Uncertainty and sensitivity analysis

Corso di Laurea Specialistica: Reliability, Safety and Risk Analysis A+B

Anno Accademico 2011-2012
Outline

- Introduction
- Uncertainty and Sensitivity Analysis
- Local vs Global Approaches
  - Local Approaches:
    - The method of moments
    - The sensitivity on the nominal range
  - Global Approaches:
    - Discrete:
      - Event and Probability Tree
      - Method of Discrete Probabilities
    - Continuous:
      - Random Sampling (Monte Carlo-based methods)
        - Linear Regression Method
        - Variance Decomposition Method
- Model (structure) uncertainty
Introduction

Description of **phenomena** → Adoption of **mathematical models** (which are for example turned into operative computer codes for simulations)

**Models** → **Deterministic** or **Stochastic**

In practice the system under analysis can not be characterized exactly and the **knowledge** of the undergoing phenomena is **incomplete**

Uncertainty on both the values of the **model parameters** and on the **hypothesis** underlying the **model structure**

Uncertainty propagates within the model and causes uncertainty of the model **outputs**
How uncertainty propagates

\[ y = m(x) \]
\[ x = \text{vector of } n \text{ uncertain input parameters} \]
\[ m(x) = \text{model structure} \]
- **Deterministic** (e.g., advection-dispersion equation, Newton law)
- **Stochastic** (e.g., Poisson model, exponential model)

\[ y = \text{output vector correspondent to } x \text{ and } m(x) \]
Two major objectives:

1. **Uncertainty analysis** and **propagation**
   
   Propagates the uncertainties of the input parameters and the model structure to the model output

2. **Sensitivity analysis**

   Identifies the relative **importance** of the contributions to the output uncertainty of the various model parameters and hypotheses.
Two possible approaches to uncertainty and sensitivity analysis:

1. Local

2. Global
Local approaches

1. Focus on nominal values of the inputs $x^0$
2. Observe what happens to $y$ for small variations around $x^0$
3. The measure of the contribution of input $x_i$ is

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

4. Typically one single parameter $x_i$ is varied one at a time around its nominal value, while maintaining the others fixed at their nominal values
5. Rigorous extension to global approaches only if the model is linear
Global approaches

1. Focus on determining the output uncertainty distribution $f_Y(y)$
2. $f_Y(y)$ contains all relevant information on the uncertainty of the model response regardless the values of the input
3. No hypotheses on the model $m$

A. **Global** approaches account for the **whole input variability range**
   **Local** approaches account for **small variations** around nominal values

B. **Global** approaches account for **interactions** between the inputs
   **Local** approaches consider variations of **one input at a time**

Better results at a higher computational expense
Local approaches considered:

1. The method of moments (analytical)

2. The sensitivity on the nominal range* (discrete)

* local/global
Local approaches:
1. The method of moments (analytical) (1)

\[
\begin{align*}
  x^0_i &= E[x_i] \\
  y^0 &= m(x^0)
\end{align*}
\]

Nominal values

\[
y = m(x^0) + \sum_{i=1}^{n} (x_i - x^0_i) \left( \frac{\partial y}{\partial x_i} \right)_{x^0} + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} (x_i - x^0_i)(x_j - x^0_j) \left( \frac{\partial^2 y}{\partial x_i \partial x_j} \right)_{x^0} + \ldots
\]

Taylor expansion
Local approaches:
1. The method of moments (analytical) (2)

UNCERTAINTY PROPAGATION:
Compute two moments of the distribution of $y$: $E[y]$ $Var[y]$

$$E[y] = E[m(x_0)] + \sum_{i=1}^{n} E[(x_i - x_i^0)] \left( \frac{\partial y}{\partial x_i} \right)_{x_0} + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} E[(x_i - x_i^0)(x_j - x_j^0)] \left( \frac{\partial^2 y}{\partial x_i \partial x_j} \right)_{x_0}$$

cov[$x_i$, $x_j$]

$$E[y] \approx m(x^0) + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \text{cov}[x_i, x_j] \left( \frac{\partial^2 y}{\partial x_i \partial x_j} \right)_{x^0}$$

