

An Optimization Technique for Estimating Sobol Sensitivity Indices

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Abstract—In this paper we proposed an optimization technique for improving the Monte Carlo approaches based on Halton and Sobol algorithms. The proposed technique is novel in the sense that the optimization of the Halton and Sobol sequences is applied for the first time and essentially improves the results by the original sequences. The results will be of great importance for the environment protection and the trustability of forecasts.

I. INTRODUCTION

WHEN it comes to decision making, the reliability of the large-scale mathematical models is questioned [9], [10], [8], [18]. To improve the reliability, the sensitivity of model outputs to variations of model inputs due to natural variability is studied and analyzed. By definition [4], [15], [17] *sensitivity analysis* is a procedure to measure how sensitive are the mathematical model outputs are to some variations of the input data. The input data in this paper for sensitivity analysis is derived through runs of the large-scale mathematical model for large-distance transportation of air pollution – **Unified Danish Eulerian Model (UNI-DEM)**. The model is created at the Danish National Environmental Research Institute (<http://www2.dmu.dk/AtmosphericEnvironment/DEM/>, [19], [20], [21]).

This model considers large geographical region (4800 × 4800 km), including Europe and the Mediterranean in full and Asia and Africa in part. It also describes the primary chemical, photochemical and physical processes between the considered species and the emissions in the environment of rapidly changing meteorological conditions. It is that model which is chosen for a case study in the paper since the chemical processes are regarded with great precision amongst the other atmospheric chemistry models [3].

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II. GLOBAL SENSITIVITY ANALYSIS – SOBOL APPROACH

The mathematical model is assumed to be represented by a model function

$$u = f(x), \quad (1)$$

where $x = (x_1, x_2, \dots, x_d) \in U^d \equiv [0; 1]^d$ is the vector of input parameters with a joint probability density function (p.d.f.) $p(x) = p(x_1, \dots, x_d)$.

The Sobol approach idea is based on a decomposition of the integrable model function f into terms of increasing dimensionality [15], [17]:

$$f(x) = f_0 + \sum_{\nu=1}^d \sum_{l_1 < \dots < l_\nu} f_{l_1 \dots l_\nu}(x_{l_1}, x_{l_2}, \dots, x_{l_\nu}), \quad (2)$$

where f_0 is some constant.

The representation (2) is called the ANOVA-representation of the model function $f(x)$ in case each term is chosen to satisfy the following condition [16]:

$$\int_0^1 f_{l_1 \dots l_\nu}(x_{l_1}, x_{l_2}, \dots, x_{l_\nu}) dx_{l_k} = 0, \quad 1 \leq k \leq \nu, \nu = 1, \dots, d.$$

This condition guarantees that the functions in the right hand-side of (2) are uniquely defined, and $f_0 = \int_{U^d} f(x) dx$. The quantities

$$D = \int_{U^d} f^2(x) dx - f_0^2, \quad D_{l_1 \dots l_\nu} = \int f_{l_1 \dots l_\nu}^2 dx_{l_1} \dots dx_{l_\nu} \quad (3)$$

are referred to as total and partial variances, respectively. An analogous decomposition holds for the total variance which is represented by the corresponding partial variances: $D = \sum_{\nu=1}^d \sum_{l_1 < \dots < l_\nu} D_{l_1 \dots l_\nu}$. The primary sensitivity measures following the Sobol approach are defined as Sobol global sensitivity indices [16], [14]:

$$S_{l_1 \dots l_\nu} = \frac{D_{l_1 \dots l_\nu}}{D}, \quad \nu \in \{1, \dots, d\}, \quad (4)$$

and the total sensitivity index (TSI) of an input parameter $x_i, i \in \{1, \dots, d\}$ defined by [16], [14]:

$$S_i^{tot} = S_i + \sum_{l_1 \neq i} S_{il_1} + \sum_{l_1, l_2 \neq i, l_1 < l_2} S_{il_1 l_2} + \dots + S_{il_1 \dots l_{d-1}}, \quad (5)$$

where S_i is named *the main effect (first-order sensitivity index)* of x_i and $S_{il_1 \dots l_{j-1}}$ is the j^{th} order sensitivity index. The higher-order terms characterize the interaction effects between the unknown input parameters $x_{i_1}, \dots, x_{i_\nu}, \nu \in \{2, \dots, d\}$ on the output variance. It is obvious that the rigorous mathematical treatment of the problem of supplying global sensitivity analysis includes evaluating total sensitivity indices (5) of corresponding order that, based on the formulae (3)-(4), results in computing multidimensional integrals.

