Adaptive Monte Carlo Approach for Sensitivity Analysis

Ivan Dimov

Institute of Information and Communication Technologies, Bulgarian Academy of Sciences (BAS)
e-mail: ivdimov@bas.bg

Intensive course on
*Advanced Monte Carlo methods - computational challenges*
February 21 - 27, 2012
Introduction

Mathematical background
- Unified Eulerian Model
- Total Sensitivity Indices
- Sobol’ Approach for Computing Global Sensitivity Indices

Adaptive Monte Carlo approach

Numerical experiments

Concluding remarks
Goal

The aim is to propose and study a new mechanism for sensitivity studies in a case study: concentrations levels of some important pollutants (like ozone $O_3$) in real-live scenarios of air pollution transport over Europe with Unified Eulerian Models.
Goal

The aim is to propose and study a new mechanism for sensitivity studies in a case study: concentrations levels of some important pollutants (like ozone $O_3$) in real-live scenarios of air pollution transport over Europe with Unified Eulerian Models.

Sensitivity analysis studies

- improving the model
- increasing the reliability of the results, and
- identifying processes that must be studied more carefully
Goal

The aim is to propose and study a new mechanism for sensitivity studies in a case study: concentrations levels of some important pollutants (like ozone $O_3$) in real-live scenarios of air pollution transport over Europe with Unified Eulerian Models.

Sensitivity analysis studies

- improving the model
- increasing the reliability of the results, and
- identifying processes that must be studied more carefully

Motivation

- assessing the influences of each input parameters on the output variability
- to provide validation, optimization, and risk analysis of simulation models
- to determine robustness, reliability, efficiency of a model
\[
\frac{\partial c_s}{\partial t} = - \frac{\partial (uc_s)}{\partial x} - \frac{\partial (vc_s)}{\partial y} - \frac{\partial (wc_s)}{\partial z} + \\
+ \frac{\partial}{\partial x} \left( K_x \frac{\partial c_s}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial c_s}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial c_s}{\partial z} \right) + \\
+ E_s + Q_s(c_1, c_2, \ldots, c_q) - (k_{1s} + k_{2s})c_s, \quad s = 1, 2, \ldots, q.
\]

- \( q \) — number of equations = number of chemical species,
- \( c_s \) — concentrations of the chemical species,
- \( u, v, w \) — components of the wind along the coordinate axes,
- \( K_x, K_y, K_z \) — diffusion coefficients,
- \( E_s \) — emissions in the space domain,
- \( k_{1s}, k_{2s} \) — coefficients of dry and wet deposition respectively,
- \( Q_s(c_1, c_2, \ldots, c_q) \) — non-linear functions that describe the chemical reactions between species.
\[
\frac{\partial c_s}{\partial t} = - \frac{\partial (uc_s)}{\partial x} - \frac{\partial (vc_s)}{\partial y} - \frac{\partial (wc_s)}{\partial z} + \\
+ \frac{\partial}{\partial x} \left( K_x \frac{\partial c_s}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial c_s}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial c_s}{\partial z} \right) + \\
+ E_s + Q_s(c_1, c_2, \ldots, c_q) - (k_{1s} + k_{2s})c_s, \quad s = 1, 2, \ldots, q.
\]

- \( q \) – number of equations = number of chemical species,
- \( c_s \) – concentrations of the chemical species,
- \( u, v, w \) – components of the wind along the coordinate axes,
- \( K_x, K_y, K_z \) – diffusion coefficients,
- \( E_s \) – emissions in the space domain,
- \( k_{1s}, k_{2s} \) – coefficients of dry and wet deposition respectively,
- \( Q_s(c_1, c_2, \ldots, c_q) \) – non-linear functions that describe the chemical reactions between species.
\[
\frac{\partial c_s}{\partial t} = - \frac{\partial (uc_s)}{\partial x} - \frac{\partial (vc_s)}{\partial y} - \frac{\partial (wc_s)}{\partial z} + \\
+ \frac{\partial}{\partial x} \left( K_x \frac{\partial c_s}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial c_s}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial c_s}{\partial z} \right) + \\
+ E_s + Q_s(c_1, c_2, \ldots, c_q) - (k_{1s} + k_{2s})c_s, \quad s = 1, 2, \ldots, q.
\]