$E[y] \equiv y^0 = m(x^0)$ only if the model is linear
Local approaches:
1. The method of moments (analytical) (3)

UNCERTAINTY PROPAGATION:

\[
Var[y] = E[(y - y_0)^2] \approx E \left[ \sum_{i=1}^{n} \left( x_i - x_i^0 \right) \left( \frac{\partial y}{\partial x_i} \right)_{x_0}^2 \right]
\]

Note that:

\[
\left( \sum_{i=1}^{n} z_i \right)^2 = \sum_{i=1}^{n} z_i^2 + 2 \sum_{i=1}^{n} \sum_{j=i+1}^{n} z_i z_j
\]

\[
Var[y] \approx \sum_{i=1}^{n} E \left[ (x_i - x_i^0)^2 \right] \left( \frac{\partial y}{\partial x_i} \right)_{x_0}^2 + 2 \sum_{i=1}^{n} \sum_{j=i+1}^{n} E \left[ (x_i - x_i^0)(x_j - x_j^0) \right] \left( \frac{\partial y}{\partial x_i} \right)_{x_0} \left( \frac{\partial y}{\partial x_j} \right)_{x_0}
\]

Input independence
Local approaches:
1. The method of moments (analytical) (4)

SENSITIVITY ANALYSIS:

\[ \text{Var}[y] = E[(y - y^0)^2] \approx \sum_{i=1}^{n} \text{Var}[x_i] \left( \frac{\partial y}{\partial x_i} \right)_{x^0}^2 \]

\[ U_M(x_i) = \text{Std}[x_i] \left( \frac{\partial y}{\partial x_i} \right)_{x^0}^0 \]

1. Approximation!
2. Partial derivative computation!

NOTICE (in this case):

uncertainty propagation:

\[
E[y] \equiv m(x^0) + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \text{cov}[x_i, x_j] \left( \frac{\partial^2 y}{\partial x_i \partial x_j} \right)_{x^0} \]

\[ \text{Var}[y] \equiv \sum_{i=1}^{n} \text{Var}[x_i] \left( \frac{\partial y}{\partial x_i} \right)^2_{x^0} \]

needs

sensitivity analysis:

\[ U_M(x_i) = \text{Std}[x_i] \left( \frac{\partial y}{\partial x_i} \right)_{x^0}^0 \]
Local/global approaches:
2. Sensitivity on the nominal range (discrete) (1)

![Diagram showing sensitivity analysis](image)

\[ U_R(x_i) = m(x_i^+, x_{j \neq i}^0) - m(x_i^-, x_{j \neq i}^0) \]

1. More than local (range)
2. Less than global (1-at-time) → no interactions considered
3. Only extreme values → no detailed analysis of the trend of the model function
Local/global approaches:
2. Sensitivity on the nominal range (discrete) (2)

Parametric analysis:
Evaluate and plot $y$ for a sequence of different values of each input, holding the others constant.

$y = m(x_1, x_2)$

- no probabilistic info considered
  (only sensitivity, no uncertainty analysis)
- difficult “visualization” when number of inputs is larger than two
Global approaches considered:

1. Discrete
   - Event and probability tree
   - Discrete probability method

2. Continuous
   - Random sampling (Monte Carlo-based methods)
     - Linear regression method
     - Variance decomposition method
1. Discrete global approaches: Event and probability tree (1)

- The input variability ranges are **discretized** in levels

\[
x_1 \quad \begin{array}{c} 0.3 \quad 1.7 \\ 0.3 \quad 1.0 \quad 1.7 \\ 0.5 \quad 1.5 \quad 0.5 \quad 1.0 \quad 1.5 \end{array}
\]

- Different **scenarios** are organized in a **tree**
  - node = uncertain parameter
  - branch = one possible level of the parameter
  - consider all possible combinations
  - scenario = value of the model output obtained in correspondence of the values of the “branches”
1. Discrete global approaches: Event and probability tree (2)

- Assign *discrete probabilities* to the branches
  - if discrete probability distributions → straightforward
  - if continuous probability distributions → discretize!
  - probabilities of the branches are *conditional* on the values of the “previous” branches

