Proceedings of the 20th Conference on Computer Science and Intelligence Systems (FedCSIS) pp. 777–781
DOI: 10.15439/2025F4849
ISSN 2300-5963 ACSIS, Vol. 43

A New Optimization Method for Evaluating Sobol' Sensitivity Indices

Venelin Todorov*†, Velichka Traneva§, Stoyan Tranev§,
Mihai Petrov§, Slavi Georgiev‡¶, Fatima Sapundzhi‖
*Department of Parallel Algorithms and Machine Learning with a Laboratory in Neurotechnologies,
Institute of Information and Communication Technologies, Bulgarian Academy of Sciences,
25A Acad. G. Bonchev Str., 1113 Sofia, Bulgaria
†Centre of Excellence in Informatics and Information and Communication Technologies,
Acad. G. Bonchev Str. Bl. 25A, 1113 Sofia, Bulgaria
‡Institute of Mathematics and Informatics, Bulgarian Academy of Sciences,
8 Acad. G. Bonchev Str., 1113 Sofia, Bulgaria
§Department of Mathematics, Informatics and Physics, Prof. Dr. Asen Zlatarov University – Bourgas,
1 Prof. Yakim Yakimov Blvd., 8010 Bourgas, Bulgaria
¶Department of Applied Mathematics and Statistics, Angel Kanchev University of Ruse,
8 Studentska Str., 7004 Ruse, Bulgaria
‖Department of Communication and computer engineering, Faculty of Engineering,
South-West University "Neofit Rilski", 2700, Blagoevgrad, Bulgaria
Email: venelin@parallel.bas.bg, veleka13@gmail.com, tranev@abv.bg,
mihpetrov@abv.bg, sggeorgiev@math.bas.bg, sggeorgiev@uni-ruse.bg, sapundzhi@swu.bg

***Abstract*—This paper presents an optimization method based on a particular polynomial lattice rule with interlaced factor two for estimating sensitivity indices in global sensitivity analysis, focusing on total, first-order and second-order Sobol indices. A comparison with one of the best available methods the Modified Sobol Sequence and component by component construction polynomial lattice rule have been done. Relative errors for key output quantities are analyzed and compared. Our results show that the proposed optimization method consistently outperforms other methods in accurately estimating both first-order and total-order sensitivity indices, especially for parameters with smaller effects. These findings highlight the strengths and limitations of each method, providing guidance for selecting appropriate stochastic sampling strategies in computational sensitivity analysis.**

I. Introduction

SENSITIVITY analysis (SA) [12], [14], [17], [21] is a fundamental technique in modeling and simulation that investigates how variations in input parameters influence the output of a given system. By identifying which inputs contribute most to uncertainty in the model results, SA provides valuable insights into the robustness and reliability of mathematical models. This approach is especially crucial in complex environmental, financial, and engineering systems, where numerous variables interact in nonlinear ways. SA not only enhances model transparency but also supports decision-making by highlighting the key drivers of system behavior.

Venelin Todorov was partially supported by the Centre of Excellence in Informatics and ICT under the Grant No BG16RFPR002-1.014-0018, financed by the Research, Innovation and Digitalization for Smart Transformation Programme 2021-2027 and co-financed by the European Union and by BNSF under Projects KP-06-N62/6 "Machine learning through physics-informed neural networks".

Quasi Monte Carlo methods (QMC) methods are powerful technique for performing SA [14], [21].

The input data for SA has been obtained during runs of a large-scale mathematical model for remote transport of air pollutants - **Uni**fied **D**anish **E**ulerian **M**odel (UNI-DEM) [11], [16], [26]. UNI-DEM is described mathematically [23], [24], [25]) by the following system of PDEs:

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

The number of studied pollutants by UNI-DEM determines the number q of equations in the system. It follows the other dimensions of the model:

c_s - pollutant concentrations,
u, v, w - wind components along the coordinate axes,
K_x, K_y, K_z - diffusion coefficients,
E_s - space emissions,
k_{1s}, k_{2s} - dry and wet deposit coefficients, respectively ($s = 1, \ldots, q$),
$Q_s(c_1, c_2, \ldots, c_q)$ - nonlinear functions describing chemical reactions between pollutants.

