PCE-based imprecise Sobol' indices

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PCE-based Imprecise Sobol' Indices

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Problem Statement & Context

A **computational model** is defined as a mapping:

$$\boldsymbol{x} \in \mathbb{D}_{\boldsymbol{X}} \subset \mathbb{R}^M \rightarrow y = \mathcal{M}(\boldsymbol{x}) \in \mathbb{R}$$

- $\boldsymbol{x}$ is modelled by an *imprecise* random vector $\boldsymbol{X}$, which accounts for both *aleatory* uncertainty (natural variability) and *epistemic* uncertainty (lack of knowledge).
- The elements of $\boldsymbol{X}$ are assumed *statistically independent*.
- The computational model is considered as a *black-box*.

Goal: Sensitivity analysis – estimate the influence of each component $X_i \in \boldsymbol{X}$ on the random response $Y = \mathcal{M}(\boldsymbol{X})$.

PCE-based Sobol' Indices

Considering a **probabilistic** input vector $\boldsymbol{X}$, then a Polynomial Chaos Expansion (PCE) meta-model surrogates $\mathcal{M}$:

$$Y = \mathcal{M}(\boldsymbol{X}) \approx \sum_{\boldsymbol{\alpha} \in \mathcal{A}} a_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{X})$$

- $\psi_{\boldsymbol{\alpha}}(\boldsymbol{X})$: multivariate *orthonormal polynomials* with respect to $\boldsymbol{X}$.
- $a_{\boldsymbol{\alpha}}$: coefficients of the polynomials.
- $\mathcal{A}$: set of $\boldsymbol{\alpha}$ indices determined by an appropriate truncation scheme.
- **Sparse PCE**: obtained with least-angle regression (**LARS**).

Then, PCE-based Sobol' indices read:

$$S^{(\mathrm{P})}_{i_1 \dots i_s} = \sum_{\boldsymbol{\alpha} \in \mathcal{I}_{i_1 \dots i_s}} a^2_{\boldsymbol{\alpha}} \Big/ \sum_{\boldsymbol{\alpha} \in \mathcal{A}, \boldsymbol{\alpha} \neq \boldsymbol{0}} a^2_{\boldsymbol{\alpha}}$$

- $\mathcal{I}_{i_1 \dots i_s} = \{\boldsymbol{\alpha} \in \mathcal{A} : \ \alpha_k > 0 \text{ for all } k \in \{i_1, \dots, i_s\}, \alpha_k = 0 \text{ otherwise}\}$.

$\rightarrow$ Postprocessing of PCE coefficients $\rightarrow$ cheap.

$\rightarrow$ Variance decomposition of probabilistic variability.

$\Rightarrow$ Extension to imprecise probabilities?

Sudret, B. (2008). *Global sensitivity analysis using polynomial chaos expansions.* Reliab. Eng. Sys. Safety 93, 964-979.

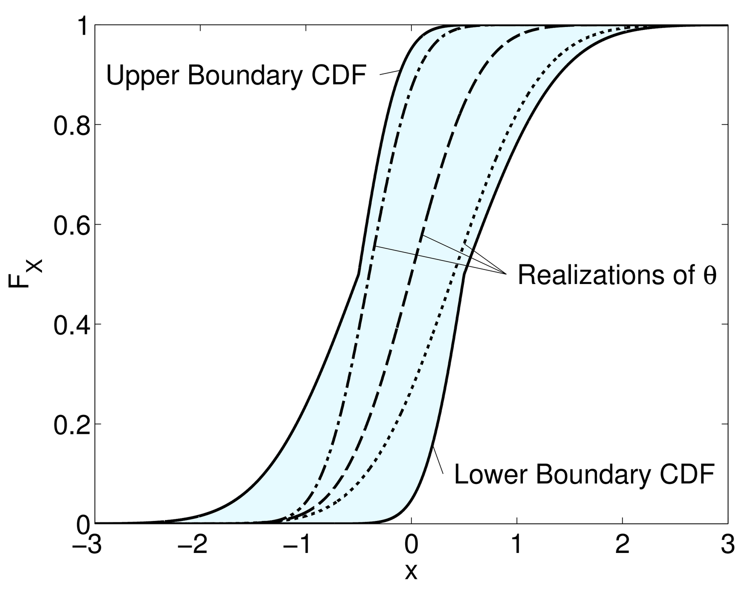
Parametric P-box

Definition: CDF F_X (aleatory uncertainty) with interval-valued distribution parameters $\boldsymbol{\theta}$ (epistemic uncertainty).

