# Adaptive Monte Carlo Approach for Sensitivity Analysis

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Intensive course on
*Advanced Monte Carlo methods - computational challengies*
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.

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- **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

$$
\begin{aligned}
\frac{\partial c_s}{\partial t} = & -\frac{\partial(uc_s)}{\partial x} - \frac{\partial(vc_s)}{\partial y} - \frac{\partial(wc_s)}{\partial z} + \\
& + \frac{\partial}{\partial x}\left(K_x \frac{\partial c_s}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial c_s}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial c_s}{\partial z}\right) + \\
& + E_s + Q_s(c_1, c_2, \ldots, c_q) - (k_{1s} + k_{2s})c_s, \quad s = 1, 2, \ldots, q.
\end{aligned}
$$

| | | |
|---|---|---|
| $q$ | – | 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, |
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- The mathematical model

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

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

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- Total Sensitivity Index of input parameter $x_i, \quad i \in \{1, \ldots, d\}$:

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

where

$S_i$ - *the main effect (first-order sensitivity index)* of $x_i$ and
$S_{il_1 \ldots l_{j-1}}$ – $j^{\text{th}}$ *order sensitivity index for parameter* $x_i$ $(2 \leq j \leq d)$.

ANalysis Of VAriances (ANOVA) HDMR of a square integrable function $f(\mathbf{x})$:

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

and $$\int_0^1 f_{l_1\ldots l_\nu}(x_{l_1}, x_{l_2}, \ldots, x_{l_\nu})\mathrm{d}x_{l_k} = 0, \quad 1 \le k \le \nu, \ \ \nu = 1, \ldots, d.$$

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

- $f_0 = \int_{U^d} f(\mathbf{x})\mathrm{d}\mathbf{x}, \quad f_{l_1}(x_{l_1}) = \int_{U^{d-1}} f(\mathbf{x}) \prod_{k \neq l_1} \mathrm{d}\mathbf{x}_k - f_0, \ l_1 \in \{1, \ldots, d\}$
- $\int_{U^d} f_{i_1\ldots i_\mu} f_{j_1\ldots j_\nu} \,\mathrm{d}\mathbf{x} = 0, \ \ (i_1, \ldots, i_\mu) \neq (j_1, \ldots, j_\nu), \ \ \mu, \nu \in \{1, \ldots, d\}.$

### Definition (Sobol')

$$S_{l_1 \ \ldots \ l_\nu} = \frac{\mathbf{D}_{l_1 \ \ldots \ l_\nu}}{\mathbf{D}}, \quad \nu \in \{1, \ldots, d\},$$

where

- partial variances $$\mathbf{D}_{l_1 \ \ldots \ l_\nu} = \int f^2_{l_1 \ \ldots \ l_\nu} \mathrm{d}x_{l_1} \ldots \mathrm{d}x_{l_\nu},$$
- total variance $$\mathbf{D} = \int_{U^d} f^2(\mathbf{x}) \mathrm{d}\mathbf{x} - f_0^2, \qquad \mathbf{D} = \sum_{\nu=1}^{d} \sum_{l_1 < \ldots < l_\nu} \mathbf{D}_{l_1 \ldots l_\nu},$$

and the following properties hold:

- $$S_{l_1 \ \ldots \ l_s} \geq 0, \qquad \sum_{s=1}^{d} \sum_{l_1 < \ldots < l_s}^{d} S_{l_1 \ \ldots \ l_s} = 1.$$

Table: Methods for evaluating global sensitivity indices.

| Method | Cost (model runs) | Sensitivity measures |
|---|---|---|
| FAST (1973) | $O(d^2)$ | $S_i, \forall i$ |
| Sobol' (1993) | $N(2d+2)$ | $S_i, S_{x_i}^{tot}, \forall i$ |
| EFAST (1999) | $dN$ | $S_i, S_{x_i}^{tot}, \forall i$ |
| Saltelli (2002) | $N(d+2)$ | $S_i, S_{x_i}^{tot}, \forall i, S_{-lj}, \forall l, j, l \neq j$ |
| Saltelli (2002) | $N(2d+2)$ | $S_i, S_{x_i}^{tot}, \forall i, S_{lj}, S_{-lj}, \forall l, j, l \neq j$ |

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 $\mathbf{y}$ : $\mathbf{D_y} = \sum_{n=1}^{m} \sum_{(i_1 < \ldots < i_n) \in K} \mathbf{D}_{i_1, \ldots, i_n}$.

