COSSAN TRAINING COURSE
on UNCERTAINTY QUANTIFICATION

Sensitivity Analysis

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Outline

1. Background to sensitivity
2. Local Sensitivity Analysis
3. Global sensitivity analysis
   - Scatter plots
   - Correlation coefficient
   - Rank correlation coefficient
   - Morris method
   - Derivative-based global sensitivity measure
   - Variance based sensitivity
4. Summary
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Sensitivity analysis

- Numerical model $y = f(t; x)$
  - Assumed to be implicitly defined (*black box model*)
- Functional dependency $t +$ uncertain parameters $x$

Sensitivity analysis: measure of the contribution of the variability of the input parameters to the variability of the output of the numerical model
Sensitivity analysis

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- Functional dependency $t + \text{uncertain parameters } x$

Sensitivity analysis: measure of the contribution of the variability of the input parameters to the variability of the output of the numerical model
Sensitivity analysis

- All the methods discussed in this lecture are applicable to input as independent RVs only
  - Correlated variables → impossible to discuss the contribution of a variable taken individually

- Multiple sensitivity metrics available in the literature
- Objective: provide an overview and comparison of some existing methods
  - Definition of various sensitivity indices
  - Little discussion of the algorithm
Local vs. Global sensitivity analysis

- **Local sensitivity analysis**
  - Performed with regards to a reference point
  - Analysis result depends on reference point
  - Often based on Gradient

- **Global sensitivity analysis**
  - Whole domain of variation of the input parameters is considered
  - Independent from reference point
  - Often numerically more demanding
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Local sensitivity analysis

- One factor at a time (OAT) methods
  - Identification of a reference point in the space of input parameters:
    \[ \mathbf{x}^{(0)} = (x_1^{(0)}, x_2^{(0)}, \ldots, x_n^{(0)}) \]
  - Example of reference point: average \( \mathbf{x}^{(0)} = (\mu_1, \mu_2, \ldots, \mu_n) \), median, mode, etc.
  - Sensitivity → small variation of model output \( y \) around reference point \( \mathbf{x}^{(0)} \) (gradient)

- Sensitivity index:
  \[ S_i \left( \mathbf{x}^{(0)} \right) = \frac{\partial y}{\partial x_i} \left( \mathbf{x}^{(0)} \right) \]
Local sensitivity analysis

Problem: Strong influence of the dimension (i.e. lengths expressed in mm, Young moduli in Gpa, etc.)

→ Need for dimensionless measure of sensitivity!

- **Elasticity coefficient**: Normalized local sensitivity measure

\[
E_i \left( x^{(0)} \right) = \frac{x_i^{(0)}}{y \left( x^{(0)} \right)} \frac{\partial y}{\partial x_i} \left( x^{(0)} \right)
\]

- Practical interpretation: \( x_i^{(0)} \) is increased by 1% → \( y \) is increased by \( E_i \) percent
Local sensitivity analysis

Problem: Strong influence of the dimension (i.e. lengths expressed in mm, Young moduli in Gpa, etc.)

→ Need for dimensionless measure of sensitivity!

- Alternative definition of a normalized sensitivity coefficient

\[ S_i \left( x^{(0)} \right) = \frac{\sigma_{X_i}}{\sigma_Y} \frac{\partial Y}{\partial X_i} \left( x^{(0)} \right) \]

- \( \sigma_{X_i} \): standard deviation of the \( X_i \) random variable input
- \( \sigma_Y \): standard deviation of the output \( Y \)
Local sensitivity analysis

Example

\[ y(x_1, x_2) = (x_1)^2 \cdot (x_2)^4 \]

with

\[ X_1 \sim U([0, 1]), \quad X_2 \sim U([0, 1]) \]

Reference point: (0.5, 0.5)

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<thead>
<tr>
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<th>( E_i )</th>
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</thead>
<tbody>
<tr>
<td>( x_1 )</td>
<td>0.0625</td>
<td>2</td>
</tr>
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Scatter plots

