

RELIABILITY
ENGINEERING
&
SYSTEM
SAFETY

Reliability Engineering and System Safety 91 (2006) 717-727

www.elsevier.com/locate/ress

Random balance designs for the estimation of first order global sensitivity indices

S. Tarantola^{a,*}, D. Gatelli^a, T.A. Mara^b

^aJoint Research Centre, European Commission, Institute of the Protection and Security of the Citizen, TP 361, Via E. Fermi 1, 21020 Ispra (VA), Italy ^bLaboratory of Industrial engineering, University of Reunion Island, BP 7151, 15 avenue René Cassin, 97 715 Saint-Denis, France

> Received 29 July 2004; accepted 17 June 2005 Available online 12 September 2005

Abstract

We present two methods for the estimation of main effects in global sensitivity analysis. The methods adopt Satterthwaite's application of random balance designs in regression problems, and extend it to sensitivity analysis of model output for non-linear, non-additive models. Finite as well as infinite ranges for model input factors are allowed. The methods are easier to implement than any other method available for global sensitivity analysis, and reduce significantly the computational cost of the analysis. We test their performance on different test cases, including an international benchmark on safety assessment for nuclear waste disposal originally carried out by OECD/NEA.

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Keywords: Computational models; Uncertainty analysis; Global sensitivity analysis

1. Introduction

The paper presents two procedures for the estimation of main effects in sensitivity analysis of model output. The estimation of main effects is the objective of a sensitivity analysis problem setting known as Factors Prioritization (FP) [1]. In this setting, the factor importance is defined as the expected amount by which the variance of the model output is reduced when a given input factor is fixed to its true, albeit unknown, value within its range of uncertainty. The larger the reduction of the output variance due to fixing one factor, the higher the main effect for that factor, and the higher the importance of that factor. In setting FP the factors are fixed one at a time, all the others being averaged over their range of variation. As known to practitioners, this setting is blind to interactions among factors [1,2,4,5,8,13, 15,16].

The ideal use of setting FP is for prioritization of research, whereby the factor most deserving of better experimental observation is identified. Setting FP is tackled

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by estimating main effects, which, in a variance-based context, are expressed as $V_{X_i}[E_{X_{-i}}(Y|X_i)]/V(Y)$ [1]. Here, Y is the model output, X_i is the generic input factor, $E_{X_{-i}}$ is the average that operates upon all the factors but X_i , and V_{X_i} is the variance that operates upon X_i .

Note that other settings exist for quantitative sensitivity analysis. For example, a very efficient screening experiment exists [2] to identify non-influential factors in large models. This is useful in the context of the setting known as 'factors fixing' (FF) [1]. The focus of this paper is on the FP setting, to which we restrain our experiments.

The proposed procedures combine Satterthwaite's random balance designs [3] with the Fourier Amplitude Sensitivity Test (FAST) (see [4] for a review, see [5] for a generalisation). In Section 2 we illustrate the two methods and in Section 3 we test their performance against the best available recipe for global sensitivity analysis, recently appeared in [1]. The tests are carried out on an analytical test function widely used for benchmarking sensitivity analysis procedures. In Section 4, another test is carried out on the Level E model, an international benchmark on safety assessment for nuclear waste disposal originally carried out by OECD/NEA [7], and largely applied in the literature. The tests show the superiority of the proposed procedures.

^{*} Corresponding author. Tel.: +39 332 789928; fax: +39 332 785733. E-mail address: stefano.tarantola@jrc.it (S. Tarantola).

2. The proposed methods

The classic FAST method [4] is based on selecting N design points over a particular space-filling curve in the k-th dimensional input space, built as to explore each dimension (factor) with a different frequency $\{\omega_1, \omega_2, ..., \omega_k\}$. A quite complex algorithm is used to set the frequencies such that they are free of interferences up to a given order M (usually M=6). The computational model is executed at each design point and the Fourier spectrum is calculated on the model output at specific frequencies $\{\omega_i, 2\omega_i, ..., M\omega_i\}$ to estimate the sensitivity index of factor X_i .