It is assumed that the mathematical model can be presented by a model function

$$\mathrm{u} = f(\mathrm{x}), \quad \text{where} \quad \mathrm{x} = (x_1, x_2, \ldots, x_s) \in U^s \equiv [0;1]^s \tag{1}$$

is a vector of input parameters with a joint **p**robability **d**ensity **f**unction (p.d.f.) $p(\mathrm{x}) = p(x_1, \ldots, x_s)$.

The concept of Sobol approach is based on a decomposition of an integrable model function f [20]:

$$f(\mathrm{x}) = f_0 + \sum_{\nu=1}^{s} \sum_{l_1<\ldots<l_\nu} f_{l_1\ldots l_\nu}(x_{l_1}, x_{l_2}, \ldots, x_{l_\nu}), \qquad (2)$$

where f_0 is a constant. The representation (2) is referred to as the ANOVA-representation of the model function $f(\mathrm{x})$ if each term satisfy [20]:

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

The quantities

$$\mathbf{D} = \int_{U^s} f^2(\mathrm{x})\mathrm{d}\mathrm{x} - f_0^2,\ \mathbf{D}_{l_1\ \ldots\ l_\nu} = \int f^2_{l_1\ \ldots\ l_\nu}\mathrm{d}x_{l_1}\ldots\mathrm{d}x_{l_\nu} \qquad (3)$$

are the so-called total and partial variances, respectively. A similar decomposition holds for the total variance that is represented by the corresponding partial variances: $\mathbf{D} = \sum_{\nu=1}^{s}\sum_{l_1<\ldots<l_\nu}\mathbf{D}_{l_1\ldots l_\nu}$. The main sensitivity measures following the Sobol approach are the so-called Sobol global sensitivity indices [20], [17] defined by

$$S_{l_1\ \ldots\ l_\nu} = \frac{\mathbf{D}_{l_1\ \ldots\ l_\nu}}{\mathbf{D}}, \quad \nu \in \{1, \ldots, s\}. \qquad (4)$$

and the **t**otal **s**ensitivity **i**ndex (TSI) of an input parameter $x_i, i \in \{1, \ldots, s\}$ defined by [20], [17]:

$$S_i^{tot} = S_i + \sum_{l_1 \ne i} S_{il_1} + \sum_{l_1, l_2 \ne i, l_1<l_2} S_{il_1l_2} + \ldots + S_{il_1\ldots l_{s-1}}, \qquad (5)$$

where S_i is called *the main effect (first-order sensitivity index)* of x_i and $S_{il_1\ldots l_{j-1}}$ is the j-th order sensitivity index. The higher-order terms describe the interaction effects between the unknown input parameters $x_{i_1}, \ldots, x_{i_\nu}, \nu \in \{2, \ldots, s\}$ on the output variance. This implies that performing global sensitivity analysis from a mathematical standpoint involves calculating total sensitivity indices (see Equation 5), which—according to the formulations in Equations 3–4—reduces to the evaluation of multidimensional integrals.

II. The Stochastic Approaches

Let us consider the following task for multidimensional integration:

$$S(f) := I = \int_{U^s} f(x)dx.$$

The first algorithm that we are going to use is the modified Sobol sequence based on procedure of shaking.

We will use a method that looks like the stratified symmetrized Monte Carlo [19]. For our Monte Carlo algorithm based on modified Sobol sequence (MCA-MSS-2-S), the original domain of integration is divided into m^s disjoint subdomains with equal volumes $\mathbf{K}_i^s, i = 1, \ldots, m^s$, where m is the number of subintervals used for the partition in each dimension. Here two pseudorandom points are generated. The first ξ_i is generated uniformly distributed inside the subdomain $\mathbf{K}_i^s$ and second $\xi_i^{'}$ is computed to be symmetric to ξ_i according to the central point s_i in $\mathbf{K}_i^s$. The concept in two-dimensional case for MCA-MSS-2-S is illustrated on Figure 1.