- Qualitative indication of variable sensitivity through plot
- Generate $M$ samples of the input variables (Monte-Carlo, Latin Hypercube, Halton, etc.)
  - $x^{(1)}, x^{(2)}, \ldots, x^{(M)}$ with $x^{(i)} = (x_1^{(i)}, x_2^{(i)}, \ldots, x_n^{(i)})$
- Compute the outputs of the numerical model $y(x^{(1)}), y(x^{(2)}), \ldots, y(x^{(M)})$
- Plot $y(x^{(i)}) = y(x_1^{(i)}, x_2^{(i)}, \ldots, x_j^{(i)}, \ldots, x_n^{(i)})$ in terms of $x_j^{(i)}$ for every sample $i = 1, \ldots, M$
  - The dependency from the other inputs is ignored in this plot (2-d scatter only)
  - Graphical representation of relation between $x_j$ and $y$
- To study the full dependency, as many plots as the number of inputs are required
Scatter plots

Example

\[ y(x_1, x_2) = (x_1)^2 + \alpha x_2, \]

\[ X_1 \sim U([0, 1]), \quad X_2 \sim U([0, 1]) \]

- **Case 1:** \( \alpha = 0 \)

\[ 0 \quad 0.2 \quad 0.4 \quad 0.6 \quad 0.8 \quad 1 \]

\[ 0 \quad 0.1 \quad 0.2 \quad 0.3 \quad 0.4 \quad 0.5 \quad 0.6 \quad 0.7 \quad 0.8 \quad 0.9 \quad 1 \]

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Scatter plots

Example

\[ y(x_1, x_2) = (x_1)^2 + \alpha x_2, \]

\[ X_1 \sim U([0, 1]), \quad X_2 \sim U([0, 1]) \]

• Case 2: \( \alpha = 0.25 \)
Scatter plots

Example

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Correlation coefficient

- Also called “Pearson correlation coefficient” or “Pearson’s $r$”
- Uses correlation (a-dimensional covariance) to measure a linear relation between inputs and outputs
  - The higher the correlation (in absolute value), the more a random variable contributes to the variability of the output
- Defined as
  \[
  \rho_{Y,X_j} = \frac{\text{Cov}(Y, X_j)}{\sqrt{\text{Var}[Y]} \cdot \sqrt{\text{Var}[X_j]}}
  \]
- Correlation coefficient can be determined numerically with Monte Carlo simulation
- Limitation: unable to quantify non-linear dependencies
Correlation coefficient

Example 1

\[ y(x_1, x_2) = (x_1)^2 + \alpha x_2, \]

\[ X_1 \sim U([0, 1]), \quad X_2 \sim U([0, 1]) \]

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Correlation coefficient

Example 1

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\[ X_1 \sim U([0, 1]), \quad X_2 \sim U([0, 1]) \]

- Case 2: \( \alpha = 0.25 \)
**Correlation coefficient**

Example 1

\[ y(x_1, x_2) = (x_1)^2 + \alpha x_2, \]

\[ X_1 \sim U([0, 1]), \quad X_2 \sim U([0, 1]) \]

- **Case 1:** \( \alpha = 4 \)
Correlation coefficient

Example 2

1 0.8 0.4 0 -0.4 -0.8 -1

Image source: wikipedia
Correlation coefficient

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Rank correlation coefficient

- Also called “Spearman’s rank correlation coefficient” or “Spearman’s $\rho$”
- Overcome the limitation of Pearson’s coefficient to linear relations
- Based on the rank of the samples output instead of their numerical values

Associate a rank to each value of $x_j$ and to the values of the output $y$ according to their increasing value

- The lowest value is associated a rank of 1
- The second lowest value is associated a rank of 2
- The highest value is associated to a rank of $M$ (= total number of samples)

Compute $\rho_s$ as the correlation between the ranks

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- Comparison between Pearson and Spearman coefficient

A bias may be introduced by the rank transformation.
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Morris method

Method applied when the random variables are $\mathbf{X} \sim U([0, 1]^n)$, uniform in $n$-dimensional hypercube