- Evaluate the *probability* of the *scenarios* $y$ (product of conditional probabilities)
1. Discrete global approaches: Event and probability tree (3)

- Extract **sensitivity information** (see sensitivity on the nominal range - parametric study)

\[
y = m(x_1, x_2)
\]

\[
x_1 = .3 \quad x_2 = 0.5 \quad y = .6
\]

\[
x_1 = .3 \quad x_2 = 1 \quad y = 1.9
\]

\[
x_1 = .33 \quad x_2 = 1.5 \quad y = 3.9
\]

\[
x_1 = .33 \quad x_2 = 0.5 \quad y = 1.6
\]

\[
x_1 = .8 \quad x_2 = 1 \quad y = 1.8
\]

\[
x_1 = .8 \quad x_2 = 1.5 \quad y = 2.2
\]

\[
x_1 = .8 \quad x_2 = 0.5 \quad y = 2.4
\]

\[
x_1 = .1 \quad x_2 = 1 \quad y = 3
\]

\[
x_1 = .1 \quad x_2 = 1.5 \quad y = 3.4
\]

- It considers interactions between the inputs
- Problem: combinatorial explosion!

\( (n \text{ inputs, } k \text{ levels } \rightarrow k^n \text{ combinations!} ) \)
Global approaches considered:

1. Discrete
   - Event and probability tree
   - Discrete probability method

2. Continuous
   - Random sampling (Monte Carlo-based methods)
     - Linear regression method
     - Variance decomposition method
1. Discrete global approaches: Discrete probability method (1)

Consider the simple model \( y = m(x, z) \)

1) The pdf’s \( f_X(x) \) and \( f_Z(z) \) are **discretized** in \( n \) and \( s \) intervals of amplitude \( \Delta_i \) e \( \Delta_j \) : two sets of pairs \( <x_i, p_i>, <z_j, q_j>, i = 1, 2, \ldots, n, j = 1, 2, \ldots, s \)

\[
p_i = \int_{\Delta_i} f_X(x) \, dx \quad x_i = \frac{1}{p_i} \int_{\Delta_i} x f_X(x) \, dx \quad i = 1, 2, \ldots, n
\]

\[
q_j = \int_{\Delta_j} f_Z(z) \, dz \quad z_j = \frac{1}{q_j} \int_{\Delta_j} z f_Z(z) \, dz \quad j = 1, 2, \ldots, s
\]
1. Discrete global approaches: Discrete probability method (2)

2) Build the **matrix** of the \( n \times s \) output values:

\[ y_{ij} = m(x_i, z_j), \ i = 1, 2, \ldots, n, \ j = 1, 2, \ldots, s \]

with probabilities \( r_{ij} = p_i q_j \) (independence of inputs!)

3) **Condense** the discrete distribution of \( y \) as:

\[ r_l = \sum_{y_{ij} \in l} r_{ij} \]

\[ y_l = \frac{1}{r_i} \sum_{y_{ij} \in l} r_{ij} y_{ij} \]

\( l = 1, 2, \ldots, t \ll n \cdot s \)
1. Discrete global approaches: Discrete probability method (3)

a) Combinatorial explosion avoided

\[
\begin{align*}
&f_X \quad (25 \text{ values}) \\
&f_Z \quad (5 \text{ values}) \\
&f_W \quad (5 \text{ values}) \\
\end{align*}
\]

(5 values instead of \(25 \times 5 = 125\))

b) Info about dependences is lost in condensation process

\[
y = x \cdot z \quad \text{where} \quad x = a \cdot b \quad \text{and} \quad z = b + c
\]

\[
\begin{align*}
& a \\
& b \\
& c \\
\end{align*}
\]

\[
\begin{align*}
& x \quad \text{(condensed)} \\
& z \quad \text{(condensed)} \\
& y \quad (\text{indep??})
\end{align*}
\]

(indep OK)
Global approaches considered:

1. Discrete
   - Event and probability tree

2. Continuous
   - Random sampling (Monte Carlo-based methods)
     - Linear regression method
     - Variance decomposition method
2. Continuous global approaches: 
Random sampling (Monte Carlo-based methods) (1)