The first method proposed here is based on random balance design (RBD). We first select N design points over a curve in the input space. Contrarily to FAST, we explore the input space using the same frequency ω , to avoid the use of the algorithm cited above. However, due to that, the curve is not space-filling but covers only a sub-set of the whole input space. Therefore, we take random permutations of the coordinates of such points, to generate a set of scrambled points that cover the input space. The model is then evaluated at each design point. Subsequently, the model outputs are re-ordered such that the design points are in increasing order with respect to factor X_i . The Fourier spectrum is calculated on the model output at the frequency ω and at its higher harmonics $\{\omega, 2\omega, ..., M\omega\}$ and yields the estimate of the sensitivity index of factor X_i . The model outputs are re-ordered with respect to the other factors (and the Fourier spectra are calculated accordingly) to obtain all the other sensitivity indices.

The second method proposed is HFR, a hybrid version that combines classic FAST and RBD.

The parametric curve used in the classic FAST is defined as:

$$X_i(s_j) = G_i(\sin \omega_i s_j),$$

$$\forall i = 1, 2, ..., k; \ \forall j = 1, 2, ..., N;$$
(1)

where X_i is the *i*-th input factor, G_i are functions to be chosen by the analyst to get the desired probability density function for X_i , s is the parametric variable varying in $(-\pi;\pi)$ which is sampled over its range using N points, and the frequencies ω_i are selected such that they are free of interferences up to a given order M (usually set to 4 or 6). For example, Eq. (1) is selected as $X_i(s) = (1/2) + (1/\pi) \arcsin(\sin \omega_i s)$ in [5] to get a uniform distribution for X_i in (0;1).

The selection of the ω_i is made using an algorithm (see [4]). The FAST sample design implies a lower bound on the sample size, which the theory fixes at $N_{\min} = 2M \max{\{\omega_i\}} + 1$. However, $\max{\{\omega_i\}}$ is an increasing function of k and, for large k, the sample size and the related computational cost, can be too high to be acceptable.

In the RBD approach all the factors are sampled using the same frequency ω , which is an arbitrary integer, set to 1 for simplicity. Anyway, ω could assume any other value up to (N-1)/2M, which is the maximum value that is allowed by

the theory: higher values would cause the frequency to exceed the sampling dimension N.

A sample of *N* points over $(-\pi;\pi)$ is generated using the parametric equation:

$$X_i(s_{ij}) = G_i(\sin \omega s_{ij}),$$

$$\forall i = 1, 2, ..., k; \ \forall j = 1, 2, ..., N.$$
(2)

where $\{s_{i1}, s_{i2}, ..., s_{iN}\}$ denotes the *i*-th random permutation of the *N* points. For each factor X_i Eq. (2) provides a different random permutation.

The model is evaluated N times over the sample of size N.

$$Y(s_j) = f(X_1(s_{1j}), X_2(s_{2j}), ..., X_k(s_{kj})) \quad \forall j = 1, 2, ..., N$$
(3)

The values of model output $Y(s_j)$, j = 1,...,N, are then reordered $(Y^R(s_j))$ such that the corresponding values of $X_1(s_{1j})$ are ranked in increasing order. By so doing, the harmonic content of X_1 propagates through f to $Y^R(s_j)$. The sensitivity of Y to X_1 is determined by the harmonic content of Y^R , which is quantified by its Fourier spectrum

$$F(\omega) = \frac{1}{\pi} \sum_{j=1}^{N} Y^{R}(s_{j}) \exp(-\operatorname{Im} k \omega s_{j})$$
 (4)

evaluated at $\omega = 1$ and its higher harmonics (in our case $\omega = 2$, $\omega = 3$,...) up to order M = 6.