The value of the integral can be approximated [6]:

$$I(f) \approx \frac{1}{2m^s}\sum_{i=1}^{m^s}\left[f(\xi_i) + f(\xi_i^{'})\right].$$

It is proved that the algorithm MCA-MSS-2-S has an optimal rate of convergence ($n^{-\frac{1}{2}-\frac{2}{s}}$) for the class of continuous functions with continuous first derivatives and bounded second derivatives [7]. Up to now this method gives one of the best results for estimating sensitivity indices [6].

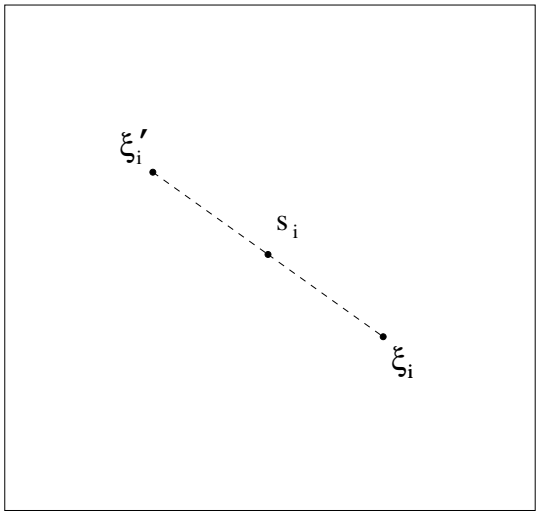

Fig. 1. Generation of a pseudorandom point $\xi_i(\xi_i') \in \mathbf{E}_i^2$.

Now we will use the so-called lattice rules. To introduce rank-1 lattice rule we will use the following formula [22]:

$$\mathbf{x}_k = \left\{\frac{k}{N}\mathbf{z}\right\},\ k = 1, \ldots, N, \qquad (6)$$

where N is an integer, $N \ge 2$, $\mathbf{z} = (z_1, z_2, \ldots z_s)$ is the generating vector and $\{z\}$ denotes the fractional part of z. For the definition of the $E_s^\alpha(c)$ and $P_\alpha(z, N)$ see [22].

In 1959 Bahvalov [1] proved that there exists an optimal choice of the generating vector $\mathbf{z}$:

$$\left|\frac{1}{N}\sum_{k=1}^{N} f\left(\left\{\frac{k}{N}\mathbf{z}\right\}\right) - \int\limits_{[0,1)^s} f(u)du\right| \le cu(s,\alpha)\frac{(\log N)^{\beta(s,\alpha)}}{N^\alpha}, \qquad (7)$$

for the function $f \in E_s^\alpha(c)$, $\alpha > 1$ and $u(s,\alpha), \beta(s,\alpha)$ do not depend on N.

The first generating vector in construction of our lattice rule is the generalized Fibonacci numbers of the corresponding dimension and the method will be called FIBO. FIBO will use the following generating vector [22]:

$$\mathbf{z} = (1, F_n^{(s)}(2), \ldots, F_n^{(s)}(s)), \qquad (8)$$

where we use that $F_n^{(s)}(j) := F_{n+j-1}^{(s)} - \sum_{i=0}^{j-2} F_{n+i}^{(s)}$ and $F_{n+l}^{(s)}$ ($l = 0, \ldots, j-1, j$ is an integer, $2 \leq j \leq s$) is the term of the s-dimensional Fibonacci sequence [22].

Now we will consider a special lattice rule based on the component by component construction method [2], [3], [18]. An optimal generating vector based on the rank-1 lattice rules with prime number of points is obtained using the component by component construction method. More specifically, let us initially set $z_1 := 1$. Then, assuming z_1 remains fixed, and $z_2 \in U^N := z \in \mathbb{N} : 1 \leq z \leq N-1,\ \gcd(z, N) = 1$ is chosen in such a way that a predefined error criterion [5], [15] is minimized in two dimensions. Then, iteratively for $i = 3, \ldots, s$, z_i is selected from U^N in such a manner that it minimizes the predefined error criterion in i dimensions. At the first step of the algorithm s dimensional optimal generating vector $\mathbf{z} = (z_1, z_2, \ldots z_s)$ is generated by the fast component by component construction method described above. On the second step of the algorithm we generate the points of lattice rule by formula $\mathbf{x}_k = \left\{ \frac{k}{N}\mathbf{z} \right\},\ k = 1, \ldots, N$. And at the third and last step of the algorithm an approximate value I_N of the multidimensional integral is evaluated by the formula:

$$I_N = \frac{1}{N} \sum_{k=1}^{N} f\left(\left\{ \frac{k}{N}\mathbf{z} \right\} \right).$$

The steps of working for the method are given on the flowchart on Fig. 2.