The procedure consists in drawing from the assigned pdf’s $f_X(x)$ a sequence of $s$ samples of each of the $n$ input parameters

$$x_j = [x_{j1}, x_{j2}, \ldots, x_{jn}] \quad j=1,2,\ldots,s$$

In correspondence of each of the $s$ generated vectors of input values, we evaluate the model and thus obtain a sequence of output values

$$y_j = m(x_{j1}, x_{j2}, \ldots, x_{jn}) \quad j=1,2,\ldots,s$$

The sequences $x_j, y_j$ can be analyzed using classical statistical techniques for uncertainty and sensitivity analysis

$$f_Y(y) = \text{pdf of } y$$
2. Continuous global approaches: Random sampling (Monte Carlo-based methods) (2)

- It covers the space of the uncertain input parameters by random sampling from the corresponding probability distributions.

- It provides a direct estimation of the output uncertainty distribution $f_y(y)$.

- It is an approximated method, but its accuracy can be easily assessed and improved by increasing the sample size $s$.

$$\sigma \propto \frac{1}{\sqrt{s}}$$

- Computational cost (i.e., time), $T_{comp}$:
  - $T_{comp}$ increases linearly with $s$.
  - For a given accuracy (i.e., for a given $s$), $T_{comp}$ increases linearly with the number of inputs $n$ (not exponentially as in the event and probability tree).
Global approaches considered:

1. Discrete
   - Event and probability tree

2. Continuous
   - Random sampling (Monte Carlo-based methods)
     - Linear regression method
     - Variance decomposition method
Let us consider the approximated linear model:

\[ y = m(x) = y^*(x) + e = x^T\beta + e = \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_n x_n + e \]

\[ x^T = \text{input vector} = [x_1, x_2, \ldots, x_n] \]
\[ \beta = [\beta_1, \beta_2, \ldots, \beta_n]^T = \text{unknown coefficients vector} \]
\[ e = \text{error term} \]

**Indicator of the uncertainty of the output \((y)\) distribution \(=\) Variance\([y]\)**

\[ V[y] = V[x^T\beta + e] = V[x^T\beta] + V[e] \]
\[ \text{e not dependent on } x \]
\[ \text{Independent inputs} \]
\[ \text{Var}[e] \text{ “negligible”} \]
\[ \text{(linear model is good approximation)} \]

**Sensitivity index**

\[ R_i^2 = \frac{\beta_i^2 \cdot V[x_i]}{V[y]} \]
2. Continuous global approaches - Random sampling: Linear regression method (2)

1) Draw from the assigned pdf’s $f_X(x)$ a sequence of $s$ samples for each of the $n$ input parameters

$$x_j = [x_{j1}, x_{j2}, \ldots, x_{jn}] \quad j = 1, 2, \ldots, s$$

2) In correspondence of each of the $s$ generated vectors of input values, evaluate the model and thus obtain a sequence of output values

$$y_j = m(x_{j1}, x_{j2}, \ldots, x_{jn}) \quad j = 1, 2, \ldots, s$$ (UNCERTAINTY PROPAGATION)

3) Estimate the following quantities:

$$E[y] \equiv \bar{y} = \frac{1}{s} \sum_{j=1}^{s} y_j$$

$$V[y] \equiv \hat{V}[y] = \frac{1}{s-1} \sum_{j=1}^{s} (y_j - \bar{y})^2$$

$$\beta_i \equiv \hat{\beta}_i = \frac{\sum_{j=1}^{s} (y_j - \bar{y})(x_{ji} - E[x_i])}{\sum_{j=1}^{s} (x_{ji} - E[x_i])^2}$$

$$\hat{R}_i^2 = \frac{\hat{\beta}_i^2 \cdot V[x_i]}{\hat{V}[y]}$$ (SENSITIVITY ANALYSIS)
Global approaches considered:

1. Discrete
   - Event and probability tree

2. Continuous
   - Random sampling (Monte Carlo-based methods)
     - Linear regression method
     - Variance decomposition method
Let us consider the following simple model (2 inputs):
\[ y = m(x_1, x_2) \]

To what extent does the variance of \( y \) **decreases** when we fix \( x_1 = x_1^* \)?

\[ V_{x_2} \left[ y \mid x_1 = x_1^* \right] \]

In general, \( x_1 \) has a **distribution** of values! \( \Rightarrow \) **Expectation**!

\[ E_{x_1} \left[ V_{x_2} \left( y \mid x_1 = x_1^* \right) \right] \]

The lower, the more important \( x_1 \) is!