In the discrete,

$$\hat{V}_1 = \text{Var}[E(Y|X_1)] = \sum_{l=1}^{M} F(\omega)|_{w=l} = \sum_{l=1}^{M} F(l)$$
 (5)

provides, in a variance-based context [1], an estimate of V_1 , i.e. the nominator of the main effect for the first factor. The procedure is then repeated for all the other factors whereby the same set of model output is just reordered according to $X_i(s_{ij})$ and Eqs. (4) and (5) are used to estimate V_i , i=2,...,k.

With the use of permutations, the total cost is kept down to N, instead of $\sim k*N$ (like in Sobol' and FAST). Note that random permutations are also used to generate replicated LHS designs for the estimation of importance measures [8].

The HFR method combines RBD with classic FAST. The k factors are partitioned in groups of equal cardinality. RBD is applied independently within each group of factors. FAST is applied between the groups: here a different frequency is associated to each group.

To make an example, in a six-factor model we can set-up three groups of two factors each, using frequencies $\omega_1 = 1$, $\omega_2 = 7$, $\omega_3 = 11$ and two different random permutations. Each random permutation, being associated with three different frequencies, provides a separate design for each factor.

In alternative, we could set up two groups of three factors each; the procedure is the same and the results are equally satisfactory.

The sampling design of HFR combines the accuracy of classic FAST with the computational cheapness of RBD, as we shall see on a number of test cases.

3. Analytic tests

3.1. The function of Sobol'

The first test function has been proposed by Sobol' and has been widely used as benchmark for sensitivity analysis (see e.g. [9]). The function is defined as:

$$f = \prod_{i=1}^{k} g_i(X_i) \tag{6}$$

where k is the number of input factors and $g_i(x_i)$ is given by

$$g_i(x_i) = \frac{|4X_i - 2| + a_i}{1 + a_i}$$
 for $0 \le X_i \le 1$ and $a_i \ge 0$. (7)

The parameter a_i is set to determine the relative importance of the X_i 's. For a_i =0 the corresponding factor X is very important, for a_i =1 it is relatively important, while for a_i =9 it becomes non-important and for a_i =99 non-significant, given that the range of uncertainty of $g_i(x_i)$ depends exclusively on the value of a_i . In a case where all the a_i 's are equal, the factors have the same level of importance; this level is in any case quantified by a_i .

The analytical partial variances of the first order (V_i) and the total unconditional variance (V) of the model output can be computed analytically:

$$V_i = \frac{1}{3(1+a_i)^2}, \qquad V = \prod_{i=1}^k (V_i + 1) - 1,$$
 (8)

from which the first order sensitivity index $S_i = V_i/V$ can be calculated.

In the first test we set the a_i as $\{0, 1, 4.5, 9, 99, 99, 99, 99\}$, so that the first factor is the most important, and the last four factors are the least important. The analytic indices S_i and the estimates at N=1000 and 10,000 are given in Table 1. With the RBD approach, all the estimated indices converge towards the analytic values, although the estimates for the least important factors are slightly overestimated. In HFR, we grouped the eight factors into two groups, associated with the frequencies $\omega=11$ and 35. The HFR estimates for the least important factors are closer to the analytic values. In summary, RBD yields better estimates for the important factors, whilst HFR better detects the non-important factors.

To better investigate the statistical properties of the two approaches, we replicate the procedure r=50 times and calculate the average and the standard deviation of the S_i over the replicates (see Table 2). The tests are repeated at increasing sample sizes N=500, 1000 and 2000. We note that the HFR seems to perform better,

Table 1 G-function's analytic values and estimates for first orders in a sample size of N=1000 and 10,000

	Analytic values	The RBD approach	Hybrid FAST–RBD
N = 1000			
Factor 1	0.716	0.7200	0.6998
Factor 2	0.1790	0.1954	0.1873
Factor 3	0.024	0.0288	0.0247
Factor 4	0.0072	0.0210	0.0140
Factor 5	7.162×10^{-5}	0.0125	0.0021
Factor 6	7.162×10^{-5}	0.0119	0.0210
Factor 7	7.162×10^{-5}	0.0103	0.0111
Factor 8	7.162×10^{-5}	0.0108	0.0062
N = 10,000			
Factor 1	0.716	0.7159	0.7091
Factor 2	0.1790	0.1790	0.1830
Factor 3	0.024	0.0250	0.0231
Factor 4	0.0072	0.0083	0.0096
Factor 5	7.162×10^{-5}	0.0015	0.0002
Factor 6	7.162×10^{-5}	0.0015	0.0011
Factor 7	7.162×10^{-5}	0.0013	0.0006
Factor 8	7.162×10^{-5}	0.0015	0.0008