e.g. an imprecise Gaussian variable

- $X \sim \mathcal{N}([\underline{\mu}_X, \overline{\mu}_X], [\underline{\sigma}_X, \overline{\sigma}_X])$
- $\boldsymbol{\theta} = \{\mu_X, \sigma_X\}$.

Ferson, S. and J. Hajagos (2004). *Arithmetic with uncertain numbers: rigorous and (often) best possible answers.* Reliab. Eng. Sys. Safety 85(1-3):135–152.



Imprecise Sobol' Indices

Idea: Separation of sources of uncertainty within Sobol' indices:

- Aleatory uncertainty $\Rightarrow$ value of conventional Sobol' indices
- Epistemic uncertainty $\Rightarrow$ interval-valued indices

Augmented PCE

Definition: Augmented input vector $\boldsymbol{V} = (\boldsymbol{C}, \boldsymbol{\Theta})$ with $C_i = F_{X_i}(X_i; \Theta_i)$ and hence $C_i \sim \mathcal{U}(0,1)$. Then:

$$W = \mathcal{M}\left(F^{-1}_{\boldsymbol{X}}(\boldsymbol{C}; \boldsymbol{\Theta})\right) \stackrel{\text{def}}{=} \mathcal{M}^{(\text{aug})}(\boldsymbol{V})$$

Consider Θ_i as *uniform distributions*, PCE meta-model for W as a function of $\boldsymbol{V}$:

$$W \approx \mathcal{M}^{(\text{PCE})}(\boldsymbol{V}) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}} a_{\boldsymbol{\alpha}} \, \psi_{\boldsymbol{\alpha}}(\boldsymbol{V})$$

where $\psi_{\boldsymbol{\alpha}}(\boldsymbol{V})$ are multivariate *orthonormal polynomials* with respect to $\boldsymbol{V}$.

PCE-based Imprecise Sobol' Indices

Reordering to a PCE in terms of $\boldsymbol{C}$ (aleatory uncertainty):

$$W(\boldsymbol{\theta}) \approx \sum_{\boldsymbol{\alpha}^*_C \in \mathcal{A}^*_C} a_{\boldsymbol{\alpha}^*_C}(\boldsymbol{\theta}) \, \psi_{\boldsymbol{\alpha}^*_C}(\boldsymbol{C})$$

where $a_{\boldsymbol{\alpha}^*_C}$ is a combination of $a_{\boldsymbol{\alpha}}$ and $\psi_{\boldsymbol{\alpha}_{\boldsymbol{\Theta}}}(\boldsymbol{\Theta})$. Then, bounds of the Sobol' indices:

$$\underline{S}^{(\mathrm{P})}_{i_1 \dots i_s} = \min_{\boldsymbol{\theta} \in \mathcal{D}_{\boldsymbol{\Theta}}} \sum_{\boldsymbol{\alpha}^*_C \in \mathcal{I}_{i_1,\dots,i_s}} a^2_{\boldsymbol{\alpha}^*_C}(\boldsymbol{\theta}) \Big/ \sum_{\boldsymbol{\alpha}^*_C \in \mathcal{A}^*_C, \boldsymbol{\alpha}^*_C \neq \boldsymbol{0}} a^2_{\boldsymbol{\alpha}^*_C}(\boldsymbol{\theta})$$

$$\overline{S}^{(\mathrm{P})}_{i_1 \dots i_s} = \max_{\boldsymbol{\theta} \in \mathcal{D}_{\boldsymbol{\Theta}}} \sum_{\boldsymbol{\alpha}^*_C \in \mathcal{I}_{i_1,\dots,i_s}} a^2_{\boldsymbol{\alpha}^*_C}(\boldsymbol{\theta}) \Big/ \sum_{\boldsymbol{\alpha}^*_C \in \mathcal{A}^*_C, \boldsymbol{\alpha}^*_C \neq \boldsymbol{0}} a^2_{\boldsymbol{\alpha}^*_C}(\boldsymbol{\theta})$$