III. SOBOLOV AND HALTON SEQUENCES AND THEIR OPTIMIZATIONS

Quasirandom or low discrepancy sequences, which vivid representatives are the Halton and Sobol sequences, are “less random” than a pseudorandom number sequence, but they are much more useful for numerical calculation of integrals in higher dimensions, since the low discrepancy sequences tend to sample space “more uniformly” than random numbers [2].

Let $\mathbf{x}_i = (x_i^{(1)}, x_i^{(2)}, \dots, x_i^{(s)})$ for $i = 1, 2, \dots$ and $n = \dots a_3(n), a_2(n), a_1(n)$ be the representation of n in base b . The respective multidimensional quasirandom sequence is defined as follows: $X_n = (\phi_{b_1}(n), \phi_{b_2}(n), \dots, \phi_{b_s}(n))$, where the bases b_i are relatively prime numbers.

Halton sequence [5], [6] is defined as:

$$s_n^{(k)} = \sum_{i=0}^{\infty} \sigma_{i+1}^{(k)} a_{i+1}^{(k)}(n) b_k^{-(i+1)},$$

where $(b_1, b_2, \dots, b_s) \equiv (2, 3, 5, \dots, p_s)$, and p_i designates the i -th prime, and $\sigma_i^{(k)}, i \geq 1$ denotes the set of permutations on $(0, 1, 2, \dots, p_k - 1)$.

Sobol sequence [1], [7] is defined by:

$$\mathbf{x}_k \in \bar{\sigma}_i^{(k)}, k = 0, 1, 2, \dots$$

where $\bar{\sigma}_i^{(k)}, i \geq 1$ are the set of permutations on every $2^k, k = 0, 1, 2, \dots$ subsequent points of the Van der Corput sequence, defined by $n = \sum_{i=0}^{\infty} a_{i+1}(n) b^i, \phi_b(n) = \sum_{i=0}^{\infty} a_{i+1}(n) b^{-(i+1)}$ when $b = 2$.

In binary for the Sobol sequence we have that: $x_n^{(k)} = \bigoplus_{i \geq 0} a_{i+1}(n) v_i$, where $v_i, i = 1, \dots, s$ is the set of direction numbers [7].

IV. OPTIMIZATION BY SCRAMBLING

The fundamental motivation of optimization targets at obtaining more uniform quasirandom sequences, especially in high dimensions. The proved convergence rate for the Scrambling Algorithms improves drastically the rate for the unscrambled nets [13], which is $n^{-1}(\log n)^{d-1}$. The idea of

scrambling is founded on randomization of a single digit at each iteration. Let

$$x^{(i)} = (x_{i,1}, x_{i,2}, \dots, x_{i,s}), i = 1, \dots, n \quad (6)$$

be quasirandom numbers in $[0, 1]^s$, and let

$$z^{(i)} = (z_{i,1}, z_{i,2}, \dots, z_{i,s}) \quad (7)$$

be the respective scrambled version of the point $x^{(i)}$. Suppose now that every $x_{i,j}$ could be represented in base b as

$$x_{i,j} = (0.x_{i1,j} x_{i2,j} \dots x_{iK,j} \dots)_b \quad (8)$$

with K being the number of digits for scrambling. To scramble the Halton sequence, we use a permutation of the radical inverse coefficients obtained by applying a reverse-radix operation to each of the possible coefficient values [11]. To scramble the Sobol sequence, we use random linear scramble blended with a random digital shift [12].

