Low-rank Tensor Approximations for Sensitivity Analysis of Complex Models with High-Dimensional Input

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Introduction

› Increasingly complex computer models are used nowadays across engineering and sciences

› Sensitivity analysis requiring repeated runs of a complex model may become intractable

› A solution is offered by meta-models that mimic the behavior of complex models while having simple functional forms
Outline

› Variance-based sensitivity analysis

› From Polynomial Chaos Expansions (PCE) to Low-rank Approximations (LRA)

› Sensitivity analysis with LRA

› Example applications
  › Structural engineering
  › Heat conduction
  › Hydro-geology
Sensitivity analysis

\( \mathbf{X} = \{X_1, \ldots, X_M\} \quad \rightarrow \quad Y = \mathcal{M}(\mathbf{X}) \)

- Variance decomposition of model response for independent input:

\[
D = \text{Var}[\mathcal{M}(\mathbf{X})] = \sum_{i=1}^{M} D_i + \sum_{1 \leq i, j \leq M} D_{i,j} + \cdots + D_{1,2,\ldots,M}
\]

- Sobol' sensitivity index:

\[
S_\mathbf{u} = \frac{D_\mathbf{u}}{D}, \quad \mathbf{u} = \{i_1, \ldots, i_s\}, \quad 1 \leq s \leq M
\]
Sensitivity analysis

- First order Sobol' sensitivity index:

\[
S_i = \frac{D_i}{D} = \frac{\text{Var}[\mathbb{E}[\mathcal{M}(\mathbf{X}|X_i)]]}{\text{Var}[\mathcal{M}(\mathbf{X})]} = \frac{\mathbb{E}[\mathbb{E}[\mathcal{M}(\mathbf{X}|X_i)]^2] - \mathbb{E}[\mathcal{M}(\mathbf{X})]^2}{\text{Var}[\mathcal{M}(\mathbf{X})]}
\]

- Total Sobol' sensitivity index:

\[
S_i^T = \sum_{\mathbf{u} \subseteq \{1,\ldots,M\}} \sum_{i \in \mathbf{u}} \frac{D_{\mathbf{u}}}{D} = 1 - \frac{\mathbb{E}[\mathbb{E}[\mathcal{M}(\mathbf{X}|X_i)]^2] - \mathbb{E}[\mathcal{M}(\mathbf{X})]^2}{\text{Var}[\mathcal{M}(\mathbf{X})]}
\]

- First order and total Sobol' sensitivity indices can also be defined for a group of variables

Konakli K, Sudret B, 2016; *Reliability Engineering & System Safety*
Uncertainty analysis with meta-models

\[ X = \{X_1, \ldots, X_M\} \rightarrow Y = \mathcal{M}(X) \]

› Polynomial chaos expansion (PCE)

\[ \hat{Y} = \sum_{\alpha \in \mathcal{A}} y_\alpha \Psi_\alpha(X) \quad \Psi_\alpha(X) = \prod_{i=1}^{M} P^{(i)}_{\alpha_i}(X_i) \]

› Low-rank tensor approximation (LRA)

\[ \hat{Y} = \sum_{l=1}^{R} b_l \left( \prod_{i=1}^{M} \sum_{k=0}^{p_i} z^{(i)}_{kl} P^{(i)}_{k}(X_i) \right) \]
Polynomial chaos expansions

› We consider the mapping \( \mathbf{X} \in D_X \subseteq \mathbb{R}^M \rightarrow Y = \mathcal{M}(\mathbf{X}) \in \mathbb{R} \)

› The PCE approximation of the model response is given by:

\[
\hat{Y} = \sum_{\alpha \in \mathcal{A}} y_\alpha \Psi_\alpha(\mathbf{X})
\]

- \( \Psi_\alpha(\mathbf{X}) \): multivariate polynomials orthogonal w.r.t. the PDF of \( \mathbf{X} \):

\[
\Psi_\alpha(\mathbf{X}) = \prod_{i=1}^{M} P_{\alpha_i}^{(i)}(X_i)
\]

- \( \mathcal{A} \): set of indices defined by an appropriate truncation scheme

- \( y_\alpha \): coefficients obtained by minimizing the difference \( (Y - \hat{Y}) \) over an experimental design (ED)
Low-rank approximations

› PCE face the curse of dimensionality:
  › exponential growth of basis size with input dimension

› In LRA, the number of unknowns grows only linearly with the input dimension:

\[
\hat{Y} = \sum_{l=1}^{R} b_l \left( \prod_{i=1}^{M} \sum_{k=0}^{p_i} z_{kl}^{(i)} P_k^{(i)}(X_i) \right)
\]

› Construction of LRA involves a sequence of small-size minimization problems:
  › Progressive adding of rank-one terms
  › Updating of coefficients along each dimension (alternated least-squares minimization)

Konakli K, Sudret B, 2016; Journal of Computational Physics
Sensitivity analysis with low-rank approximations