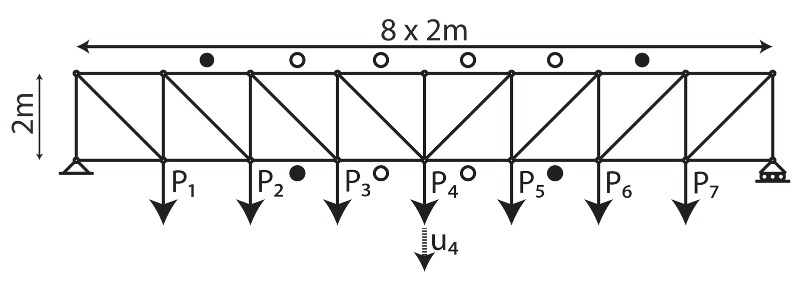
$\Rightarrow$ Postprocessing of augmented PCE $\Rightarrow$ **cheap optimizations**.

Schöbi, R. and B. Sudret (2015). *Propagation of uncertainties modelled by parametric p-boxes using sparse polynomial chaos expansions.* In Proc. 12th Int. Conf. on Applications of Stat. and Prob. in Civil Engineering (ICASP12), Vancouver, Canada.

Example: Simply Supported Truss

Problem: assess deflection $u_4(\boldsymbol{p})$ of truss (Hurtado, 2013):

- Loads P_i, $i = 1, \dots, 7$ independent.
- $\mu_{P_i} \in [95, 105]$ kN, $\sigma_{P_i} \in [13, 17]$ kN.

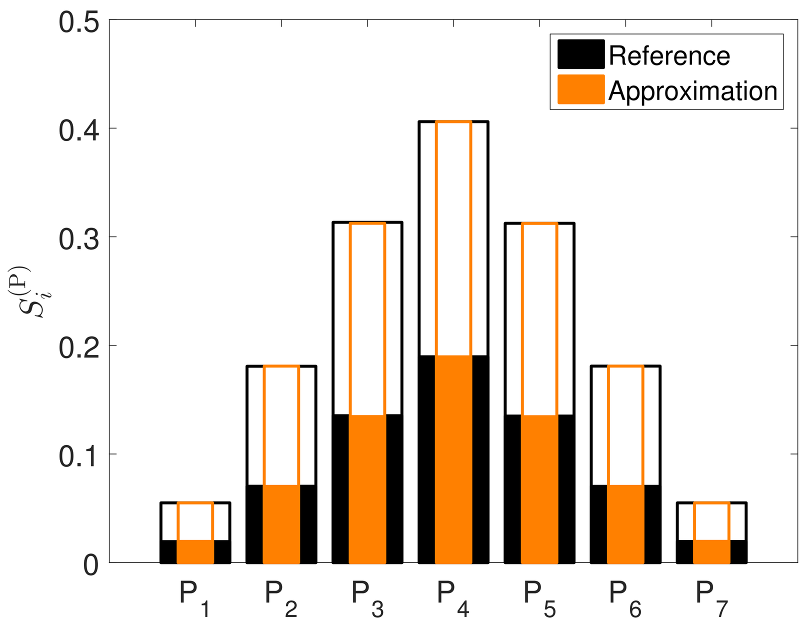


Augmented PCE: $N = 100$ LHS samples.

Results:

- Computation of first order indices
- $\begin{cases} \underline{S} \rightarrow \text{solid bar} \\ \overline{S} \rightarrow \text{hollow bar} \end{cases}$

$\Rightarrow$ High accuracy in estimates of Sobol' indices



Hurtado, J.E. (2013). *Assessment of reliability intervals under input distributions with uncertain parameters.* Prob. Eng. Mech., 32:80-92.

Conclusions

- The augmented input space allows for a **distinction between aleatory and epistemic uncertainty** in $\boldsymbol{X}$.
- **Imprecise Sobol' indices** allow for a distinction between aleatory and epistemic uncertainty in sensitivity analysis.
- **Augmented PCE** makes sensitivity analysis tractable for expensive-to-evaluate models with random input described by parametric p-boxes.

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