Introduction to Sensitivity and Uncertainty Analysis in Reactor Physics

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Outline

- Sensitivity analysis
- Uncertainty analysis
- Methods
- Application to reactor physics
- Example calculation
Sensitivity

- **Starting point**: mathematical model containing uncertain parameters and response dependent on this model

- **Question**: If one of the parameters is perturbed, how will this affect the response?

- **Mathematical definition**:
  - Simplest case: local sensitivity of response \( R \) with respect to parameter \( \alpha \) at point \( \alpha = \alpha_0 \) is the derivative
    \[
    s_\alpha = \left( \frac{dR}{d\alpha} \right)_{\alpha=\alpha_0}
    \]  
    \( \text{(1)} \)
  - This generalizes easily to more general mathematical systems (e.g. parameters that are functions and responses that are functionals)
**Sensitivity Analysis**

- **Objective**: Compute derivatives with respect to all parameters of interest

- Brute-force approach:
  - Variate the parameters one-by-one and compute the response
  - Inefficient when there are several parameters

- Deterministic approach:
  - Formulate the problem mathematically and compute the derivatives
  - Very efficient if a mathematical concept called *adjoint* is utilized
Uncertainty

- **Starting point**: a mathematical model containing uncertain parameters and response dependent on this model

- **Question**: How to quantify the uncertainty related to the parameters?
  - Bayesian probability definition: knowledge about a parameter presented as probability distribution
  - Variance (one parameter) or covariance (several parameters) of the distribution may be chosen as the descriptive statistic for the uncertainty
Uncertainty Analysis

- **Objective**: Compute the probability distribution of the response based on the probability distributions of the uncertain parameters.

- Determination of the exact distribution usually extremely difficult.
  - Compute only variance/covariance due to uncertain parameters OR estimate distribution based on simulations.

- Inaccuracy related to numerical methods or approximation errors not included in classical uncertainty analysis.
Uncertainty Analysis Methods

- **Deterministic approach:**
  1. Calculate response sensitivity vector $s$
  2. Linearize response
     \[
     R \approx s\alpha
     \]
  3. Compute respective variance/covariance
     \[
     \text{Cov}[R] \approx \text{Cov}[s\alpha] = s\text{Cov}[\alpha]s^T.
     \]

- **Statistical approach**
  1. Sample points from distribution $p(\alpha)$
  2. Compute $R$ corresponding to each sample
  3. Compute uncertainty estimates based on simulated $p(R)$
Application to Reactor Physics

- **Mathematical model**: transport (or diffusion) equation, potentially combined with a depletion model

- **Responses**: multiplication factor, reaction rates, homogenized cross-sections etc.

- **Uncertain parameters**: neutron cross-sections, initial nuclide concentrations, system dimensions etc.
Application to Reactor Physics: Adjoint-based Approach

+ Computationally very efficient
+ Yields detailed sensitivity profiles
  − Best-suited for deterministic codes
  − Requires extensive modifications in the code
  − Has not been applied to depletion problems
Application to Reactor Physics: Statistical Approach

+ Well-suited for both deterministic and Monte Carlo codes
+ Code can be treated as a black box (depletion does not cause any difficulties!)
+ Yields additional information about the distribution $p(R)$ (besides variance/covariance)
  – Computationally expensive
  – Does not yield sensitivity information
S&U analysis with Monte Carlo method

- Statistical approach
  - Sample from Gaussian distribution based on covariance data
  - Total Monte Carlo:
    - Suitable for burnup calculations

- Adjoint-based approach
  - exploit the physical interpretation of adjoint:
    - Suitable for problems covered by generalized perturbation theory
Example of S&U Calculation

- Calculation code: CASMO-4
- Source of uncertainty: neutron cross-sections
- S&U analysis method: Adjoint-based
- Test case: a $7 \times 7$ BWR assembly [1]

<table>
<thead>
<tr>
<th>Rod type</th>
<th>$^{235}\text{U}$ (wt.%)</th>
<th>$\text{Gd}_2\text{O}_3$ (wt.%)</th>
<th>No. of rods</th>
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<tbody>
<tr>
<td>1</td>
<td>2.93</td>
<td>0</td>
<td>26</td>
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<tr>
<td>2</td>
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<td>1.69</td>
<td>0</td>
<td>6</td>
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<td>4</td>
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<td>6B</td>
<td>2.93</td>
<td>3.0</td>
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K. Ivanov et al., Benchmark for uncertainty analysis in modeling (UAM) for design, operation, and safety analysis of LWRs, Volume I: Specification and Support Data for the Neutronics Cases (Phase I), Version 2.0 , NEA/NSC/DOC(2011)
Example: flux and adjoint flux
Example: $k_{\text{inf}}$ S&U profiles (1)