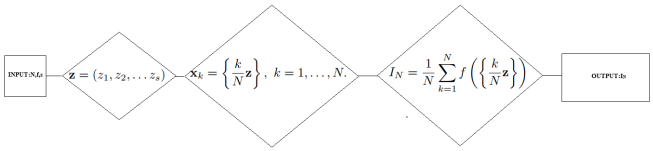

Fig. 2. The flowchart of the algorithm

Now we will continue with our optimization method based on polynomial lattice rule with special generating matrices never used for this computational task before. Let b be prime, let p be a polynomial and $deg\ p = m$ with coefficients in Z_b, and let $q_1, \ldots q_s$ be polynomials and $deg(q_1, \ldots, q_s) \leq m-1$ with coefficients in Z_b. Then we will choose C_j, the j^{th} generating matrix.

Let for $u_1, u_2, \cdots \in Z_b$:

$$\frac{q_j(x)}{p(x)} = \frac{u_1}{x} + \frac{u_2}{x^2} + \ldots.$$

Then set

$$\mathbf{C_j} = \begin{pmatrix} u_1 & u_2 & u_3 & \ldots & u_m \\ u_2 & u_3 & \ldots & \ldots & u_{m+1} \\ u_3 & \ldots & \ldots & \ldots & u_{m+2} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ u_m & u_{m+1} & u_{m+2} & \ldots & u_{2m-1} \end{pmatrix} \in Z_b^{m \times m}. \tag{9}$$

The digital net [4] with $C_1, \ldots, C_s$ is named a polynomial lattice point set (PLPS), and a QMC rule using a polynomial lattice point set is named a polynomial lattice rule, where p is the modulus, and $(q_1, \ldots, q_s)$ is the generating vector of polynomials [13].

Let $m, s, d \in \mathbb{N}$ be defined with $d > 1$. Let $p \in Z_b$ be defined as $\deg(p) = m$ and let $q = (q_1, \ldots, q_{ds}) \in (Z_b)^{ds}$. An interlaced polynomial lattice rule of order d is actually a point set composed by b_m points $x_0, \ldots, x_b^{m-1}$ which are defined as [4]

$$x_n := D_d(z_n),$$

the n^{th} point z_n of a PLPS $P_{b^m,ds}(q, p)$ is presented by

$$z_n := \left(v_m\left(\frac{n(x)q_1(x)}{p(x)} \right), v_m\left(\frac{n(x)q_2(x)}{p(x)} \right), \ldots, v_m\left(\frac{n(x)q_{ds}(x)}{p(x)} \right) \right) \in [0,1)^{ds}$$

for $0 \leq n < b^m$. For explanation of $n(x)$ see [13]. A QMC rule, that uses this point set is called an interlaced polynomial lattice rule (of order d). Generating matrices used for the construction of interlaced polynomial lattice point sets were based on the implementation of the Sobol sequence with interlacing factor $d = 2$, as described in [15].

III. Case study - UNI-DEM model

The efficient MC algorithms for multidimensional numerical integration described above have been applied to sensitivity studies of concentration variations of air pollutants with respect to emission levels and some chemical reactions rates. More information can be found in [8], [9], [10].

A. Sensitivity Studies with Respect to Emission Levels

TABLE I
COMPARISON OF RELATIVE ERRORS FOR SENSITIVITY INDICES ESTIMATION USING VARIOUS STOCHASTIC APPROACHES ($n \approx 65536$).