- Iso-probabilistic transformation to physical space if differently distributed

1. Create a regular grid in the hypercube of inputs ($\rightarrow$ samples)

2. Select a step size $\Delta > 0.5$

3. For a given sample $j$, compute the **elementary effect** of each input variable:

$$EE_1^{(j)} = \frac{y(x_1^{(j)} + \Delta, x_2^{(j)}) - y(x_1^{(j)}, x_2^{(j)})}{\Delta}$$

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Morris method

4 Generate **trajectories** of samples
   - Select a random starting sample
   - Randomly select sequence of input but increase/decrease the input value to stay inside the hypercube

5 Evaluate and collect all the elementary effects on each trajectory
Morris method

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Morris indices

\[ \mu_j^* = \frac{1}{N} \sum_{i=1}^{N} \left| EE^{(i)}_j \right| \]

and

\[ \sigma_j^2 = \frac{1}{N} \sum_{i=1}^{N} \left( EE^{(i)}_j - \mu_j \right)^2, \text{ where } \mu_j = \frac{1}{N} \sum_{i=1}^{N} EE^{(i)}_j \]

- Sensitivity identified by two indices
- No clear ranking of the RVs
  - high \( \mu_j^* \) \( \rightarrow \) \( y \) is highly sensitive to \( j \)-th input
  - high \( \sigma_j^2 \) \( \rightarrow \) non-linear dependency from \( j \)-th input or high interaction with other input parameters
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Derivative-based global sensitivity measure

- Method applied when the random variables are $\mathbf{X} \sim U([0, 1]^n)$, uniform in $n$-dimensional hypercube
  - Iso-probabilistic transformation to physical space if differently distributed

- Extension of the local gradient-based methods

- Sensitivity identified with two indices
  $$\mu^*_j = E \left[ \left| \frac{\partial y}{\partial x_j} \right| \right] \text{ and } \sigma^2_j = \text{Var} \left[ \frac{\partial y}{\partial x_j} \right]$$

  - $\mu^*_j$ measure of the importance of $x_j$ (on average)
  - $\sigma^2_j$ quantifies the non-linear effects
Derivative-based global sensitivity measure

Monte Carlo implementation:

1. Generate $M$ reference point $x^{(i)}$

2. For each sample $x^{(i)}$ evaluate the local sensitivity index with regards to the input $j$

$$S_j^{(i)} = \frac{\partial y}{\partial x_j}(x^{(i)})$$

3. Estimate the mean and variance of the collected local sensitivity indices

$$\mu_j^* = \frac{1}{N} \sum_{i=1}^{N} \left| S_j^{(i)} \right| \quad \text{and} \quad \sigma_j^2 = \frac{1}{N} \sum_{i=1}^{N} \left( S_j^{(i)} - \mu_j \right)^2$$
Derivative-based global sensitivity measure

Example

\[ y(x_1, x_2) = (x_1)^2 \cdot (x_2)^4 \]

with

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Decomposition of variance

Any square integrable function $y$ of $n$-dimensional random inputs $x$ can be expressed as

$$y(x) = y_0 + \sum_{i=1}^{n} y_i(x_i) + \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} y_{ij}(x_i, x_j) + \cdots + y_{1,2,...,n}(x_1, x_2, \ldots, x_n)$$

$$y_0 = E[y(x)] = \int y(x) f_X(x) \, dx$$

$$y_i(x_i) = E_{\sim x_i}[y | X_i] - y_0,$$ where $E_{\sim x_i}$ expectation computed over all the variables except $X_i$: $E_{\sim x_i}[y | X_i] = \int y(x) f_{X_{\sim i}}(x_{\sim i}) \, dx_{\sim i}$ with

$$f_{x_{\sim i}}(x_{\sim i}) = f_{x_1}(x_1) f_{x_2}(x_2) \cdots f_{x_{i-1}}(x_{i-1}) f_{x_{i+1}}(x_{i+1}) \cdots f_{x_n}(x_n)$$

$$y_{ij}, y_{ijk}, \text{ etc.}, \text{ similarly defined recursively}$$

Orthogonal decomposition $\rightarrow \int y_i(x_i) y_j(x_j) \, dx_i dx_j = 0$ if $i \neq j$
Decomposition of variance

