X)|X_1) &= P_{1,\ell_1}(X_1)\mathbb{E}(\prod_{i=2}^{d} P_{i,\ell_i}(X_i)|X_1) \\ &= P_{1,\ell_1}(X_1)\mathbb{E}(\prod_{i=2}^{d} P_{i,\ell_i}(X_i)) = P_{1,\ell_1}(X_1)\prod_{i=2}^{d}\mathbb{E}(P_{i,\ell_i}(X_i)) = P_{1,\ell_1}(X_1)\prod_{i=2}^{d}\delta_{\ell_i,0}\end{aligned}$$

   Hence,

$$\mathbb{E}(P_{\underline{\ell}}(X)|X_1) = \begin{cases} P_{\underline{\ell}}(X) & \text{if } \ell_2 = \cdots = \ell_d = 0 \\ 0 & \text{otherwise}\end{cases}$$

4. Deduce that the first main effect of f is obtained by choosing the tensors that involve *only* X_1, defined by the subset $\mathcal{I}_1 = \{\underline{\ell}\in\mathcal{I} \text{ s.t. } \ell_1 \geq 1, \ell_2 = \cdots = \ell_d = 0\}$. Compute the corresponding Sobol index S_1 in function of the $c_{\underline{\ell}}$.

   The first part is obvious from the previous question, and we thus have

$$f_1(x) = \sum_{\underline{\ell}\in\mathcal{I}_1} c_{\underline{\ell}} P_{\underline{\ell}}(x).$$

   Then, by orthogonality, $D_1 = \sum_{\underline{\ell}\in\mathcal{I}_1} c_{\underline{\ell}}^2$. *Finally* $S_1 = \frac{D_1}{D} = \frac{\sum_{\underline{\ell}\in\mathcal{I}_1} c_{\underline{\ell}}^2}{\sum_{\underline{\ell}\in\mathcal{I}\setminus\underline{0}} c_{\underline{\ell}}^2}$.

5. Similarly, compute $\mathbb{E}(P_{\underline{\ell}}(X)|X_{-1}) = \mathbb{E}(P_{\underline{\ell}}(X)|X_2,\ldots,X_d)$.
   Show that the first total effect of f is obtained by choosing the tensors that involve *at least* X_1, defined by $\mathcal{I}_1^{\text{tot}} = \{\underline{\ell}\in\mathcal{I} \text{ s.t. } \ell_1 \geq 1\}$. Give the expression of the total Sobol index S_1^{tot}.

   Similarly,

$$\mathbb{E}(P_{\underline{\ell}}(X)|X_{-1}) = \mathbb{E}(P_{1,\ell_1}(X_1))\prod_{i=2}^{d} P_{i,\ell_i}(X_i) = \delta_{\ell_1,0}\prod_{i=2}^{d} P_{i,\ell_i}(X_i) = \delta_{\ell_1,0}P_{\underline{\ell}}(X)$$

   Hence, the part of the ANOVA decomposition involving at least x_1 *is:*

$$f_1^{tot}(x) = f(x) - \mathbb{E}(f(X)|X_{-1} = x_{-1}) = \sum_{\underline{\ell}\in\mathcal{I}_1^{tot}} c_{\underline{\ell}} P_{\underline{\ell}}(x).$$

   Then, by orthogonality, $D_1^{tot} = \sum_{\underline{\ell}\in\mathcal{I}_1^{tot}} c_{\underline{\ell}}^2$. *Finally* $S_1 = \frac{D_1^{tot}}{D} = \frac{\sum_{\underline{\ell}\in\mathcal{I}_1^{tot}} c_{\underline{\ell}}^2}{\sum_{\underline{\ell}\in\mathcal{I}} c_{\underline{\ell}}^2}$.