**Variance of the output distribution (VARIANCE DECOMPOSITION)**
\[ V[y] = V_{x_1} \left[ E_{x_2} \left( y \mid x_1 \right) \right] + E_{x_1} \left[ V_{x_2} \left( y \mid x_1 \right) \right] \]

**Sensitivity index**
\[ \eta_1^2 = \frac{V_{x_1} \left[ E_{x_2} \left( y \mid x_1 \right) \right]}{V[y]} \]
2. Continuous global approaches - Random sampling: Variance decomposition method (2)

\[ \eta_1^2 = \frac{V_{x_1}[E_{x_2}(y \mid x_1)]}{V[y]} \]

DOES IT MAKE SENSE?

WHAT IS \( E_{x_2}(y \mid x_1) \)?

The expected value of the output \( y \), computed with respect to \( x_2 \), when \( x_1 \) is given:

\[ E_{x_2}(y \mid x_1) = \int_{x_2} m(x_1, x_2) f(x_2 \mid x_1) dx_2 \]

\( \Rightarrow \text{function of } x_1! \)

WHAT IS \( V_{x_1}[E_{x_2}(y \mid x_1)] \)?

The variance of the function above!

The “expected” (part of) variability of the output \( y \) which is due to \( x_1 \) alone:

\[ V_{x_1}[E_{x_2}(y \mid x_1)] = \int_{x_1} \left[ E_{x_2}(y \mid x_1) - E(y) \right]^2 f(x_1) dx_1 \]
2. Continuous global approaches - Random sampling: Variance decomposition method (3)

\[ \eta_1^2 = \frac{V_{x_1}[E_{x_2}(y | x_1)]}{V[y]} \]

1) Sample \( s \) random values for \( x_1 \) from \( f_{x_1}(x_1), \{x_1^1, x_1^2, ..., x_1^j, ..., x_1^s\} \)

**NOTE:** \( f_{x_1}(x_1) = \int_{x_2} f_{x_1,x_2}(x_1,x_2)dx_2 \)

2) For each \( x_1^j \) (i.e., \( j = 1, 2, ..., s \))

   a) Sample \( r \) values of \( x_2 \) from \( f_{x_2|x_1}(x_2 | x_1 = x_1^j): \{x_2^1, x_2^2, ..., x_2^k, ..., x_2^r\} \)

   **NOTE:** \( f_{x_2|x_1}(x_2 | x_1) = f_{x_1,x_2}(x_1,x_2) / f_{x_1}(x_1) \)

   b) Evaluate the \( r \) output values \( y^{jk} = m(x_1^j, x_2^k), k = 1, 2, ..., r \)

   **(UNCERTAINTY PROPAGATION)**

   c) Estimate the expected value:

   \[ \hat{y}^*(x_1^j) = \frac{1}{r} \sum_{k=1}^{r} y^{jk} \approx E_{x_2}[y | x_1 = x_1^j] \]

End For (\( j \))
2. Continuous global approaches - Random sampling: Variance decomposition method (4)

\[ E_{X_2} [y \mid x_1 = x_1^1], E_{X_2} [y \mid x_1 = x_1^2], \ldots, E_{X_2} [y \mid x_1 = x_1^s] \]