V. SENSITIVITY STUDIES WITH RESPECT TO EMISSION LEVELS

In this section we give the outcomes for the sensitivity of UNI-DEM output (particularly the monthly ammonia mean concentrations) with respect to the data variation of anthropogenic emissions as input. The input itself comprises 4 different constituents

$\mathbf{E} = (\mathbf{E}^A, \mathbf{E}^N, \mathbf{E}^S, \mathbf{E}^C)$:

- \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 domain into consideration is the 4-dimensional hypercube $[0.5, 1]^4$.

Results regarding the relative error estimation for the quantities f_0 , the total variance \mathbf{D} , the first-order (S_i) and the total (S_i^{tot}) sensitivity indices are presented in Tables I, II, III, respectively. f_0 is represented by a 4-dimensional integral, while the rest of the above quantities are represented by 8-dimensional integrals, following the ideas of the *correlated sampling* technique to compute sensitivity measures in a robust way (see [8], [17]). Four different stochastic approaches employed for numerical integration are given in separate columns in the tables.

For $n = 2^{24}$ for the model function f_0 the best algorithm is the Halton scrambled sequence, followed by the Halton sequence – see the results in Tables I for the maximum number of samples. For number of samples $n = 2^{24}$ for the total variance D the best algorithm is the Sobol sequence, followed by the Halton scrambled sequence – see the results in Tables II for the maximum number of samples. The performance of the algorithms can be seen on Fig. 1.

It can be seen in Table III that the optimized SOBOPT and HALOPT improve the results in most of the cases, and most importantly for the small in value sensitivity indices $S_2, S_4, S_2^{tot}, S_4^{tot}$. These are the most important cases because they determine the reliability of the model results.

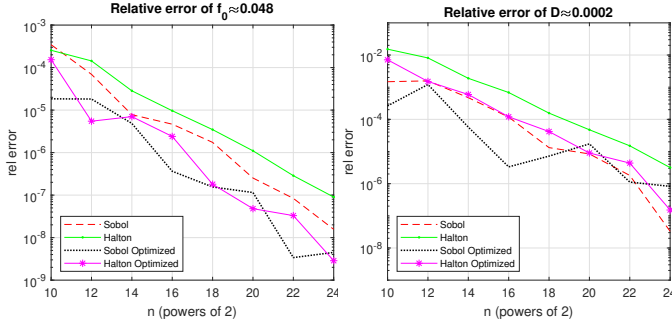


Fig. 1. Relative errors for the calculation of $f_0 \approx 0.048$ (left) and $D \approx 0.0002$ (right)

TABLE I
RELATIVE ERROR FOR THE EVALUATION OF $f_0 \approx 0.048$.

#	SOBOL	HALTON	SOBOPT	HALOPT
	Relative error	Relative error	Relative error	Relative error
2^{16}	4.6585e-06	9.6538e-06	3.6422e-07	2.3992e-06
2^{20}	2.5234e-07	1.1020e-06	1.1501e-07	4.7965e-08
2^{24}	1.5669e-08	9.0096e-08	4.4868e-09	2.8637e-09

VI. SENSITIVITY STUDIES WITH RESPECT TO CHEMICAL REACTIONS RATES

In this section we explore the sensitivity of the ozone concentration values in the air over Genova with respect to the rate variation of some chemical reactions of the condensed CBM-IV scheme ([19]), in particular: # 1, 3, 7, 22 (time-dependent) and # 27, 28 (time independent). The reduced equations of the

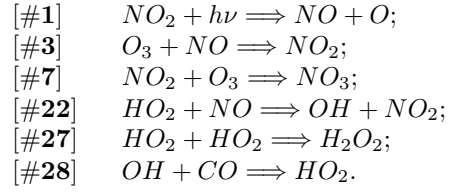
TABLE II
RELATIVE ERROR FOR THE EVALUATION OF THE TOTAL VARIANCE $D \approx 0.0002$.