- $k_{\text{inf}} = 1.1055$
- $\Delta k_{\text{inf}}/k_{\text{inf}} = 0.5076\%$

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>Param.pair</th>
<th>Rel. sensitivity</th>
<th>Rel. uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{238}\text{U}$</td>
<td>$\sigma_c, \sigma_c$</td>
<td>$-2.448 \times 10^{-1}$</td>
<td>$3.198 \times 10^{-1}$</td>
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<td>$^{235}\text{U}$</td>
<td>$\nu, \nu$</td>
<td>$9.161 \times 10^{-1}$</td>
<td>$2.720 \times 10^{-1}$</td>
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<td>$^{235}\text{U}$</td>
<td>$\sigma_c, \sigma_c$</td>
<td>$-1.010 \times 10^{-1}$</td>
<td>$1.423 \times 10^{-1}$</td>
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<tr>
<td>$^{235}\text{U}$</td>
<td>$\sigma_f, \sigma_f$</td>
<td>$4.157 \times 10^{-1}$</td>
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</tr>
<tr>
<td>$^{238}\text{U}$</td>
<td>$\sigma_s, \sigma_s$</td>
<td>$-1.499 \times 10^{-2}$</td>
<td>$1.320 \times 10^{-1}$</td>
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<tr>
<td>$^{235}\text{U}$</td>
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<td></td>
<td>$1.242 \times 10^{-1}$</td>
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<td>$^{235}\text{U}$</td>
<td>$\chi, \chi$</td>
<td>$9.161 \times 10^{-1}$</td>
<td>$1.030 \times 10^{-1}$</td>
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<tr>
<td>$^{238}\text{U}$</td>
<td>$\nu, \nu$</td>
<td>$6.107 \times 10^{-2}$</td>
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<td>$^1\text{H}$</td>
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<td>$1.263 \times 10^{-1}$</td>
<td>$5.061 \times 10^{-2}$</td>
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Example: $k_{\text{inf}}$ S&U profiles (2)

- Sensitivity plots

  ![Sensitivity plots](image)

- $^{238}\text{U}$ capture covariance matrix

  ![Covariance matrix](image)
Example: Homogenized two-group cross-section uncertainties

<table>
<thead>
<tr>
<th>Response</th>
<th>Value</th>
<th>Relative uncertainty $\frac{\Delta R}{R}$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu \Sigma_{f,1}$</td>
<td>$4.976 \times 10^{-3}$</td>
<td>$8.399 \times 10^{-1}$</td>
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<tr>
<td>$\nu \Sigma_{f,2}$</td>
<td>$6.922 \times 10^{-2}$</td>
<td>$4.490 \times 10^{-1}$</td>
</tr>
<tr>
<td>$\Sigma_{a,1}$</td>
<td>$7.283 \times 10^{-3}$</td>
<td>$7.526 \times 10^{-1}$</td>
</tr>
<tr>
<td>$\Sigma_{a,2}$</td>
<td>$5.494 \times 10^{-2}$</td>
<td>$2.122 \times 10^{-1}$</td>
</tr>
<tr>
<td>$\Sigma_{c,1}$</td>
<td>$5.348 \times 10^{-3}$</td>
<td>$1.098 \times 10^{0}$</td>
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<tr>
<td>$\Sigma_{c,2}$</td>
<td>$2.653 \times 10^{-2}$</td>
<td>$5.066 \times 10^{-1}$</td>
</tr>
<tr>
<td>$\Sigma_{f,1}$</td>
<td>$1.935 \times 10^{-3}$</td>
<td>$5.563 \times 10^{-1}$</td>
</tr>
<tr>
<td>$\Sigma_{f,2}$</td>
<td>$2.841 \times 10^{-2}$</td>
<td>$3.244 \times 10^{-1}$</td>
</tr>
</tbody>
</table>
Example: generalized adjoints

Energy (eV)

$\nu \sum_{f,1}$

$\nu \sum_{f,2}$

Energy (eV)
Example: S&U profiles for $\nu \Sigma_{f,2}$

- $\nu \Sigma_{f,2} = 6.922 \times 10^{-2}$, relative uncertainty $4.490 \times 10^{-1}\%$

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>Param. pair</th>
<th>Sensitivity</th>
<th>Contribution to $\frac{\Delta R}{R}$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{235}U$</td>
<td>$\bar{\nu}, \bar{\nu}$</td>
<td>$9.996 \times 10^{-1}$</td>
<td>$3.105 \times 10^{-1}$</td>
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<tr>
<td>$^{235}U$</td>
<td>$\sigma_f, \sigma_f$</td>
<td>$7.985 \times 10^{-1}$</td>
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<td>$^{235}U$</td>
<td>$\sigma_f, \sigma_c$</td>
<td>$7.985 \times 10^{-1}$</td>
<td>$1.134 \times 10^{-1}$</td>
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<tr>
<td>$^{238}U$</td>
<td>$\sigma_c, \sigma_c$</td>
<td>$-4.406 \times 10^{-2}$</td>
<td>$7.257 \times 10^{-2}$</td>
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<tr>
<td>$^{235}U$</td>
<td>$\sigma_c, \sigma_c$</td>
<td>$-3.599 \times 10^{-2}$</td>
<td>$5.613 \times 10^{-2}$</td>
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</tbody>
</table>
Summary

- Sensitivity analysis
  - Adjoint-based approach
  - Brute force method

- Uncertainty analysis
  - Deterministic (requires sensitivities)
  - Statistical sampling

- S&U analysis with Monte Carlo method
  - Statistical sampling based on covariance data
  - Total Monte Carlo
  - Adjoint-based (exploit physical interpretation of adjoint)