The estimates are calculated both with the RBD and the Hybrid FAST-RBD approach.

both in terms of average (in 21 cases out of 24) and standard deviation (in 18 cases out of 24). In other words, in HFR the average is better approximating the analytic values, and the standard deviation is smaller than in RBD, indicating a smaller dispersion of the 50 estimates around the average value.

3.2. Performance for large-dimensional models and comparison with the method of Sobol' as extended by Saltelli

We test the performance of the proposed methods in the case of models with a large number of factors. We consider the function of Sobol' with k=100 factors.

Four factors are very important $(a_i=0)$, four other factors are fairly important $(a_i=1)$, two other factors are less important $(a_i=9)$ and the remaining 90 factors are irrelevant $(a_i=99)$.

The analytic values for these four groups of factors are, respectively, $\{0.0982\ 0.0245\ 9.8173\times10^{-004}\ 9.8173\times10^{-006}\}$

We test the performance of the RBD approach against the method of Sobol' as extended by Saltelli [6], with N=100 and total computational cost C=N(k+2)=10,200. Indeed, with the Sobol' or Saltelli's methods the computational cost depends on the number of factors (k), while with the proposed methods the computational cost is equal to the sample size (C=N). Therefore, with a small number of model runs, we can estimate the first order sensitivity indices for models with a very large number of factors.

Fig. 1 displays the results of this test case. The method of Sobol' gives better estimates for the less important factors,

Table 2
Results of the two proposed methods under different conditions

	Analytic values	The RBD approach		Hybrid FAST-RBD	
		Mean	Standard deviation	Mean	Standard deviation
N = 500, n	o. of experim	ents = 50			
Factor 1	0.7160	0.7196	0.0173	0.7079	0.0136
Factor 2	0.1790	0.1986	0.0249	0.1833	0.0235
Factor 3	0.0240	0.0482	0.0189	0.0399	0.0144
Factor 4	0.0072	0.0318	0.0117	0.0223	0.0108
Factor 5	0.0001	0.0236	0.0083	0.0044	0.0022
Factor 6	0.0001	0.0237	0.0073	0.0122	0.0053
Factor 7	0.0001	0.0238	0.0107	0.0152	0.0071
Factor 8	0.0001	0.0253	0.0083	0.0188	0.0077
N = 1000,	no. of experin	ments = 50			
Factor 1	0.7160	0.7168	0.0096	0.7073	0.0112
Factor 2	0.1790	0.1873	0.0167	0.1815	0.0207
Factor 3	0.0240	0.0348	0.0088	0.0311	0.0094
Factor 4	0.0072	0.0172	0.0064	0.0143	0.0058
Factor 5	0.0001	0.0110	0.0040	0.0021	0.0010
Factor 6	0.0001	0.0122	0.0044	0.0057	0.0028
Factor 7	0.0001	0.0128	0.0038	0.0069	0.0030
Factor 8	0.0001	0.0113	0.0046	0.0084	0.0043
N = 2000,	no. of experin	ments = 50			
Factor 1	0.7160	0.7171	0.0069	0.7057	0.0061
Factor 2	0.1790	0.1849	0.0133	0.1783	0.0147
Factor 3	0.0240	0.0304	0.0074	0.0277	0.0066
Factor 4	0.0072	0.0127	0.0046	0.0114	0.0045
Factor 5	0.0001	0.0062	0.0026	0.0012	0.0006
Factor 6	0.0001	0.0057	0.0024	0.0036	0.0017
Factor 7	0.0001	0.0058	0.0022	0.0043	0.0016
Factor 8	0.0001	0.0060	0.0027	0.0043	0.0025

The estimates are calculated as the mean of the estimates obtained in the 50 repetitions of the exercise. This has been done for three different sample sizes.

but this is not interesting in the context of setting FP. The proposed method with C=2000 yields better estimates than the method of Sobol' with C=10,200 for the most important factors in terms of setting FP.