EQ	RV	MSS-2S	IPLR2	CBCCM	FIBO
f_0	0.048	**2e-08**	7e-06	8e-06	9e-06
$\mathbf{D}$	0.0002	**2e-06**	8e-05	6e-04	3e-04
S_1	9e-01	5e-04	**2e-05**	**2e-05**	4e-04
S_2	2e-04	7e-02	**3e-03**	4e-01	2e-01
S_3	1e-01	1e-02	**9e-05**	3e-03	3e-03
S_4	4e-05	6e-01	**1e-02**	1e+00	5e-01
S_1^{tot}	9e-01	1e-03	**1e-05**	3e-04	5e-04
S_2^{tot}	2e-04	3e-03	**2e-03**	1e-01	3e-01
S_3^{tot}	1e-01	4e-03	**8e-05**	9e-04	2e-03
S_4^{tot}	5e-05	1e-01	**2e-02**	4e-01	5e-01

Firstly we will study the sensitivity of the model output (in terms of mean monthly concentrations of several important pollutants) with respect to variation of input emissions of the anthropogenic pollutants. The anthropogenic emissions input consist of 4 different components $\mathbf{E} = (\mathbf{E^A}, \mathbf{E^N}, \mathbf{E^S}, \mathbf{E^C})$ as follows:

$\mathbf{E^A}$ – ammonia (NH_3);
$\mathbf{E^S}$ – sulphur dioxide (SO_2);
$\mathbf{E^N}$ – nitrogen oxides $(NO + NO_2)$;
$\mathbf{E^C}$ – anthropogenic hydrocarbons.

The output of the model is mean monthly concentration of the following 3 pollutants:

- s_1 – ozone (O_3);
- s_2 – ammonia (NH_3);
- s_3 – ammonium sulphate and ammonium nitrate ($NH_4SO_4 + NH_4NO_3$).

In our particular case we are interested in sensitivity studies of the mean monthly concentrations of ammonia in Milan. The domain under consideration is the 4-dimensional hypercubic domain $[0.5, 1]^4$).

This table I compares the relative errors (RE) for estimating sensitivity indices of various input parameters using four stochastic approaches, with a sample size of approximately 65536. The Reference Values (RV) are included for context. for the model function MSS-2S stands out with the smallest relative error (2e-08), indicating exceptional accuracy in estimating the mean output. IPLR2, CBCCM, and FIBO are all orders of magnitude less precise here (errors in the range of 7e-06 to 9e-06). This suggests MSS-2S is highly efficient for estimating basic function averages. For the total variance ($\mathbf{D}$) MSS-2S again shows the lowest RE (2e-06), confirming its strength in capturing overall variance. IPLR2 (8e-05) and FIBO (3e-04) are better than CBCCM (6e-04) but lag behind MSS-2S.

For S_1 (most influential parameter), both IPLR2 and CBCCM achieve the best RE (2e-05), outperforming MSS-2S and FIBO. This suggests these two methods are more precise in estimating dominant first-order effects. For S_2, IPLR2 performs best (3e-03), significantly better than MSS-2S (7e-02), CBCCM (4e-01), and FIBO (2e-01). For S_3 and S_4, IPLR2 consistently has the smallest errors (9e-05 and 1e-02 respectively), with MSS-2S and FIBO trailing and CBCCM performing worst. This indicates IPLR2 is very efficient at estimating sensitivity for less dominant variables. For S_1^{tot} IPLR2 outperforms others with 1e-05 error, better than CBCCM (3e-04), MSS-2S (1e-03), and FIBO (5e-04). For S_2^{tot} IPLR2 again leads with 2e-03, while MSS-2S (3e-03) performs well but CBCCM and FIBO lag behind (0.1 and 0.3). For S_3^{tot} and S_4^{tot}, IPLR2 maintains the best accuracy with relative errors of 8e-05 and 2e-02, respectively, indicating strong performance on total effect indices across less influential parameters.

To summarize, in this case, if the goal is to accurately estimate the mean and total variance, MSS-2S is the method of choice. For detailed sensitivity analysis—precisely estimating both first-order and total-order indices, especially those with smaller magnitude—IPLR2 offers superior accuracy. CBCCM and FIBO show relatively larger errors, suggesting they may be less suitable for high-precision sensitivity studies with this sample size.