- \( q \) – number of equations = number of chemical species,
- \( c_s \) – concentrations of the chemical species,
- \( u, v, w \) – components of the wind along the coordinate axes,
- \( K_x, K_y, K_z \) – diffusion coefficients,
- \( E_s \) – emissions in the space domain,
- \( k_{1s}, k_{2s} \) – coefficients of dry and wet deposition respectively,
- \( Q_s(c_1, c_2, \ldots, c_q) \) – non-linear functions that describe the chemical reactions between species.
\[
\frac{\partial c_s}{\partial t} = - \frac{\partial (uc_s)}{\partial x} - \frac{\partial (vc_s)}{\partial y} - \frac{\partial (wc_s)}{\partial z} +
+ \frac{\partial}{\partial x} \left( K_x \frac{\partial c_s}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial c_s}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial c_s}{\partial z} \right) +
+E_s + Q_s(c_1, c_2, \ldots, c_q) - (k_{1s} + k_{2s})c_s, \quad s = 1, 2, \ldots, q.
\]

\( q \) – number of equations = number of chemical species,

\( c_s \) – concentrations of the chemical species,

\( u, v, w \) – components of the wind along the coordinate axes,

\( K_x, K_y, K_z \) – diffusion coefficients,

\( E_s \) – emissions in the space domain,

\( k_{1s}, k_{2s} \) – coefficients of dry and wet deposition respectively,

\( Q_s(c_1, c_2, \ldots, c_q) \) – non-linear functions that describe

the chemical reactions between species.

Ivan Dimov, BAS
Adaptive Monte Carlo Approach for Sensitivity Analysis
\[
\frac{\partial c_s}{\partial t} = -\frac{\partial (uc_s)}{\partial x} - \frac{\partial (vc_s)}{\partial y} - \frac{\partial (wc_s)}{\partial z} + \\
+ \frac{\partial}{\partial x} \left( K_x \frac{\partial c_s}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial c_s}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial c_s}{\partial z} \right) + \\
+ E_s + Q_s(c_1, c_2, \ldots, c_q) - (k_{1s} + k_{2s})c_s, \quad s = 1, 2, \ldots, q.
\]

\(q\) — number of equations = number of chemical species,
\(c_s\) — concentrations of the chemical species,
\(u, v, w\) — components of the wind along the coordinate axes,
\(K_x, K_y, K_z\) — diffusion coefficients,
\(E_s\) — emissions in the space domain,
\(k_{1s}, k_{2s}\) — coefficients of dry and wet deposition respectively,
\(Q_s(c_1, c_2, \ldots, c_q)\) — non-linear functions that describe the chemical reactions between species.
\[
\frac{\partial c_s}{\partial t} = -\frac{\partial (uc_s)}{\partial x} - \frac{\partial (vc_s)}{\partial y} - \frac{\partial (wc_s)}{\partial z} + \\
+ \frac{\partial}{\partial x} \left( K_x \frac{\partial c_s}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial c_s}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial c_s}{\partial z} \right) + \\
+ E_s + Q_s(c_1, c_2, \ldots, c_q) - (k_{1s} + k_{2s})c_s, \quad s = 1, 2, \ldots, q.
\]

- \( q \) – number of equations = number of chemical species,
- \( c_s \) – concentrations of the chemical species,
- \( u, v, w \) – components of the wind along the coordinate axes,
- \( K_x, K_y, K_z \) – diffusion coefficients,
- \( E_s \) – emissions in the space domain,
- \( k_{1s}, k_{2s} \) – coefficients of dry and wet deposition respectively,
- \( Q_s(c_1, c_2, \ldots, c_q) \) – non-linear functions that describe the chemical reactions between species.
\[
\frac{\partial c_s}{\partial t} = -\frac{\partial (uc_s)}{\partial x} - \frac{\partial (vc_s)}{\partial y} - \frac{\partial (wc_s)}{\partial z} + \\
+ \frac{\partial}{\partial x} \left( K_x \frac{\partial c_s}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial c_s}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial c_s}{\partial z} \right) + \\
+ E_s + Q_s(c_1, c_2, \ldots, c_q) - (k_{1s} + k_{2s})c_s, \quad s = 1, 2, \ldots, q.
\]