3.3. Performance for large number of important factors and comparison with the classic FAST

Before licensing the computational scheme proposed in this paper we believe important to check whether it works also when the number of important factors in the model is very large. In fact, important factors are easier to detect when they are few. As their number rises, the computational method needs to be very accurate to identify them all. We test the performance of the RBD method on a model with a high fraction of important factors. We consider the G-function with 10 very important factors and 10 non-significant factors. The result is given in Fig. 2(a). We note that, even at relatively small sample size (C=N=5000), the important factors can be clearly distinguished from the non-significant ones.

We also test the hybrid version and compare it against the classic FAST. This latter requires a minimum sample size of N=8377 under the same conditions. In the hybrid version we choose five groups of factors each composed by four factors. Frequencies for the groups have been set at 11, 21, 27, 35, 39.

Fig. 2(a) shows that classic FAST gives better results for non-significant factors while it overestimates the important ones. The proposed methods give similar results, yet the hybrid approach has a lower variance and better approximates analytic values (see Table 3). Note that the variance of the estimates for the important and the non-important factors has been obtained across each set of 10 factors, and not by replicating the experiments.

We also try an extreme case considering a model with 20 factors, 15 of each are very important (Fig. 2(b)). The proposed methods can detect the important factors from the non-significant ones at C=N=10,000. Again, the classic FAST performs better for non-significant factors, while the important factors are overestimated. The HFR version, implemented in the same way as in the previous case, provides the more

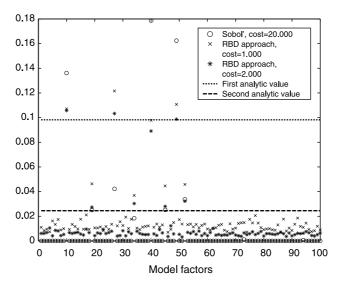


Fig. 1. First test case: G-function. Estimation of first order sensitivity indices using the RBD approach at 1000 runs, at 2000 runs and the method of Sobol' at 20,000 runs.

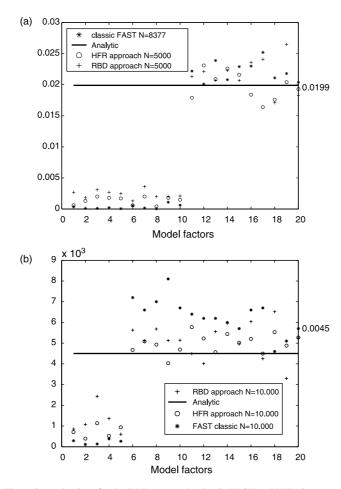


Fig. 2. (a): First test case: G-function. The estimated values for the RBD approach, classic FAST and HFR, in a case study with a large number of important factors (10 very important and 10 non-significant ones). N=5000 for the HFR and the RBD approaches, while N=8377 for the classic FAST. (b): First test case: G-function. The estimated values for the RBD approach, classic FAST and HFR, in a case study with a large number of important factors (15 very important and 5 non-significant ones), N=10,000.

accurate estimates for important factors with respect to the other two methods. Comparing Fig. 2(a) with Fig. 2(b), and also Tables 3 and 4, as the number of significant factors increases, the hybrid version becomes the most precise.