B. Sensitivity Studies with Respect to Chemical Reactions Rates

In this part we will study the sensitivity of the ozone concentration in Genova according to the rate variation of some chemical reactions: ## $1, 3, 7, 22$ (time-dependent) and $27, 28$ (time independent) reactions of the condensed CBM-IV scheme ([23]). The simplified chemical equations of these reactions are as follows:

$$
\begin{aligned}
&[\#\mathbf{1}] \quad NO_2 + h\nu \Longrightarrow NO + O;\\
&[\#\mathbf{3}] \quad O_3 + NO \Longrightarrow NO_2;\\
&[\#\mathbf{7}] \quad NO_2 + O_3 \Longrightarrow NO_3;\\
&[\#\mathbf{22}] \quad HO_2 + NO \Longrightarrow OH + NO_2;\\
&[\#\mathbf{27}] \quad HO_2 + HO_2 \Longrightarrow H_2O_2;\\
&[\#\mathbf{28}] \quad OH + CO \Longrightarrow HO_2.
\end{aligned}
$$

The domain under consideration is the 6-dimensional hypercubic domain $[0.6, 1.4]^6$).

TABLE II
COMPARISON OF RELATIVE ERRORS (RE) FOR AE OF SIS ACROSS SELECTED METHODS ($n \approx 2^{16}$).

EQ	RV	MSS-2S	D-α2-Cs-1	CBCCM	FIBO
f_0	0.27	**5e-07**	8.4e-06	1e-05	3e-04
$\mathbf{D}$	0.0025	1e-04	**2.8e-05**	1e-04	2e-03
S_1	4e-01	2e-02	**2.4e-04**	3e-03	4e-02
S_2	3e-01	6e-02	**1.2e-04**	5e-03	1e-02
S_3	5e-02	8e-02	**2.3e-04**	4e-03	5e-01
S_4	3e-01	4e-03	**1.2e-05**	5e-04	1e-02
S_5	4e-07	2e+02	**5.9e-01**	2e+02	3e+03
S_6	2e-02	4e-02	**1.0e-03**	3e-02	1e+00
S_1^{tot}	4e-01	5e-02	**2.2e-04**	7e-03	8e-02
S_2^{tot}	3e-01	3e-02	**2.8e-04**	2e-03	3e-02
S_3^{tot}	5e-02	4e-02	**5.9e-04**	2e-02	1e+00
S_4^{tot}	3e-01	4e-02	**5.8e-05**	1e-03	4e-01
S_5^{tot}	2e-04	1e+00	**1.5e-02**	2e-01	9e+01
S_6^{tot}	2e-02	4e-02	**1.1e-03**	3e-03	2e+00
S_{12}	6e-03	7e-01	**2.8e-03**	3e-01	3e+00
S_{14}	5e-03	1e+00	**6.5e-03**	3e-02	8e+00
S_{24}	3e-03	1e+00	**4.5e-03**	5e-02	1e+01
S_{45}	1e-05	4e+00	**3.3e-02**	1e+00	4e+01

This table II compares the relative errors (RE) for estimating sensitivity indices of various input parameters using four stochastic approaches, with a sample size of approximately 65536.

FIBO performs poorly overall, especially in detecting higher-order and small-effect indices. It delivers acceptable errors only for dominant first-order indices, such as S_1 and S_2, but is far less accurate for total-effect and interaction indices. Also, it is characterized with substantial divergence in weak-effect indices like S_5, S_5^{tot}, and interaction terms—REs are several orders of magnitude larger than other methods. FIBO is inadequate for high-precision sensitivity analysis, particularly in higher-dimensional or low-sensitivity contexts.

CBCCM offers moderately good performance, better than FIBO but generally not better than MSS-2S or IPLR2 It excels in select indices like S_1^{tot} and S_2^{tot} but is not the best in any single row of the table. It tends to perform worse than IPLR2 in detecting fine-grained or subtle effects, although it outperforms MSS-2S and FIBO in some higher-order interactions. CBCCM is reliable but not exceptional. It represents a solid compromise between computational cost and accuracy.