- The components $y_i$, $y_{ij}$, etc. are rarely analytically known.
- $y_i$ represents the effect of varying $X_i$ alone, and so on
- These function can be used to compute the variance as

$$
\text{Var}[y] = \sum_{i=1}^{n} V_i + \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} V_{ij} + \cdots + V_{12\cdots n}
$$

where

$$
V_i = \text{Var}_{X_i}[E_{\sim X_i}[y|X_i]], \\
V_{ij} = \text{Var}_{X_{ij}}[E_{\sim X_i, X_j}[y|X_i, X_j]] - V_i - V_j
$$
Sobol’ indices

First order index

- First order sensitivity indices (or main effect)
- Variance based measure of sensitivity

\[ S_i = \frac{V_i}{\text{Var}[y]} \]

- \( S_i \) indicates how much of the variance of the output is contributed by \( X_i \) alone
- Higher order index \( S_{ij} \) analyse the interaction between \( X_i \) and \( X_j \)
- \( \sum_{i=1}^{n} S_i + \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} S_{ij} + \cdots + S_{12\ldots n} = 1 \)
- To consider all the possible interactions \( 2^d - 1 \) indices need to be evaluated
Sobol’ indices

Total effect index

- $S_{Ti}$ indicates how much of the variance of the output is contributed by $X_i$ including the interactions with all the other variables

$$S_{Ti} = \frac{E_{X_{\sim i}}[\text{Var}_{X_i}(Y|X_{\sim i})]}{\text{Var}[Y]}$$

$$= 1 - \frac{\text{Var}_{X_{\sim i}}[E_{X_i}(Y|X_{\sim i})]}{\text{Var}[Y]}$$

- Note that $\sum_{i=1}^{n} S_{Ti} \geq 1$

The computation of $S_i$ and $S_{Ti}$ is numerically demanding!
**Sobol’ indices**

**Total effect index**

- $S_{Ti}$ indicates how much of the variance of the output is contributed by $X_i$ **including the interactions** with all the other variables

\[
S_{Ti} = \frac{E_{X_{\sim i}}[\text{Var}_i(Y|X_{\sim i})]}{\text{Var}[y]}
\]

\[
= 1 - \frac{\text{Var}_{X_{\sim i}}[E_i(Y|X_{\sim i})]}{\text{Var}[y]}
\]

- Note that $\sum_{i=1}^{n} S_{Ti} \geq 1$

**The computation of $S_i$ and $S_{Ti}$ is numerically demanding!**
Monte Carlo computation of Sobol’ indices

- Generate 2 $M \times n$ matrix of samples $\mathbf{A}$ and $\mathbf{B}$

\[
\mathbf{A} = \begin{bmatrix}
X_1^{(1)} & X_2^{(1)} & \cdots & X_j^{(1)} & \cdots & X_n^{(1)} \\
X_1^{(2)} & X_2^{(2)} & \cdots & X_j^{(2)} & \cdots & X_n^{(2)} \\
\vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\
X_1^{(N)} & X_2^{(N)} & \cdots & X_j^{(N)} & \cdots & X_n^{(N)}
\end{bmatrix}
\]

\[
\mathbf{B} = \begin{bmatrix}
X_{n+1}^{(1)} & X_{n+2}^{(1)} & \cdots & X_{n+j}^{(1)} & \cdots & X_{2n}^{(1)} \\
X_{n+1}^{(2)} & X_{n+2}^{(2)} & \cdots & X_{n+j}^{(2)} & \cdots & X_{2n}^{(2)} \\
\vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\
X_{n+1}^{(N)} & X_{n+2}^{(N)} & \cdots & X_{n+j}^{(N)} & \cdots & X_{2n}^{(N)}
\end{bmatrix}
\]
Monte Carlo computation of Sobol’ indices