4. Application: the Level-E model

We apply the method to a real test case. The Level E was used both as a benchmark of Monte Carlo

Table 3 Comparison between the estimates obtained with the three methods under analysis (classic Fast, RBD, Hybrid FAST–RBD) in a case-study with 10 very important factors (a_i =0) and 10 non-significant factors (a_i =99)

	Analytic values		The RBD approach	Hybrid FAST-RBD	Classic FAST
Important factors	0.0199	Mean Variance	$0.0217 \\ 1.1014 \times 10^{-005}$	$0.0198 \\ 5.0911 \times 10^{-006}$	0.0221 8.2378×10^{-006}
Non-important factors	1.988×10^{-006}	Mean Variance	$0.0024 \\ 6.7384 \times 10^{-006}$	$0.0014 \\ 2.4595 \times 10^{-006}$	$3.2799 \times 10^{-004} $ 2.3382×10^{-007}

Table 4 Comparison between the estimates obtained with the three methods under analysis (classic FAST, RBD, Hybrid FAST–RBD) in a case-study with 15 very important factors (a_i =0) and 5 non-significant factors (a_i =99)

	Analytic values		The RBD approach	Hybrid FAST-RBD	Classic FAST
Important factors	0.0045	Mean Variance	0.0086 3.1128×10^{-006}	0.0047 1.2586×10^{-006}	0.0063 7.2886×10^{-007}
Non-important factors	4.514×10^{-007}	Mean Variance	$0.0025 \\ 3.9133 \times 10^{-007}$	$6.4000 \times 10^{-004} $ 2.8000×10^{-008}	$2.3720 \times 10^{-004} $ 1.2315×10^{-008}

Table 5
Description of the input parameters and their probability distributions for the Level-E exercise

Notation	Definition	Distribution	Range	Units
\overline{T}	Containment time	Uniform	/100,1000/	yr
$k_{ m I}$	Leach rate for iodine	Log-uniform	$/10^{-3}$, 10^{-2} /	yr ⁻¹
$k_{\rm C}$	Leach rate for Np chain nuclides	Log-uniform	$/10^{-6}, 10^{-5}/$	yr ⁻¹
$v^{(1)}$	Water vel. In geosphere's 1st layer	Log-uniform	$/10^{-3}$, 10^{-1} /	m/yr
$I^{(1)}$	Length of geosphere's 1st layer	Uniform	/100, 500/	m
$R_{ m I}^{(1)}$	Retention factor for I (1st layer)	Uniform	/1, 5/	_
$R_{\rm C}^{(1)}$ $v^{(2)}$	Factor to compute ret. coeff. For Np (1st layer)	Uniform	/3, 30/	_
v ⁽²⁾	Water vel. In geosphere's 2nd layer	Log-uniform	$/10^{-2}$, 10^{-1} /	m/yr
$I^{(2)}$	Length of geosphere's 2nd layer	Uniform	/50, 20/	m
$R_{\rm I}^{(2)}$	Retention factor for I (2nd layer)	Uniform	/1, 5/	- .
$R_{\rm C}^{(2)}$	Factor to compute ret. coeff. For Np (2nd layer)	Uniform	/3, 30/	_
W	Stream flow rate	Log-uniform	$/10^5, 10^7/$	m ³ /yr

computation ([10,11]) and as a benchmark for sensitivity analysis methods (Level S, [7]). This test case has been extensively used by several authors, see [12] for a review. The model predicts the radiological dose to humans over geological time scales due to the

underground migration of radionuclides from a nuclear waste disposal site through a system of natural and engineered barriers.

The model has a total of 33 parameters, 12 of which are taken as independent uncertain parameters (Table 5);

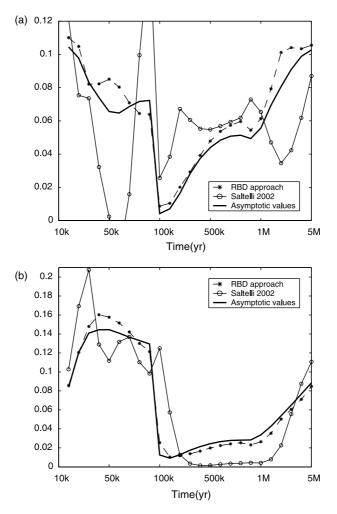


Fig. 3. (a): Second test case: Level-E. Comparison between the method of [6] and the RBD approach, for input factor 4. (b): Second test case: Level-E. Comparison between the method of [6] and the RBD approach, for input factor 12