First-order Sobol' sensitivity index:

\[
\hat{S}_i = \frac{\mathbb{E} \left[ \mathbb{E} \left( \hat{M}(X|X_i) \right) \right]^2 - \mathbb{E} \left[ \hat{M}(X) \right]^2}{\text{Var} \left[ \hat{M}(X) \right]}
\]

\[
\mathbb{E} \left[ \mathbb{E} \left[ \hat{M}(X|X_i) \right] \right]^2 = \sum_{l=1}^{R} \sum_{l'=1}^{R} b_l b_{l'} \left( \prod_{j \neq i}^{M} z_{0l}^{(j)} z_{0l'}^{(j)} \right) \left( \sum_{k=0}^{p_i} z_{kl}^{(i)} z_{k'l}^{(i)} \right)
\]

\[
\mathbb{E} \left[ \hat{M}(X) \right] = \sum_{l=1}^{R} b_l \left( \prod_{i=1}^{M} z_{0l}^{(i)} \right)
\]

\[
\text{Var} \left[ \hat{M}(X) \right] = \sum_{l=1}^{R} \sum_{l'=1}^{R} b_l b_{l'} \left( \prod_{i=1}^{M} z_{kl}^{(i)} z_{k'l}^{(i)} \right) - \left( \prod_{i=1}^{M} z_{0l}^{(i)} z_{0l'}^{(i)} \right)
\]

Similar expressions are derived for the total sensitivity indices Konakli K, Sudret B, 2016; Reliability Engineering & System Safety
Truss deflection

Dimensionality: $M = 10$

- $A_1, E_1$: properties of horizontal bars
- $A_2, E_2$: properties of diagonal bars

<table>
<thead>
<tr>
<th>Variable</th>
<th>Distribution</th>
<th>Mean</th>
<th>CoV</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1 \text{ (m}^2\text{)}$</td>
<td>Lognormal</td>
<td>0.002</td>
<td>0.10</td>
</tr>
<tr>
<td>$A_2 \text{ (m}^2\text{)}$</td>
<td>Lognormal</td>
<td>0.001</td>
<td>0.10</td>
</tr>
<tr>
<td>$E_1, E_2 \text{ (GPa)}$</td>
<td>Lognormal</td>
<td>210</td>
<td>0.10</td>
</tr>
<tr>
<td>$P_1, \ldots, P_6 \text{ (KN)}$</td>
<td>Gumbel</td>
<td>50</td>
<td>0.15</td>
</tr>
</tbody>
</table>
Truss deflection

Total sensitivity indices
ED based on Sobol sequences, Reference solution based on $10^6$ points

Konakli K, Sudret B, 2016; Reliability Engineering & System Safety
Truss deflection

**Total sensitivity indices**
ED based on LHS, Reference solution based on $10^6$ points

Konakli K, Sudret B, 2016; *Reliability Engineering & System Safety*
Truss deflection

Total sensitivity indices
ED based on LHS, Reference solution based on $10^6$ points

Konakli K, Sudret B, 2016; Reliability Engineering & System Safety
Heat conduction

Dimensionality: $M = 53$

**Thermal conductivity**

- Gaussian random field with square-exponential auto-correlation function
- Underlying standard normal random field approximated as:

$$g(z) \approx \sum_{i=1}^{M} \frac{\xi_{i}}{\sqrt{l_{i}}} \phi_{i}^{T}C_{z}$$

$\xi_{i}$: standard normal random variables
$\phi_{i}^{T}C_{z}$: deterministic spatial functions
Heat conduction

First 20 spatial modes

Finite element discretization

Konakli K, Sudret B, 2016; Reliability Engineering & System Safety
Heat conduction

Example realizations

Konakli K, Sudret B, 2016; *Reliability Engineering & System Safety*
Heat conduction

Total sensitivity indices
ED based on Sobol sequences

Konakli K, Sudret B, 2016; Reliability Engineering & System Safety

N=2000
Heat conduction

Total sensitivity indices
ED based on Sobol sequences

Konakli K, Sudret B, 2016; Reliability Engineering & System Safety
Heat conduction

Sensitivity measures using the Spearman rank correlation
(based on 10,000 model evaluations)

Konakli K, Sudret B, 2016; Reliability Engineering & System Safety
Application in computational hydrogeology

- Sensitivity analysis of Mean Lifetime Expectancy (MLE) in layered hydrogeological model [Deman G, Konakli K, et al., 2016; Reliability Engineering & System Safety]

- Fictitious repository located in highly impermeable layer, encompassed by two aquifers

- Computational model consists of 15 layers with uniform thickness and homogeneous properties

- 2D cross-section discretized in square elements of 5m-size

- Steady-state flow with Dirichlet boundary conditions
Application in computational hydrogeology

- d=78 independent input random variables
- In each of the 15 layers:
  - Porosity
  - Anisotropy in components of hydraulic conductivity tensor
  - Euler angle of hydraulic conductivity tensor
  - Longitudinal component of dispersivity tensor
  - Anisotropy in components of dispersivity tensor
- Hydraulic gradients at 3 zones
Application in computational hydrogeology

Cross-validation error
LHS-based ED with 2,000 points

Generalized error
validation set with 2,000 points
Application in computational hydrogeology

LRA-based sensitivity indices

Sobol’ Indices Order 1
Application in computational hydrogeology

LRA-based sensitivity indices

Total Sobol' Indices

\[ \sum_{i}^{T} \sigma_{i}^{LRA} \]
Application in computational hydrogeology

Boxplots of sensitivity indices
20 replications, EDs of size N = 500 randomly extracted from the original ED
Application in computational hydrogeology

Comparison between LRA and PCE

Sobol’ Indices Order 1

Total Sobol’ Indices

\( \phi^D_4 \) \( \phi^C_3ab \) \( \phi^L_1b \) \( \phi^L_1a \) \( \phi^C_1 \)
Application in computational hydrogeology

Univariate effects
References


LRA methods are implemented in a MATLAB code integrated in software UQLab (for further information, please visit www.uqlab.com)
Thank you!