**Theorem (Sobol')**

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

**Motivation**

If $\mathbf{D_y} << f_0^2 \quad \Rightarrow$ a loss of accuracy.

Let $\mathbf{x} = (\mathbf{y}, \mathbf{z}) \in \mathbb{R}^d$, $\mathbf{y} = (x_{k_1}, \ldots, x_{k_m}) \in \mathbb{R}^m$, $K = (k_1, \ldots, k_m)$.
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### Reducing the Mean Value (I.M. Sobol', 1990)

- Choose a constant $c \sim f_0$ and set the function $\varphi(\mathbf{x}) = f(\mathbf{x}) - c$.
- Obtain

$$\mathbf{D_y} = \int \varphi(\mathbf{x})\, \varphi(\mathbf{y}, \mathbf{z}')\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{z}' - \omega^2, \qquad \text{where} \quad \omega = \int \varphi(\mathbf{x})\mathrm{d}\mathbf{x},$$

$$\mathbf{D} = \int \varphi^2(\mathbf{x})\mathrm{d}\mathbf{x} - \omega^2, \qquad \omega = f_0 - c.$$

Let $\mathbf{x} = (\mathbf{y}, \mathbf{z}) \in \mathbb{R}^d$, $\mathbf{y} = (x_{k_1}, \ldots, x_{k_m}) \in \mathbb{R}^m$, $K = (k_1, \ldots, k_m)$.
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### Theorem (Sobol')

$$\mathbf{D}_{\mathbf{y}} = \int f(\mathbf{x})\, f(\mathbf{y}, \mathbf{z}') \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{z}' - f_0^2$$

### 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 $f(\mathbf{x})$:

$$\mathbf{D}_{\mathbf{y}} = \int \varphi(\mathbf{x})\, [\varphi(\mathbf{y}, \mathbf{z}') \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{z}' - \varphi(\mathbf{x}')] \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{x}',$$

$$\mathbf{D} = \int \varphi(\mathbf{x})[\varphi(\mathbf{x}) - \varphi(\mathbf{x}')]\, \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{x}'.$$

Let $\mathbf{x} = (\mathbf{y}, \mathbf{z}) \in \mathbb{R}^d$, $\mathbf{y} = (x_{k_1}, \ldots, x_{k_m}) \in \mathbb{R}^m$, $K = (k_1, \ldots, k_m)$.
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## 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).

$$f(x) = (1 + \sum_{i=1}^{d} a_i\ x_i)^{-(d+1)}$$

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

$$I[f] = \int_{U^d} f(x) \mathrm{d}\mathbf{x}$$

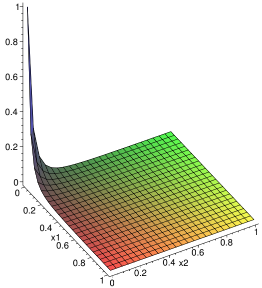


Figure: Genz integrand function with a corner peak in two dimensions

Table: Relative error and CPU time for dimension $d = 5$, $I[f] = 0.21214\mathbf{e} - 05$, $a = (5, 5, 5, 5, 4)$.

| Adaptive Monte Carlo Algorithm | | | | Plain Monte Carlo Algorithm | | | |
|---|---|---|---|---|---|---|---|
| $N$ | $I_N[f]$ $\times 10^5$ | Rel. error | Time (s) | $N$ | $I_N[f]$ $\times 10^5$ | Rel. error | Time (s) |
| 100 | 0.213 | 0.008 | 0.01 | $94.10^2$ | 0.18 | 0.13 | 0.01 |
| 1000 | 0.211 | 0.007 | 0.13 | $94.10^3$ | 0.19 | 0.08 | 0.06 |
| 10000 | 0.212 | 0.001 | 1.42 | $94.10^4$ | 0.22 | 0.02 | 0.55 |
| 100000 | 0.212 | 0.0009 | 14.05 | $94.10^5$ | 0.20 | 0.04 | 5.38 |

Calculations have been carried out on a PC with Intel(R) Pentium(R) 4 Processor.