\( q \) – number of equations = number of chemical species,

\( c_s \) – concentrations of the chemical species,

\( u, v, w \) – components of the wind along the coordinate axes,

\( K_x, K_y, K_z \) – diffusion coefficients,

\( E_s \) – emissions in the space domain,

\( k_{1s}, k_{2s} \) – coefficients of dry and wet deposition respectively,

\( Q_s(c_1, c_2, \ldots, c_q) \) – non-linear functions that describe the chemical reactions between species.
\[
\frac{\partial c_s}{\partial t} = - \frac{\partial (uc_s)}{\partial x} - \frac{\partial (vc_s)}{\partial y} - \frac{\partial (wc_s)}{\partial z} + 
+ \frac{\partial}{\partial x} \left( K_x \frac{\partial c_s}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial c_s}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial c_s}{\partial z} \right) + 
+ E_s + Q_s(c_1, c_2, \ldots, c_q) - (k_{1s} + k_{2s})c_s, \quad s = 1, 2, \ldots, q.
\]

- Number of equations = number of chemical species, \(q\)
- Concentrations of the chemical species, \(c_s\)
- Components of the wind along the coordinate axes, \(u, v, w\)
- Diffusion coefficients, \(K_x, K_y, K_z\)
- Emissions in the space domain, \(E_s\)
- Coefficients of dry and wet deposition respectively, \(k_{1s}, k_{2s}\)
- Non-linear functions that describe the chemical reactions between species, \(Q_s(c_1, c_2, \ldots, c_q)\)
The mathematical model

\[ u = f(x), \quad \text{where} \quad x = (x_1, x_2, \ldots, x_d) \in U^d \equiv [0, 1]^d \]

is a vector of inputs with a joint p.d.f. \( p(x) = p(x_1, \ldots, x_d) \).
The mathematical model

\[ u = f(x), \quad \text{where} \quad x = (x_1, x_2, \ldots, x_d) \in U^d \equiv [0, 1]^d \]

is a vector of inputs with a joint p.d.f. \( p(x) = p(x_1, \ldots, x_d) \).

Total Sensitivity Index of input parameter \( x_i \), \( i \in \{1, \ldots, d\} \):

\[
S_{x_i}^{tot} = S_i + \sum_{l_1 \neq i} S_{il_1} + \sum_{l_1, l_2 \neq i, l_1 < l_2} S_{il_1l_2} + \ldots + S_{il_1\ldots l_{d-1}},
\]

where

- \( S_i \) - the main effect (first-order sensitivity index) of \( x_i \) and
- \( S_{il_1\ldots l_{j-1}} \) - \( j^{th} \) order sensitivity index for parameter \( x_i \) (\( 2 \leq j \leq d \)).
ANalysis Of VAriances (ANOVA) HDMR of a square integrable function $f(x)$:

$$f(x) = f_0 + \sum_{\nu=1}^{d} \sum_{l_1 < \ldots < l_\nu} f_{l_1 \ldots l_\nu}(x_{l_1}, x_{l_2}, \ldots, x_{l_\nu}), \quad \text{where } f_0 = \text{const},$$

and $\int_{0}^{1} f_{l_1 \ldots l_\nu}(x_{l_1}, x_{l_2}, \ldots, x_{l_\nu}) dx_{l_k} = 0, \quad 1 \leq k \leq \nu, \quad \nu = 1, \ldots, d.$

The functions in the right-hand side are defined in a unique way:

- $f_0 = \int_{U^d} f(x) dx, \quad f_{l_1}(x_{l_1}) = \int_{U^{d-1}} f(x) \prod_{k \neq l_1} dx_k - f_0, \quad l_1 \in \{1, \ldots, d\}$

- $\int_{U^d} f_{i_1 \ldots i_\mu} f_{j_1 \ldots j_\nu} dx = 0, \quad (i_1, \ldots, i_\mu) \neq (j_1, \ldots, j_\nu), \quad \mu, \nu \in \{1, \ldots, d\}.$
Definition (Sobol’)

\[ S_{l_1 \ldots l_\nu} = \frac{D_{l_1 \ldots l_\nu}}{D}, \quad \nu \in \{1, \ldots, d\}, \]

where

- partial variances
  \[ D_{l_1 \ldots l_\nu} = \int f_{l_1}^2 \ldots l_\nu \, dx_{l_1} \ldots dx_{l_\nu}, \]

- total variance
  \[ D = \int_{U^d} f^2(x) \, dx - f_0^2, \quad D = \sum_{\nu=1}^{d} \sum_{l_1 < \ldots < l_\nu} D_{l_1 \ldots l_\nu}, \]

and the following properties hold:

