Variance-based sensitivity analysis for functional inputs

Methodology

We observe an application h from n fields $(\boldsymbol{X_1}, \ldots, \boldsymbol{X_n})$
of the associated input process $\boldsymbol{X}$ and n vectors $(\boldsymbol{Y_1}, \ldots, \boldsymbol{Y_n})$

$$h : \left| \begin{array}{ccc} \mathcal{M}_N \times (\mathbb{R}^d)^N & \rightarrow & \mathbb{R}^p \\ \boldsymbol{X} & \mapsto & \boldsymbol{Y} \end{array} \right.$$

We propose the following steps to lead to sensitivity analysis.

- 1. Identify blocks of independent inputs
- 2. Dimension reduction via Karhunen-Loeve for each input block
- 3. Approximate of the link between KL coefficients and vectorial outputs by chaos
- 4. Post-process functional chaos coefficients to derive Sobol‘ indices

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Methodology step 1/3: Dimension reduction by Karhunen-Loeve

We use the Karhunen-Loeve decomposition to find the $(\lambda_k, \boldsymbol{\varphi}_k)_{k\geq 1}$ solutions of the Fredhlom equation:

$$\int_{\mathcal{D}} \boldsymbol{C}(\boldsymbol{s}, \boldsymbol{t})\varphi_k(\boldsymbol{t})\, d\boldsymbol{t} = \lambda_k \varphi_k(\boldsymbol{s}) \quad \forall \boldsymbol{s} \in \mathcal{D}$$

The SVD decomposition helps to approach the covariance function $\boldsymbol{C}$ by its empirical estimator.

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Methodology step 1/3: Dimension reduction by Karhunen-Loeve

The linear projection function $\pi_{\boldsymbol{\lambda},\varphi}$ of the Karhunen-Loeve decomposition writes:

$$\pi_{\boldsymbol{\lambda},\varphi} : \left| \begin{array}{ccc} L^2(\mathcal{D},\mathbb{R}^d) & \rightarrow & \mathcal{S}^{\mathbb{N}} \\ f & \mapsto & \left(\dfrac{1}{\sqrt{\lambda_k}} \int_{\mathcal{D}} f(\boldsymbol{t}) \varphi_k(\boldsymbol{t})\, d\boldsymbol{t} \right)_{k\geq 1} \end{array} \right.$$

This integral is replaced by a specific weighted and finite sum and to write the projections of the j-th marginal of i-th input field $\boldsymbol{X_i^j}$ by multiplication with the projection matrix $\boldsymbol{M^j} \in \mathbb{R}^{K_j} \times \mathbb{R}^{Nd}$:

$$\boldsymbol{M_j X_i^j} = \begin{pmatrix} \xi_1^j \\ \dots \\ \xi_{K_j}^j \end{pmatrix} \in \mathbb{R}^{K_j}, \forall i \in [1,n], \forall j \in [1,d]$$

with K_j the retained number of modes in the decomposition of the j-th input

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Methodology step 1/3: Dimension reduction by Karhunen-Loeve

The projections of all the d components of n fields are assembled in the Q matrix:

$$\boldsymbol{Q} = \boldsymbol{M}\boldsymbol{X} = \begin{pmatrix} \boldsymbol{M_1}\boldsymbol{X^1} \\ \dots \\ \boldsymbol{M_d}\boldsymbol{X^d} \end{pmatrix} \in \mathbb{R}^{K_T} \times \mathbb{R}^{n}$$

with $K_T = \sum_{j=1}^{d} K_j$ the total number of modes accross input components

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Methodology step 2/3: Link KL coefficients to ouputs

Then a functional chaos decomposition is built between the projected modes sample $\boldsymbol{Q}$ and the output samples $\boldsymbol{Y}$

$$\tilde{g}(x) = \sum_{k=1}^{K_c} \beta_{\boldsymbol{\alpha}_k} \Psi_{\boldsymbol{\alpha}_k}(x)$$

The final metamodel consists in the composition of the Karhunen-Loeve projections and the functional chaos metamodel.

$$\tilde{h} : \left| \begin{array}{ccccc} \mathcal{M}_N \times (\mathbb{R}^d)^N & \rightarrow & \mathbb{R}^{K_T} & \rightarrow & \mathbb{R}^p \\ \boldsymbol{X} & \mapsto & \boldsymbol{Q} & \mapsto & \boldsymbol{Y} \end{array} \right.$$

A limitation of this approach is that the projected modes sample has a dimension K_T so the dimension of the input fields $\boldsymbol{X_i}$ and the associated number of modes must remain modest.

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Methodology step 2/3: Link KL coefficients to ouputs

From the chaos decomposition:

$$\tilde{g}(x) = \sum_{k=1}^{K_c} \beta_{\boldsymbol{\alpha}_k} \Psi_{\boldsymbol{\alpha}_k}(x)$$

Lets expand the multi indices notation:

$$\Psi_{\boldsymbol{\alpha}}(x) = \prod_{j=1}^{K_T} P^j_{\alpha_j}(x_j)$$

with α that contains the marginal degrees associated to the K_T input components

$$\boldsymbol{\alpha} \in \mathbb{N}^{K_T} = \{\underbrace{\alpha_1, \ldots, \alpha_{K_1}}_{K_1}, \ldots, \underbrace{\alpha_{K_T - K_d}, \ldots, \alpha_{K_T}}_{K_d}\}$$

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Methodology step 3/3: Derive Sobol' indices from chaos coefficients

Sobol indices of the input field component $j \in [1, d]$ can be computed from the coefficients of the chaos decomposition that involve the matching KL coefficients.

For the first order Sobol indices we sum over the multi-indices $\boldsymbol{\alpha}_k$ that are non-zero on the K_j indices corresponding to the KL decomposition of j-th input and zero on the other $K_T - K_j$ indices (noted G_j):

$$S_j = \frac{\sum_{k=1, \boldsymbol{\alpha}_k \in G_j}^{K_c} \beta_{\boldsymbol{\alpha}_k}^2}{\sum_{k=1}^{K_c} \beta_{\boldsymbol{\alpha}_k}^2}$$

For the total order Sobol indices we sum over the multi-indices $\boldsymbol{\alpha}_k$ that are non-zero on the K_j indices corresponding to the KL decomposition of the j-th input (noted GT_j):

$$S_{T_j} = \frac{\sum_{k=1, \boldsymbol{\alpha}_k \in GT_j}^{K_c} \beta_{\boldsymbol{\alpha}_k}^2}{\sum_{k=1}^{K_c} \beta_{\boldsymbol{\alpha}_k}^2}$$

This generalizes to higher order indices.

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Outlook

- Development is settling down
- Expected to land in OT 1.20 (fall 2022)
- Extension to Vector $\mapsto$ Field, Field $\mapsto$ Field ?