Table: Relative error and CPU time for dimension $d = 18$, $I[f] = 0.99186\mathbf{e} - 05$, $a = \left(\frac{1}{9}, \frac{2}{27}, \frac{2}{27}, \frac{1}{9}, \frac{2}{27}, \frac{1}{9}, \frac{1}{9}, \frac{4}{27}, \frac{2}{27}, \frac{1}{9}, \frac{1}{9}, \frac{2}{27}, \frac{2}{27}, \frac{1}{9}, \frac{1}{9}, \frac{4}{27}, \frac{1}{9}, \frac{1}{9}\right)$.

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

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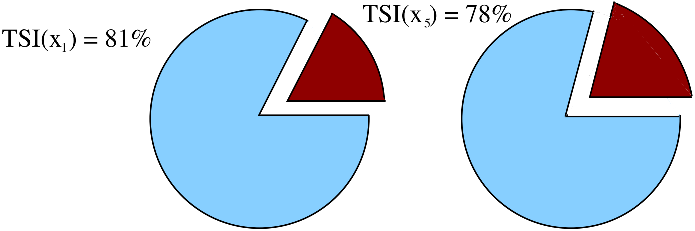


Figure: Total sensitivity indices of input parameters.

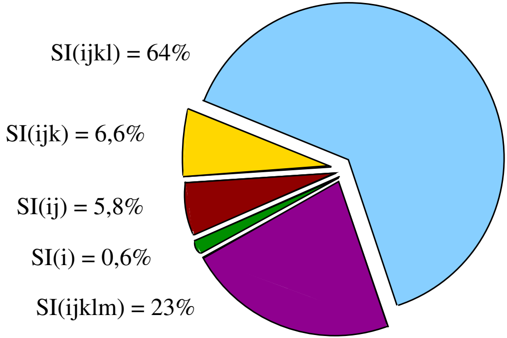


Figure: First-, second-, third-, fourth-, fifth-order effects.

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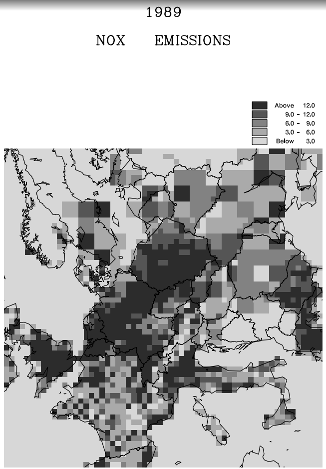


Figure: European nitrogen oxides

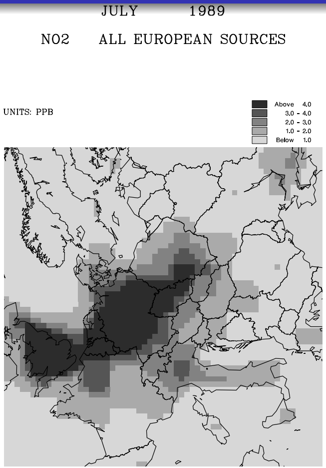


Figure: Nitrogen di-oxide

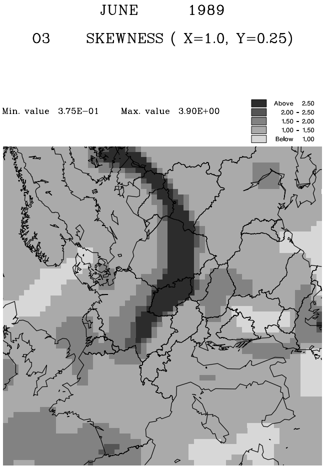


Figure: Skewness of the ozone concentrations (variance 0.50)

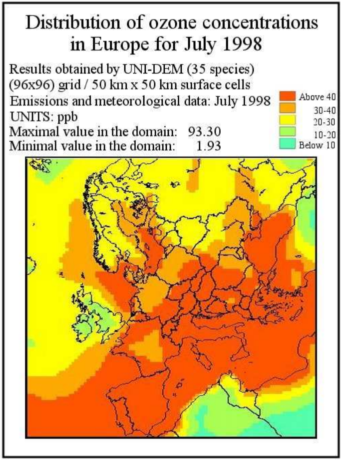


Figure: Distribution of ozone concentrations (July 1998).