- \[ S_{l_1 \ldots l_s} \geq 0, \quad \sum_{s=1}^{d} \sum_{l_1 < \ldots < l_s} S_{l_1 \ldots l_s} = 1. \]
Mathematical Representation of UNI-DEM

Sensitivity Analysis Studies - The Mathematical Model Presentation

Sobol’ Approach for Evaluating Sensitivity Measures (Sobol’, 1990)

Sobol’ Global Sensitivity Indices

Methods for evaluating global sensitivity indices

Approaches for Small Sensitivity Indices

---

**Table:** Methods for evaluating global sensitivity indices.

<table>
<thead>
<tr>
<th>Method</th>
<th>Cost (model runs)</th>
<th>Sensitivity measures</th>
</tr>
</thead>
<tbody>
<tr>
<td>FAST (1973)</td>
<td>$O(d^2)$</td>
<td>$S_i$, $\forall i$</td>
</tr>
<tr>
<td>Sobol’ (1993)</td>
<td>$N(2d + 2)$</td>
<td>$S_i$, $S_{tot}$, $\forall i$</td>
</tr>
<tr>
<td>EFAST (1999)</td>
<td>$dN$</td>
<td>$S_i$, $S_{tot}$, $\forall i$</td>
</tr>
<tr>
<td>Saltelli (2002)</td>
<td>$N(d + 2)$</td>
<td>$S_i$, $S_{tot}$, $\forall i$, $S_{-lj}$, $\forall l, j, l \neq j$</td>
</tr>
<tr>
<td>Saltelli (2002)</td>
<td>$N(2d + 2)$</td>
<td>$S_i$, $S_{tot}$, $\forall i$, $S_{lj}$, $S_{-lj}$, $\forall l, j, l \neq j$</td>
</tr>
</tbody>
</table>
Let $x = (y, z) \in \mathbb{R}^d$, $y = (x_{k_1}, \ldots, x_{k_m}) \in \mathbb{R}^m$, $K = (k_1, \ldots, k_m)$. Variance of the subset $y$:

$$D_y = \sum_{n=1}^{m} \sum_{(i_1, \ldots, i_n) \in K} D_{i_1, \ldots, i_n}.$$

**Theorem (Sobol’)**

$$D_y = \int f(x) f(y, z')dx dz' - f_0^2$$

**Motivation**

If $D_y \ll f_0^2$ $\Rightarrow$ a loss of accuracy.
Let \( \mathbf{x} = (\mathbf{y}, \mathbf{z}) \in \mathbb{R}^d \), \( \mathbf{y} = (x_{k_1}, \ldots, x_{k_m}) \in \mathbb{R}^m \), \( K = (k_1, \ldots, k_m) \).

Variance of the subset \( \mathbf{y} \):
\[
D_y = \sum_{n=1}^{m} \sum_{(i_1<\ldots<i_n)\in K} D_{i_1,\ldots,i_n}.
\]

**Theorem (Sobol')**

\[
D_y = \int f(x) f(y, z')dx dz' - f_0^2
\]

**Reducing the Mean Value (I.M. Sobol', 1990)**

- Choose a constant \( c \sim f_0 \) and set the function \( \varphi(x) = f(x) - c \).
- Obtain
\[
D_y = \int \varphi(x) \varphi(y, z')dx dz' - \omega^2, \quad \text{where} \quad \omega = \int \varphi(x)dx,
\]
\[
D = \int \varphi^2(x)dx - \omega^2, \quad \omega = f_0 - c.
\]
Let \( \mathbf{x} = (\mathbf{y}, \mathbf{z}) \in \mathbb{R}^d \), \( \mathbf{y} = (x_{k_1}, \ldots, x_{k_m}) \in \mathbb{R}^m \), \( K = (k_1, \ldots, k_m) \).

Variance of the subset \( \mathbf{y} \) :
\[
D_y = \sum_{n=1}^{m} \sum_{(i_1 < \ldots < i_n) \in K} D_{i_1, \ldots, i_n}.
\]

**Theorem (Sobol')**

\[
D_y = \int f(\mathbf{x}) f(\mathbf{y}, \mathbf{z}') d\mathbf{x} d\mathbf{z}' - f_0^2
\]