MSS-2S delivers excellent accuracy for f_0 and $\mathbf{D}$, both with errors as low as 10^{-7} to 10^{-4}. It performs well for low-to-moderate variance indices (e.g., S_1, S_2, S_3), but poorly on

higher-order or subtle interactions like S_{24} and S_{45}. It notably fails in estimating some higher-order interactions and weak effects (e.g., very high RE in the smallest in value S_5 and S_5^{tot} which are very important for the reliability of the results). MSS-2S is accurate and efficient for dominant effects, but may be unstable for weak sensitivities or higher-order interactions.

Among all methods, IPLR2 provides the lowest RE for the majority of first-order and total-effect indices, including: S_1, S_2, S_3, S_4, S_1^{tot} through S_6^{tot} and many second-order terms like S_{12}, S_{14}, S_{24}, and S_{45}. It is exceptionally robust across both low and high sensitivity parameters, and particularly effective in capturing small effect sizes (e.g., S_5). It is very competitive even for interaction terms, where other methods tend to diverge. IPLR2 stands out as the most consistently accurate and robust method, particularly effective for precise SI estimation across the full spectrum of effects.

IV. Conclusion

The computational experiments reveal that the optimization method IPLR2 developed are amongst the most effective stochastic strategies currently available for determining sensitivity indices, particularly for the most challenging task – assessing the least value sensitivity indices, which are crucial for the dependability of the model's outcomes. These findings are of considerable significance for environmental conservation and the credibility of future predictions.

The results underscore the trade-off between method complexity and accuracy: MSS-2S excels in some global measures, while IPLR2 is more balanced for all sensitivity indices. Among the evaluated methods for estimating sensitivity indices, our optimization method IPLR2 consistently delivers the most accurate and robust results, especially across both dominant and subtle effects, including higher-order interactions. MSS-2S performs well for main effects but lacks stability in weak or complex interactions. CBCCM offers balanced performance but is never the top performer. In contrast, FIBO and RV show significant limitations in accuracy and should be avoided in precision-critical sensitivity analyses. Overall, the proposed optimization method is the recommended method for comprehensive and reliable global sensitivity estimation.

Acknowledgment

Venelin Todorov was partially supported by the Centre of Excellence in Informatics and ICT under the Grant No BG16RFPR002-1.014-0018, financed by the Research, Innovation and Digitalization for Smart Transformation Programme 2021-2027 and co-financed by the European Union and by BNSF under Project KP-06-N62/6 "Machine learning through physics-informed neural networks".

References

[1] N. Bahvalov. On the Approximate Computation of Multiple Integrals. *Vestn. Mosc. State Univ.* **1959**, *4*, 3–18.

[2] J. Baldeaux, J. Dick, G. Leobacher, D. Nuyens, F. Pillichshammer, Efficient calculation of the worst-case error and (fast) component-by-component construction of higher order polynomial lattice rules, *Numer. Algorithms* **2012**, *59*, 403–431.

[3] R. Cools, F. Kuo, D. Nuyens, Constructing Embedded Lattice Rules for Multivariate Integration, *SIAM J. Sci. Comput.* **2006** *28*, 2162–2188.

[4] J. Dick, F. Pillichshammer, 2010. Digital Nets and Sequences: Discrepancy Theory and Quasi-Monte Carlo Integration. Cambridge University Press, Cambridge.

[5] I. Dimov, Monte Carlo Methods for Applied Scientists, New Jersey, London, Singapore, World Scientific, (2008).

[6] I.T. Dimov, R. Georgieva, Monte Carlo Method for Numerical Integration based on Sobol' Sequences, Numerical Methods and Applications (I. Dimov, S. Dimova, N. Kolkovska - Eds.), LNCS 6046, Springer, 2011, 50–59.

[7] I. T. Dimov, R. Georgieva, Multidimensional Sensitivity Analysis of Large-scale Mathematical Models. O.P. Iliev et al. (eds.), Numerical Solution of Partial Differential Equations: Theory, Algorithms, and Their Applications, Springer Proceedings in Mathematics & Statistics 45, Springer Science+Business Media, New York, 2013, 137–156.