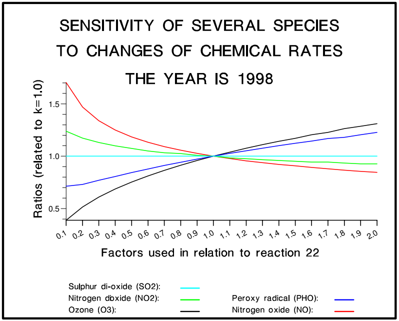


Figure: Sensitivity of several species to changes of chemical rates (1998).

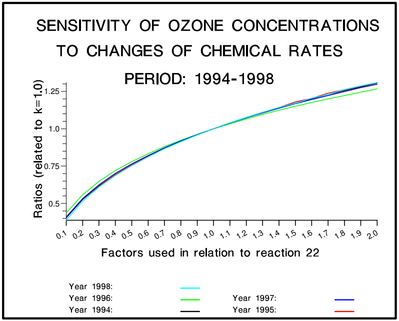


Figure: Sensitivity of ozone concentrations to changes of chemical rates (period 1994-1998).

Table: Total sensitivity indices of input parameters obtained using different variance-based approaches for sensitivity analysis.

| approach / estimated quantity | Standard (Sobol') | | Approaches for small indices | |
|---|---|---|---|---|
| | | | red. of the m.v. | combined |
| | $\mathbf{x} \in [0.1; 2.0]^3$ | $\mathbf{x} \in [0.6; 1.4]^3$ | $\mathbf{x} \in [0.6; 1.4]^3$ | $\mathbf{x} \in [0.6; 1.4]^3$ |
| integrand $g(\mathbf{x})$ | $f(\mathbf{x})$ | $f(\mathbf{x})$ | $f(\mathbf{x}) - c$ | $f(\mathbf{x}) - c$ |
| $c$ | - | - | 0.51737 | 0.51737 |
| $g_0$ | 0.51520 | 0.51634 | 0.25145 | 0.25145 |
| $\mathbf{D}$ | 0.26181 | 0.26446 | 0.07061 | 0.00530 |
| $S_1$ | 0.26386 | 0.26530 | 0.27354 | 0.52979 |
| $S_2$ | 0.26447 | 0.26359 | 0.26713 | 0.46142 |
| $S_3$ | 0.25348 | 0.25209 | 0.22406 | 0.00222 |
| $\sum_{i=1}^{3} S_i$ | 0.78182 | 0.78097 | 0.76474 | 0.99342 |

Table: Total sensitivity indices of input parameters obtained using different variance-based approaches for sensitivity analysis.

| approach / estimated quantity | Standard (Sobol') | | Approaches for small indices | |
|---|---|---|---|---|
| | | | red. of the m.v. | combined |
| | $\mathbf{x} \in [0.1; 2.0]^3$ | $\mathbf{x} \in [0.6; 1.4]^3$ | $\mathbf{x} \in [0.6; 1.4]^3$ | $\mathbf{x} \in [0.6; 1.4]^3$ |
| $S_{12}$ | 0.06885 | 0.06941 | 0.07994 | 0.00628 |
| $S_{13}$ | 0.06598 | 0.06634 | 0.06845 | 0.00009 |
| $S_{23}$ | 0.06613 | 0.06592 | 0.06686 | 0.00021 |
| $\sum_{i,j=1,i\leq j}^{3} S_{ij}$ | 0.20096 | 0.20167 | 0.21525 | 0.00658 |
| $S_{123}$ | 0.01722 | 0.01736 | 0.02001 | 0.000003 |
| $S_{x_1}^{tot}$ | 0.41592 | 0.41841 | 0.44195 | 0.53615 |
| $S_{x_2}^{tot}$ | 0.41667 | 0.41627 | 0.43395 | 0.46791 |
| $S_{x_3}^{tot}$ | 0.40281 | 0.40170 | 0.37938 | 0.00252 |

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

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