**Combined Approach (Saltelli, 2002, Kucherenko, 2007)**

- Choose a constant \( c \sim f_0 \) and set the function \( \varphi(\mathbf{x}) = f(\mathbf{x}) - c \).
- Use \( \varphi(\mathbf{x}) \) rather than \( f(\mathbf{x}) \):

\[
D_y = \int \varphi(\mathbf{x}) [\varphi(\mathbf{y}, \mathbf{z}') d\mathbf{x} d\mathbf{z}' - \varphi(\mathbf{x}')] d\mathbf{x} d\mathbf{x}',
\]

\[
D = \int \varphi(\mathbf{x})[\varphi(\mathbf{x}) - \varphi(\mathbf{x}')] d\mathbf{x} d\mathbf{x}'.
\]
Let \( \mathbf{x} = (\mathbf{y}, \mathbf{z}) \in \mathbb{R}^d, \mathbf{y} = (x_{k_1}, \ldots, x_{k_m}) \in \mathbb{R}^m, K = (k_1, \ldots, k_m) \).

Variance of the subset \( \mathbf{y} : \quad D_y = \sum_{n=1}^{m} \sum_{(i_1 < \ldots < i_n) \in K} D_{i_1, \ldots, i_n}.

**Theorem (Sobol’)**

\[
D_y = \int f(\mathbf{y}, \mathbf{z}')d\mathbf{x}d\mathbf{z}' - f_0^2
\]

**Remark**

We also have shown that for some considerations *small* sensitivity indices are important. To be able to get relevant estimates of *small* indices one needs to apply a special combined technique which includes a variance reduction method and correlated sampling.
Example (integrand with computational irregularities).

\[ f(x) = \left(1 + \sum_{i=1}^{d} a_i x_i\right)^{-(d+1)} \]

\[ \|a\|_1 = \frac{600}{d^2} \]

\[ I[f] = \int_{U^d} f(x) dx \]

**Figure:** Genz integrand function with a corner peak in two dimensions.
Table: Relative error and CPU time for dimension $d = 5$, $I[f] = 0.21214 \times 10^{-5}$, $a = (5, 5, 5, 5, 4)$.

<table>
<thead>
<tr>
<th></th>
<th>Adaptive Monte Carlo Algorithm</th>
<th></th>
<th>Plain Monte Carlo Algorithm</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$</td>
<td>$l_N[f]$ $\times 10^5$</td>
<td>Rel. error</td>
<td>Time (s)</td>
</tr>
<tr>
<td>100</td>
<td>0.213</td>
<td>0.008</td>
<td>0.01</td>
</tr>
<tr>
<td>1000</td>
<td>0.211</td>
<td>0.007</td>
<td>0.13</td>
</tr>
<tr>
<td>10000</td>
<td>0.212</td>
<td>0.001</td>
<td>1.42</td>
</tr>
<tr>
<td>100000</td>
<td>0.212</td>
<td>0.0009</td>
<td>14.05</td>
</tr>
</tbody>
</table>

Calculations have been carried out on a PC with Intel(R) Pentium(R) 4 Processor.
Table: Relative error and CPU time for dimension $d = 18$, $I[f] = 0.99186 \times 10^5$, $a = (1, 2, 2, 1, 2, 1, 1, 4, 2, 1, 1, 2, 2, 1, 1, 4, 1, 1)$.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$I_N[f] \times 10^5$</th>
<th>Rel. error</th>
<th>Time (s)</th>
<th>$N$</th>
<th>$I_N[f] \times 10^5$</th>
<th>Rel. error</th>
<th>Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.9923</td>
<td>0.0005</td>
<td>7</td>
<td>2621440</td>
<td>0.989</td>
<td>0.002</td>
<td>6</td>
</tr>
<tr>
<td>100</td>
<td>0.9918</td>
<td>0.00005</td>
<td>75</td>
<td>26214400</td>
<td>0.909</td>
<td>0.084</td>
<td>60</td>
</tr>
<tr>
<td>1000</td>
<td>0.9919</td>
<td>0.00008</td>
<td>758</td>
<td>262144000</td>
<td>0.510</td>
<td>0.48</td>
<td>600</td>
</tr>
</tbody>
</table>

Calculations have been carried out on a PC with Intel(R) Pentium(R) 4 Processor.
TSI($x_1$) = 81% 

Figure: Total sensitivity indices of input parameters.
Adaptive Monte Carlo Approach for Sensitivity Analysis

SI(ijkl) = 64%
SI(ijk) = 6,6%
SI(ij) = 5,8%
SI(i) = 0,6%
SI(ijklm) = 23%

Figure: First-, second-, third-, fourth-, fifth-order effects.