[8] I. T. Dimov, R. Georgieva, Tz. Ostromsky, Z. Zlatev, Variance-based Sensitivity Analysis of the Unified Danish Eulerian Model According to Variations of Chemical Rates, – In: I. Dimov, I. Faragó, and L. Vulkov (Eds.) Proc. NAA 2012, LNCS 8236, Springer, 2013, 247–254.

[9] I. T. Dimov, R. Georgieva, Tz. Ostromsky, Z. Zlatev, Sensitivity Studies of Pollutant Concentrations Calculated by UNI-DEM with Respect to the Input Emissions. Central European Journal of Mathematics, Numerical Methods for Large Scale Scientific Computing Vol. 11, No 8, 2013, 1531–1545.

[10] I.T. Dimov, R. Georgieva, Tz. Ostromsky, Z. Zlatev, Advanced Algorithms for Multidimensional Sensitivity Studies of Large-scale Air Pollution Models based on Sobol Sequences, Special issue of Computers and Mathematics with Applications 65 (3), Efficient Numerical Methods for Scientific Applications, Elsevier, 2013, 338 - 351.

[11] I. Dimov, Z. Zlatev, Testing the sensitivity of air pollution levels to variations of some chemical rate constants, *Notes Numer. Fluid Mech.* **1997**, *62*, 167–175.

[12] F. Ferretti, A. Saltelli, S. Tarantola, Trends in sensitivity analysis practice in the last decade, Journal of Science of the Total Environment 568, (2016), 666–670.

[13] T. Goda, 2015. Good interlaced polynomial lattice rules for numerical integration in weighted Walsh spaces. Journal of Computational and Applied Mathematics 285, 279–294.

[14] T. Homma, A. Saltelli, Importance measures in global sensitivity analysis of nonlinear models, Reliability Engineering and System Safety 52, (1996), 1–17.

[15] S. Joe, F. Kuo, 2008. Constructing Sobol' sequences with better two-dimensional projections. SIAM J. Sci. Comput. 30, 2635–2654.

[16] T. Ostromsky, (2022). Performance and Scalability Experiments with a Large-scale Air Pollution Model on the EuroHPC Petascale Supercomputer DISCOVERER. In FedCSIS (Communication Papers) (pp. 81-84).

[17] A. Saltelli, S. Tarantola, F. Campolongo, M. Ratto, Sensitivity Analysis in Practice: A Guide to Assessing Scientific Models, Halsted Press, New York, (2004).

[18] I.H. Sloan A.V. Reztsov, Component-by-component construction of good lattice rules, *Math. Comp.* **2002**, *71*, 263–273.

[19] I. Sobol, Numerical methods Monte Carlo, Nauka, Moscow, (1973).

[20] I.M. Sobol, Sensitivity estimates for nonlinear mathematical models, Mathematical Modeling and Computational Experiment 1(4), (1993), 407–414.

[21] I.M. Sobol, S. Tarantola, D. Gatelli, S. Kucherenko, W. Mauntz, Estimating the approximation error when fixing unessential factors in global sensitivity analysis, Reliability Engineering & System Safety 92, (2007), 957–960.

[22] Y. Wang, F.J. Hickernell, An historical overview of lattice point sets, In *Monte Carlo and Quasi-Monte Carlo Methods 2000*; Fang, KT., Niederreiter, H., Hickernell, F.J., Eds.; Springer: Berlin/Heidelberg, Germany, 2002, pp. 158–167.

[23] Z. Zlatev, Computer Treatment of Large Air Pollution Models, KLUWER Academic Publishers, Dorsrecht-Boston-London, (1995).

[24] Z. Zlatev, I.T. Dimov, K. Georgiev, Three-dimensional version of the Danish Eulerian model, Z. Angew. Math. Mech. 76(S4), (1996), 473–476.

[25] Z. Zlatev, I.T. Dimov, Computational and Numerical Challenges in Environmental Modelling, Elsevier, Amsterdam, (2006).

[26] The Danish Eulerian Model, Available online: http://www2.dmu.dk/AtmosphericEnvironment/DEM/