#	SOBOL	HALTON	SOBOPT	HALOPT
	Relative error	Relative error	Relative error	Relative error
2^{16}	1.1726e-04	6.8346e-04	3.3306e-06	1.2015e-04
2^{20}	8.4017e-06	4.7374e-05	1.7242e-05	8.9747e-06
2^{24}	3.2922e-08	3.1611e-06	8.2382e-07	1.5148e-07

TABLE III
RELATIVE ERROR FOR ESTIMATION OF SENSITIVITY INDICES OF INPUT PARAMETERS USING DIFFERENT QUASI-MONTE CARLO APPROACHES ($n \approx 2^{16}$).

EQ	RV	SOBOL	HALTON	SOBOPT	HALOPT
S_1	9e-01	5.4870e-06	2.9981e-04	2.3006e-05	7.7156e-05
S_2	2e-04	4.2469e-03	3.2104e-02	2.2210e-03	1.1998e-02
S_3	1e-01	1.3725e-04	2.3291e-03	3.2724e-04	4.7869e-04
S_4	4e-05	4.5620e-02	1.1969e-01	1.7836e-02	7.2187e-02
S_1^{tot}	9e-01	1.8865e-05	2.9900e-04	4.2060e-05	6.1643e-05
S_2^{tot}	2e-04	5.1886e-03	3.1544e-02	1.3834e-03	1.2575e-04
S_3^{tot}	1e-01	1.5898e-05	2.2959e-03	1.8409e-04	6.2183e-04
S_4^{tot}	5e-05	5.5960e-02	1.1911e-01	3.9446e-02	4.3995e-02

chemical reactions follow:



The domain in consideration is the 6-dimensional hypercube $[0.6, 1.4]^6$.

The authors of [8] argue which formulation of

$$f_0^2 = \left(\int_{U^d} f(x) dx \right)^2 \quad (9)$$

is better when expressing the total variance and the Sobol global sensitivity measures. The first formula is

$$f_0^2 \approx \frac{1}{n} \sum_{i=1}^n f(x_{i,1}, \dots, x_{i,d}) f(x'_{i,1}, \dots, x'_{i,d}) \quad (10)$$

and the second one is

$$f_0^2 \approx \left\{ \frac{1}{n} \sum_{i=1}^n f(x_{i,1}, \dots, x_{i,d}) \right\}^2 \quad (11)$$

where x and x' are two independent sample vectors. If one estimates sensitivity indices of a fixed order, the expression (10) is better (as it is recommended in [8]), and this is why we apply it here as well.

The relative error estimation for the quantities f_0 , the total variance D and a part of the sensitivity indices are provided in Tables IV, V and VI, respectively.

The quantity f_0 is represented by 6-dimensional integral, while the rest are represented by 12-dimensional integrals, following the concept of *correlated sampling*.

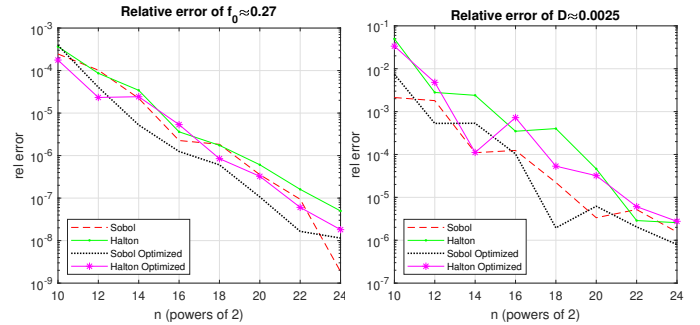


Fig. 2. Relative errors for the calculation of $f_0 \approx 0.27$ (left) and $D \approx 0.0025$ (right)

For $n = 2^{24}$ for the model function f_0 the best algorithm is the Sobol scrambled sequence, followed by the Sobol sequence – see the results in Tables IV for the maximum number of samples. For number of samples $n = 2^{24}$ for the total variance D the best algorithm is again the Sobol scrambled sequence, followed again by the Sobol sequence – see the results in Tables V for the maximum number of samples. The behaviour of the algorithms can be seen on Fig. 2.