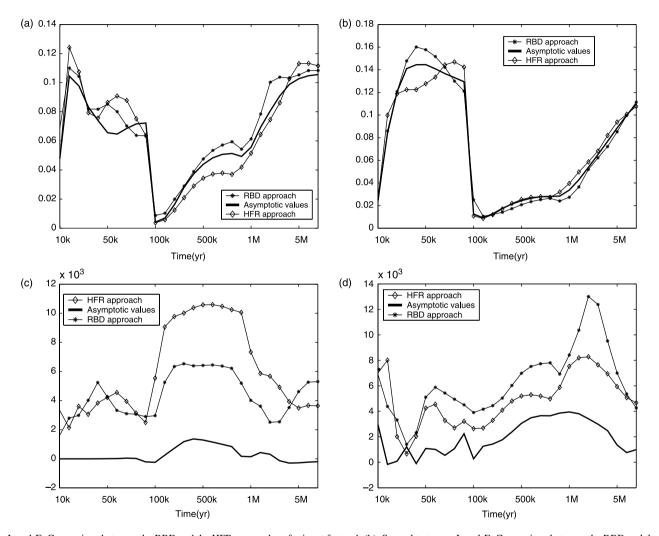


Fig. 4. (a): Second test case: Level-E. Comparison between the RBD and the HFR approaches, for input factor 4. (b): Second test case: Level-E. Comparison between the RBD and the HFR approaches, for input factor 3. (d): Second test case: Level-E. Comparison between the RBD and the HFR approaches, for input factor 9.

the core of the model is a set of partial differential equations which describes the nuclide migration in the geosphere. (See [1] for a complete description of the model).

The model is time dependent: the simulated time frame ranges from 2×10^4 to 9×10^6 years. The predictive uncertainty about Y(t) is due to uncertainties in model parameters.

The probability distributions for the factors have been selected on the basis of expert judgment. For in-depth discussion of the model and its predictions, see [7] and [11]).

After generating the sample (N=4000) and running the Level-E model, we used the output to calculate, with the RBD approach, the main effects over the simulated period. Results of the main effects for the two most influential factors (stream flow rate and water travel speed in the first geosphere layer) are given in Fig. 3.

Homma and Saltelli [13] showed how the approach proposed by Sobol' [14] to estimate main effects outperforms both crude Monte Carlo sampling and Latin Hypercube sampling. Here, we compare our proposed approach against that proposed by Saltelli [6], which is a further improvement with respect to that of Sobol' [14]. We consider a case with N=550 for the method of Saltelli [6].

The RBD approach better approximates the asymptotic values (obtained at very large sample size using the method of Saltelli) than the one implemented by Saltelli himself (Fig. 3). Besides, the computational cost of the method of Saltelli is equal to $C=N(2k+2)=550\times26=14,300$ while the cost of the proposed methods is only C=4000.

In Fig. 4 we compare the performance of the RBD approach against the hybrid HFR approach for the estimation of the main effects. The hybrid approach is

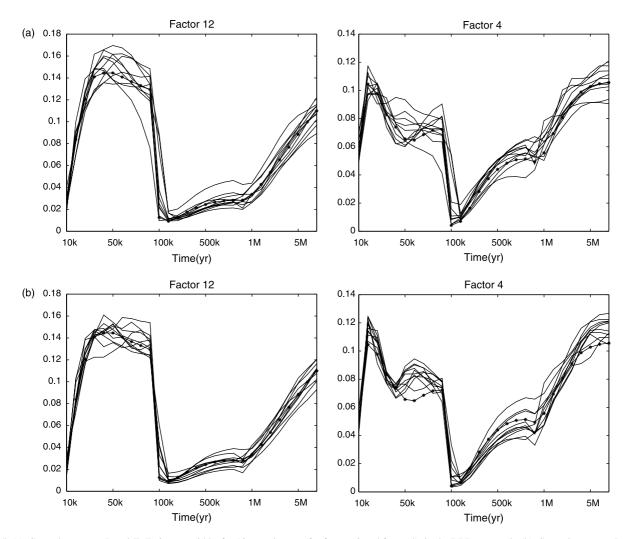


Fig. 5. (a): Second test case: Level-E. Estimates widths for 10 experiments (for factor 12 and factor 4), in the RBD approach. (b): Second test case: Level-E. Estimates widths for 10 experiments (for factor 12 and factor 4), in the HFR approach.