Komentar: vyrhu izhodniq rezultat po-syshtestveno vliqnie imat indeksite ot po-visok red
Figure: European nitrogen oxides

Ivan Dimov, BAS

Adaptive Monte Carlo Approach for Sensitivity Analysis
Figure: Skewness of the ozone concentrations (variance 0.50)
Figure: Distribution of ozone concentrations (July 1998).
**Figure:** Sensitivity of several species to changes of chemical rates (1998).

**Figure:** Sensitivity of ozone concentrations to changes of chemical rates (period 1994-1998).
**Table:** Total sensitivity indices of input parameters obtained using different variance-based approaches for sensitivity analysis.

<table>
<thead>
<tr>
<th>estimated quantity</th>
<th>Standard (Sobol’)</th>
<th>Approaches for small indices</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$x \in [0.1; 2.0]^3$</td>
<td>$x \in [0.6; 1.4]^3$</td>
</tr>
<tr>
<td>integrand $g(x)$</td>
<td>$f(x)$</td>
<td>$f(x)$</td>
</tr>
<tr>
<td>$c$</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$g_0$</td>
<td>0.51520</td>
<td>0.51634</td>
</tr>
<tr>
<td>$D$</td>
<td>0.26181</td>
<td>0.26446</td>
</tr>
<tr>
<td>$S_1$</td>
<td>0.26386</td>
<td>0.26530</td>
</tr>
<tr>
<td>$S_2$</td>
<td>0.26447</td>
<td>0.26359</td>
</tr>
<tr>
<td>$S_3$</td>
<td>0.25348</td>
<td>0.25209</td>
</tr>
<tr>
<td>$\sum_{i=1}^{3} S_i$</td>
<td>0.78182</td>
<td>0.78097</td>
</tr>
</tbody>
</table>
### Table: Total sensitivity indices of input parameters obtained using different variance-based approaches for sensitivity analysis.

<table>
<thead>
<tr>
<th>Estimated quantity</th>
<th>Standard (Sobol')</th>
<th>Approaches for small indices</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>red. of the m.v.</td>
</tr>
<tr>
<td>$x \in [0.1; 2.0]^3$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$x \in [0.6; 1.4]^3$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$S_{12}$</td>
<td>0.06885</td>
<td>0.06941</td>
</tr>
<tr>
<td>$S_{13}$</td>
<td>0.06598</td>
<td>0.06634</td>
</tr>
<tr>
<td>$S_{23}$</td>
<td>0.06613</td>
<td>0.06592</td>
</tr>
<tr>
<td>$\sum_{i,j=1,i\leq j}^3 S_{ij}$</td>
<td>0.20096</td>
<td>0.20167</td>
</tr>
<tr>
<td>$S_{123}$</td>
<td>0.01722</td>
<td>0.01736</td>
</tr>
<tr>
<td>$S_{tot}^{x_1}$</td>
<td>0.41592</td>
<td>0.41841</td>
</tr>
<tr>
<td>$S_{tot}^{x_2}$</td>
<td>0.41667</td>
<td>0.41627</td>
</tr>
<tr>
<td>$S_{tot}^{x_3}$</td>
<td>0.40281</td>
<td>0.40170</td>
</tr>
</tbody>
</table>
An adaptive MC algorithm using Sobol’s approach for providing sensitivity analysis has been developed and applied for a test integrand family. The Sobol’ approach is a widely used technique because it is a global and model-free approach. The results of this work can be outlined as follows.

- Both techniques plain Monte Carlo and adaptive Monte Carlo are applicable depending on the particular mathematical model.
- Plain Monte Carlo is preferable for relatively small dimensions up to \((d = 5)\) when the needed accuracy is not very high (the relative error is up to 10\%). This approach can be applied to relatively simple mathematical models containing up to 5 input parameters.
- Adaptive Monte Carlo is preferable when large-scale models are analysed. When the number of dimensions is up to 18 the algorithm still produces accurate results for Sobol’ sensitivity indices in a reasonable time. The relative error is approximately 0.01\%, or smaller. The computational complexity is fairly good.
- Our experience dealing with random but controlled high sharpness outputs (typical for some outputs of non-linear large-scale environmental models) shows that the higher order sensitivity indices are more influential than lower order sensitivity indices.

Future plans

---

Ivan Dimov, BAS

Adaptive Monte Carlo Approach for Sensitivity Analysis