TABLE IV
RELATIVE ERROR FOR THE EVALUATION OF $f_0 \approx 0.27$.

n	SOBOL	HALTON	SOBOPT	HALOPT
	Relative error	Relative error	Relative error	Relative error
2^{16}	2.2604e-06	3.6220e-06	1.2498e-06	5.3505e-06
2^{20}	3.5561e-07	6.0821e-07	1.0645e-07	3.2548e-07
2^{24}	1.8639e-09	4.9903e-08	1.1468e-09	1.8102e-08

TABLE V
RELATIVE ERROR FOR THE EVALUATION OF THE TOTAL VARIANCE $D \approx 0.0025$.

n	SOBOL	HALTON	SOBOPT	HALOPT
	Relative error	Relative error	Relative error	Relative error
2^{16}	1.2418e-04	3.4838e-04	1.0328e-04	7.2396e-04
2^{20}	3.3461e-06	4.6222e-05	6.2125e-06	3.2061e-05
2^{24}	1.5526e-06	2.5678e-06	7.9422e-07	2.7586e-06

It can be seen in Table VI that the optimized SOBOPT and HALOPT improve the results in most of the cases, and for very important small in value sensitivity indices S_5 . The basic algorithm is better for the two way interaction sensitivity indices, but for the most important first order sensitivity indices our optimization methods produce the best results.

TABLE VI
RELATIVE ERROR FOR ESTIMATION OF SENSITIVITY INDICES OF INPUT PARAMETERS USING DIFFERENT QUASI-MONTE CARLO APPROACHES ($n \approx 2^{16}$).

EQ	RV	SOBOL	HALTON	SOBOPT	HALOPT
S_1	4e-01	3.2231e-04	2.8340e-03	9.5066e-05	4.0386e-04
S_2	3e-01	3.8337e-04	3.7322e-03	2.2260e-04	4.6835e-04
S_3	5e-02	6.5037e-04	7.5211e-03	9.6837e-04	8.1435e-04
S_4	3e-01	4.3936e-04	2.2956e-03	3.3630e-04	2.3527e-04
S_5	4e-07	9.8860e+00	4.5383e+01	9.4627e+00	6.9084e+01
S_6	2e-02	1.7170e-03	1.3009e-02	2.3921e-04	1.4770e-04
S_1^{tot}	4e-01	2.6837e-04	2.7466e-03	1.3978e-04	2.8687e-04
S_2^{tot}	3e-01	5.6342e-04	3.2551e-03	6.7337e-05	5.6446e-04
S_3^{tot}	5e-02	8.6595e-04	6.6357e-03	9.9762e-04	4.3254e-04
S_4^{tot}	3e-01	2.1786e-04	2.1826e-03	5.9956e-04	9.0355e-05
S_5^{tot}	2e-04	1.3627e-01	2.5437e-02	6.6954e-02	3.3439e-02
S_6^{tot}	2e-02	2.5998e-03	1.0451e-02	5.3173e-04	3.0023e-03
S_{12}	6e-03	1.4614e-03	7.5509e-03	6.6880e-03	6.2554e-03
S_{14}	5e-03	1.3828e-03	9.7965e-03	3.3325e-03	8.0309e-03
S_{24}	3e-03	3.3757e-03	1.6310e-02	1.8226e-02	7.6253e-03
S_{45}	1e-05	4.3069e-01	8.2357e-01	6.2288e-01	5.1080e-01

VII. CONCLUSION

We have investigated the computational efficiency of several stochastic algorithms for multidimensional numerical integration in terms of relative error and computational effort. The case study is the sensitivity analysis of the UNI-DEM model output to variation of the input emissions of the anthropogenic pollutants and of the rates of a couple of chemical reactions. It is considered the influence of emission levels over very important air pollutants, in particular ammonia, ozone, ammonium sulphate and ammonium nitrate.