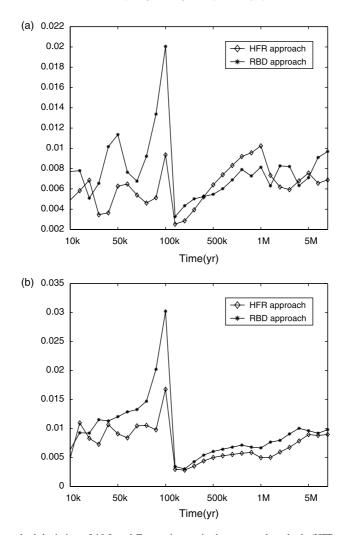


Fig. 6. (a): Comparison between the standard deviation of 10 Level-E experiments in the proposed methods (HFR and RBD) for factor 4. (b): Comparison between the standard deviation of 10 Level-E experiments in the proposed methods (HFR and RBD) for factor 12.

implemented with three groups of (four) factors, to which we assign the frequencies 11, 27 and 39. The hybrid approach is worse for the two most important factors (Fig. 4(a) and (b)), while both methods perform equally well for the non-significant factors (Fig. 4(c) and (d)).

To give more evidence of the performance of the two methods, we run each of them 10 times so that the width of the estimates can be evaluated and compared. In Fig. 5 the estimates widths of factors 4 and 12 are shown, for both methods. This HFR approach yields less varying estimates, especially at t=100,000 year, as confirmed by the standard deviation calculated across the 10 estimates (see Fig. 6). The means of the main effects over the 10 experiments for factor 4 show that the hybrid version is less precise than the RBD approach. Instead, for factor 12, the means of the hybrid approach are closer to the asymptotic values. In summary, it is

difficult to establish which method to prefer, as their performance depends on the factor considered and on the time Fig. 7.

5. Conclusions

Our analysis shows that the two new methods proposed in this paper, that based on random balance designs (RBD) and the Hybrid FAST-RBD (HFR), have computational advantages over all other strategies for the estimate of variance-based measures currently employed in the literature.

The two methods are substantially equivalent, as each of them can perform better or worst in different case studies. Of the two proposed methods, the HFR is slightly more complex to implement than RBD, and it is up to the analyst the choice of the frequencies and

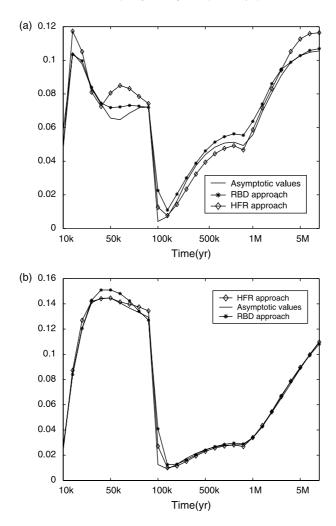


Fig. 7. (a): Comparison between the means of 10 Level-E experiments in the proposed methods (HFR and RBD) for factor 4. (b): Comparison between the means of 10 Level-E experiments in the proposed methods (HFR and RBD) for factor 12.

the selection of the subsets of factors. The persisting drawback is that we can employ these approaches only for setting FP, as the proposed methods only supply estimates for main effects.

Acknowledgements

The authors would like to acknowledge Professor Max Morris (Iowa State University, IA) and Andrea Saltelli (Joint Research Centre, Italy) for their kind support and useful suggestions.

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