- Generate \( n M \times n \) matrix of samples \( \mathbf{C}_j \) where all the columns are taken from matrix \( \mathbf{B} \) except for the \( j \)-th column, which is taken from \( \mathbf{A} \)

\[
\mathbf{C}_j = \begin{bmatrix}
\mathbf{x}^{(1)}_{n+1} & \mathbf{x}^{(1)}_{n+2} & \cdots & \mathbf{x}^{(1)}_j & \cdots & \mathbf{x}^{(1)}_{2n} \\
\mathbf{x}^{(2)}_{n+1} & \mathbf{x}^{(2)}_{n+2} & \cdots & \mathbf{x}^{(2)}_j & \cdots & \mathbf{x}^{(2)}_{2n} \\
\vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\
\mathbf{x}^{(N)}_{n+1} & \mathbf{x}^{(N)}_{n+2} & \cdots & \mathbf{x}^{(N)}_j & \cdots & \mathbf{x}^{(N)}_{2n}
\end{bmatrix}
\]

- Compute the model output using the sample matrices \( \mathbf{A} \), \( \mathbf{B} \) and \( \mathbf{C}_j \) obtaining \( M \times 1 \) vectors of outputs \( y_A \), \( y_B \) and \( y_{C_j} \)

- Estimate \( S_j = \frac{(1/N) \sum_{i=1}^{N} y_A^{(i)} y_{C_j}^{(i)} - f_0^2}{(1/N) \sum_{i=1}^{N} y_A^{(i)} y_A^{(i)} - f_0^2} \) where \( f_0 = \frac{1}{N} \sum_{i=1}^{N} y_A^{(i)} \)
Monte Carlo computation of Sobol’ indices

- Generate \( n \) \( M \times n \) matrix of samples \( \mathbf{C}_j \) where all the columns are taken from matrix \( \mathbf{B} \) except for the \( j \)-th column, which is taken from \( \mathbf{A} \)

\[
\mathbf{C}_j = \begin{bmatrix}
X_{n+1}^{(1)} & X_{n+2}^{(1)} & \cdots & X_j^{(1)} & \cdots & X_{2n}^{(1)} \\
X_{n+1}^{(2)} & X_{n+2}^{(2)} & \cdots & X_j^{(2)} & \cdots & X_{2n}^{(2)} \\
\vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\
X_{n+1}^{(N)} & X_{n+2}^{(N)} & \cdots & X_j^{(N)} & \cdots & X_{2n}^{(N)}
\end{bmatrix}
\]

- Compute the model output using the sample matrices \( \mathbf{A}, \mathbf{B} \) and \( \mathbf{C}_j \) obtaining \( M \times 1 \) vectors of outputs \( y_A, y_B \) and \( y_{C_j} \)

- Similarly \( S_{Tj} = 1 - \frac{(1/N) \sum_{i=1}^{N} y_B^{(i)} y_{C_j}^{(i)} - f_0^2}{(1/N) \sum_{i=1}^{N} y_A^{(i)} y_A^{(i)} - f_0^2} \)
First order and Total effect indices

Example

\[ y(x_1, x_2) = (x_1)^2 \cdot (x_2)^4 \]

with

\[ X_1 \sim U([0, 1]), \quad X_2 \sim U([0, 1]) \]

<table>
<thead>
<tr>
<th></th>
<th>( S_j )</th>
<th>( S_{Tj} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x_1 )</td>
<td>0.2</td>
<td>0.55</td>
</tr>
<tr>
<td>( x_2 )</td>
<td>0.44</td>
<td>0.79</td>
</tr>
</tbody>
</table>
Outline

1. Background to sensitivity
2. Local Sensitivity Analysis
3. Global sensitivity analysis
   - Scatter plots
   - Correlation coefficient
   - Rank correlation coefficient
   - Morris method
   - Derivative-based global sensitivity measure
   - Variance based sensitivity
4. Summary
Summary

- Multiple methods for sensitivity available
- Higher accuracy methods are numerically more demanding
- Computational expenses depend on the number of random variables and problem complexity

<table>
<thead>
<tr>
<th>Sensitivity Method</th>
<th>Required number of model evaluations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gradient</td>
<td>1 per random input</td>
</tr>
<tr>
<td>Scatterplot</td>
<td>$10^2 — 10^3$ per random input</td>
</tr>
<tr>
<td>Morris, DSGM</td>
<td>$10^2 — 10^3$ per random input</td>
</tr>
<tr>
<td>Sobol’ indices</td>
<td>$10^3 — 10^4$ per random input</td>
</tr>
</tbody>
</table>