The numerical experiments show that the obtained optimization methods are one of the best available stochastic

approaches for computing sensitivity indices and especially the most difficult task – the smallest in value sensitivity indices which are very important for the model results reliability. The results will be of great importance for the environment protection and the trustability of forecasts.

REFERENCES

- [1] I. Antonov, V. Saleev, An economic method of computing LP_T -sequences, USSR Comput. Math. Phys. 19, (1979), 252–256.
- [2] I. Dimov, Monte Carlo Methods for Applied Scientists, New Jersey, London, Singapore, World Scientific, (2008).
- [3] I.T. Dimov, R. Georgieva, Tz. Ostrowsky, Z. Zlatev, Advanced algorithms for multidimensional sensitivity studies of large-scale air pollution models based on Sobol sequences, Computers and Mathematics with Applications 65(3), "Efficient Numerical Methods for Scientific Applications", Elsevier, (2013), 338–351.
- [4] 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.
- [5] J. Halton, On the efficiency of certain quasi-random sequences of points in evaluating multi-dimensional integrals, Numerische Mathematik 2, (1960), 84–90.
- [6] J. Halton, G.B. Smith, Algorithm 247: radical-inverse quasi-random point sequence, Communications of the ACM 7, (1964), 701–702.
- [7] S. Joe, F. Kuo, Remark on algorithm 659: implementing Sobol's quasirandom sequence generator, ACM Transactions on Mathematical Software 29(1), (2003), 49–57.
- [8] T. Homma, A. Saltelli, Importance measures in global sensitivity analysis of nonlinear models, Reliability Engineering and System Safety 52, (1996), 1–17.
- [9] A. Karaivanova, E. Atanassov, T. Gurov, R. Stevanovic, K. Skala, Variance reduction MCMs with application in eEnvironmental studies: sensitivity analysis. AIP Conference Proceedings 1067(1), (2008), 549–558.
- [10] A. Karaivanova, I. Dimov, S. Ivanovska, A quasi-Monte Carlo method for integration with improved convergence, In International Conference on Large-Scale Scientific Computing, Springer, Berlin, Heidelberg, (2001), 158–165.
- [11] L. Kocis, W. J. Whiten, Computational investigations of low-discrepancy sequences, ACM Transactions on Mathematical Software 23(2), (1997), 266–294.
- [12] J. Matousek, On the L2-discrepancy for anchored boxes, Journal of Complexity 14(4), (1998), 527–556.
- [13] G. Ökten, A. Göncüb, Generating low-discrepancy sequences from the normal distribution: Box–Muller or inverse transform?, Mathematical and Computer Modelling 53, (2011), 1268–1281.
- [14] A. Saltelli, S. Tarantola, F. Campolongo, M. Ratto, Sensitivity Analysis in Practice: A Guide to Assessing Scientific Models, Halsted Press, New York, (2004).
- [15] I. Sobol, Numerical methods Monte Carlo, Nauka, Moscow, (1973).
- [16] I.M. Sobol, Sensitivity estimates for nonlinear mathematical models, Mathematical Modeling and Computational Experiment 1(4), (1993), 407–414.
- [17] 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.
- [18] S.L. Zaharieva, I.R. Georgiev, V.A. Mutkov, Y.B. Neikov, Arima approach for forecasting temperature in a residential premises part 2, in 2021 20th International Symposium INFOTEH-JAHORINA (INFOTEH), IEEE, (2021), 1–5.
- [19] Z. Zlatev, Computer Treatment of Large Air Pollution Models, KLUWER Academic Publishers, Dordrecht-Boston-London, (1995).
- [20] Z. Zlatev, I.T. Dimov, K. Georgiev, Three-dimensional version of the Danish Eulerian model, Z. Angew. Math. Mech. 76(S4), (1996), 473–476.
- [21] Z. Zlatev, I.T. Dimov, Computational and Numerical Challenges in Environmental Modelling, Elsevier, Amsterdam, (2006).