3) Evaluate the following quantities:

\[ E[y] = E_{X_1} \left[ E_{X_2} [y \mid x_1] \right] \approx \frac{1}{s} \sum_{j=1}^{s} E_{X_2} [y \mid x_1 = x_1^j] = \frac{1}{s} \sum_{j=1}^{s} \hat{y}^*(x_1^j) = \bar{y} \]

\[ \hat{V}_{X_1} \left[ E_{X_2} (y \mid x_1) \right] \approx \frac{1}{s-1} \cdot \sum_{j=1}^{s} \left[ \hat{y}^*(x_1^j) - \bar{y} \right]^2 \]

\[ \hat{V}[y] \approx \frac{1}{s \cdot r - 1} \cdot \sum_{j=1}^{s} \sum_{k=1}^{r} \left[ y_{jk} - \bar{y} \right]^2 \]

\[ \hat{\eta}_1^2 = \frac{\hat{V}_{X_1} \left[ E_{X_2} (y \mid x_1) \right]}{\hat{V}[y]} \]

(SENSITIVITY ANALYSIS)

- no hypotheses on the model
- possible interactions considered
- problem: computational cost!

(s \cdot r model evaluations \rightarrow around 10^6!)
2. Continuous global approaches - Random sampling: Variance decomposition method (5)

\[ y = m(x_1, x_2, x_3) \]

\[ V[y] = V_{x_1} \left[ E_{x_2, x_3} (y | x_1) \right] + E_{x_1} \left[ V_{x_2, x_3} (y | x_1) \right] \]

\[ V[y] = V_1 + V_2 + V_3 + V_{12} + V_{13} + V_{23} + V_{123} \]

- \( V_i \) = contribution of input \( x_i \) alone
- \( V_{ij} \) = contribution exclusively due to the interaction of \( x_i \) and \( x_j \)
- \( V_{123} \) = contribution exclusively due to the interaction of \( x_1 \) and \( x_2 \) and \( x_3 \)

Note that:

\[ V_1 = V_{x_1} \left[ E_{x_2, x_3} (y | x_1) \right] \]

\[ V_{12} = V_{x_1, x_2} \left[ E_{x_3} (y | x_1, x_2) \right] - V_1 - V_2 \]

= only interaction!

Example:

\[ y = x_1 + x_2^2 + x_1 \cdot x_3^2 \]

\[ V_{12} = 0 \]

but notice that \( V_{x_1, x_2} \left[ E_{x_3} (y | x_1, x_2) \right] \neq 0 \)

\[ V_{23} = 0 \]

\[ V_{123} = 0 \]
Model (structure) uncertainty:

1. The alternative model approach

2. The perturbative treatment of the reference model
Model (structure) uncertainty: The alternative model approach

Consider a set of \( M \) plausible models \( m_i, i=1,2,\ldots,M \), each characterized by a set of uncertain parameters \( a_i \) with distribution \( \pi(a_i | m_i) \)

\[
y_i(x, a_i) = m_i(x, a_i)
\]

\[
y_i(x) = \int_{a_i} m_i(x, a_i) \pi(a_i | m_i) da_i
\]

Model uncertainty quantified by a discrete probability distribution \( p(m_i), i = 1, 2, \ldots, M \)

output \( y \) estimation \( \rightarrow \) total probability theorem

\[
y(x) = \sum_{i=1}^{M} p(m_i) \int_{a_i} m_i(x, a_i) \pi(a_i | m_i) da_i
\]
Model (structure) uncertainty: The perturbative treatment of the reference model

- One single model $m^*$ is considered, typically the most plausible, and a perturbation is directly introduced in the model output.
- The perturbation is a sort of error term with which one accounts for the structural uncertainties due to the incomplete knowledge of the phenomenon.
- In practice, one adopts additional or multiplicative perturbative terms.

$$y = m^*(x,a^*) + D_a^*$$

$$y = m^*(x,a^*) D_m^*$$

The perturbations $D_a^*$ e $D_m^*$ are not exactly known, but they may be described in terms of opportune probability distributions.
Back-up slides
Discretization of a continuous probability distribution function

Preserve the **total probability** and the **mean value** at each interval

Discretized the pdf \( f_X(x) \) in \( n \) intervals of amplitude \( \Delta_i \)

\[ p_i = \int_{\Delta_i} f_X(x) \, dx \]

(probability of discrete element \( x_i \))

\[ x_i = \frac{1}{p_i} \int_{\Delta_i} x f_X(x) \, dx \]

\( (x_i = \text{mean value of } X \text{ over interval } \Delta_i) \)

\( \text{Exp}(\lambda) = \exp(1) \)