Available online at www.sciencedirect.com
ScienceDirect
Reliability Engineering and System Safety 92 (2007) 957–960
RELIABILITY ENGINEERING & SYSTEM SAFETY
www.elsevier.com/locate/ress

Estimating the approximation error when fixing unessential factors in global sensitivity analysis

I.M. Sobol'[a], S. Tarantola[b], D. Gatelli[b,*], S.S. Kucherenko[c], W. Mauntz[d]

[a]*Institute for Mathematical Modelling of the Russian Academy of Sciences, Moscow, Russia*
[b]*Joint Research Centre of the European Commission, TP361, Institute of the Protection and Security of the Citizen, Via E. Fermi 1, 21020 Ispra (VA), Italy*
[c]*Imperial College London, UK*
[d]*Department of Biochemical and Chemical Engineering, Dortmund University, Germany*

Received 20 April 2006; received in revised form 5 July 2006; accepted 6 July 2006
Available online 28 August 2006

Abstract

One of the major settings of global sensitivity analysis is that of fixing non-influential factors, in order to reduce the dimensionality of a model. However, this is often done without knowing the magnitude of the approximation error being produced. This paper presents a new theorem for the estimation of the average approximation error generated when fixing a group of non-influential factors. A simple function where analytical solutions are available is used to illustrate the theorem. The numerical estimation of small sensitivity indices is discussed.

Keywords: Sobol' method; Approximation error; Sensitivity analysis by groups; Sensitivity indices

1. Introduction

This work is related to global sensitivity analysis based on the use of ANOVA decomposition and global sensitivity indices (see [1,6–8] for theory, and [3,4] for applications). Definitions of the sensitivity indices can be found in Section 2.

Different settings for sensitivity analysis are available, depending on the modeler's needs. One of these is the factors fixing setting. It is used for identifying non-influential factors in the model (those factors that can be fixed at any value in their domains without significantly reducing the output variance). A limit with factor fixing is that of fixing unessential factors without knowing the magnitude of the approximation error that is being produced. In Section 2, we prove one new theorem which quantifies this approximation error of the model output when one factor or a group of factors is fixed. So, once we know from total indices that a factor is unessential, we will also have an estimate of the error that is generated by fixing it.

In this paper we study a model function $f(x_1,\ldots,x_n)$, where the factors $x_1,\ldots,x_n$ are non-random independent scaled variables: $0\leqslant x_1\leqslant 1,\ldots,0\leqslant x_n\leqslant 1$. Thus the point $x=(x_1,\ldots,x_n)$ is defined in the n-dimensional unit hypercube with Lebesgue measure. Clearly the factors $x_1,\ldots,x_n$ can be regarded as independent random variables uniformly distributed in the unit interval [0,1]. In this case the quantities that are called variances are real variances of certain random variables.

The sensitivity analysis based on ANOVA decomposition and global sensitivity indices can be easily (mutatis mutandis) generalized to independent random factors $x_1,\ldots,x_n$ with arbitrary distribution functions $F_1(x_1),\ldots,F_n(x_n)$ (e.g., [8]). However, the requirement of independence is important.

Section 2 contains a new theorem, Section 3—an illustration of the theorem, and in Section 4 numerical estimation of small sensitivity indices is discussed.

*Corresponding author. Tel.: +39 0332 789928; fax: +39 0332 785733.
E-mail addresses: stefano.tarantola@jrc.it (S. Tarantola), debora.gatelli@jrc.it (D. Gatelli).

0951-8320/$ - see front matter © 2006 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ress.2006.07.001

2. The proposed theorem

Let $x=(x_1,\ldots,x_n)$ be a point in the n-dimensional unit hypercube with Lebesgue measure. We denote by y an arbitrary subset consisting of s variables and let z be the set of $n-s$ complementary variables, $1\leqslant s\leqslant n-1$. Thus $x\equiv(y,z)$ and $\mathrm{d}x=\mathrm{d}y\,\mathrm{d}z$. All the integrals below are from 0 to 1 in each variable. The set of variables z can be regarded as non-essential if the sensitivity index $S_z^{\mathrm{tot}}\ll 1$. The common practice in such a situation is to fix somehow a value z_0 and to use $f(y,z_0)$ as an approximation to $f(x)$. The approximation error depends on the choice of z_0:

$$\delta(z_0)=\frac{1}{D}\int[f(x)-f(y,z_0)]^2\,\mathrm{d}x, \tag{1}$$

where D is the variance of $f(x)$: $D=\int f^2\,\mathrm{d}x-f_0^2$, $f_0=\int f\,\mathrm{d}x$. The model function is assumed to be square integrable.

The following theorem shows that $\delta(z_0)$ is of the same order as S_z^{tot}.

Theorem. *For an arbitrary z_0 the error $\delta(z_0)\geqslant S_z^{\mathrm{tot}}$. If z_0 is assumed to be random and uniformly distributed, then the expected value is $E\delta(z_0)=2S_z^{\mathrm{tot}}$.*

A corollary of the theorem is the following assertion from [5]: for an arbitrary $\varepsilon>0$ with probability exceeding $1-\varepsilon$

$$\delta(z_0)<\left(1+\frac{1}{\varepsilon}\right)S_z^{\mathrm{tot}}.$$

In particular (at $\varepsilon=0.5$), the inequality $\delta(z_0)<3S_z^{\mathrm{tot}}$ holds with probability exceeding 0.50.

Proof. The ANOVA decomposition of $f(x)$ can be written in the form

$$f(x)=f_0+g_1(y)+g_2(z)+g_{12}(x), \tag{2}$$

where $g_1(y)$ is the sum of all terms that depend on y variables only and similarly $g_2(z)$ is the sum of all terms that depend on z only; g_{12} is the remainder.

From the definition of ANOVA, one can see that $\int g_1\,\mathrm{d}y=\int g_2\,\mathrm{d}z=\int g_{12}\,\mathrm{d}y=\int g_{12}\,\mathrm{d}z=0$.

Consider the variances $D_y=\int g_1^2\,\mathrm{d}y$, $D_z=\int g_2^2\,\mathrm{d}z$, $D_{yz}=\int g_{12}^2\,\mathrm{d}x$.

Squaring (2) and integrating over $\mathrm{d}x$ we obtain the relation $D=D_y+D_z+D_{yz}$ that allows a direct definition of the sensitivity indices for the sets y and z:

$$S_z=\frac{D_z}{D},\quad S_z^{\mathrm{tot}}=\frac{D_z+D_{yz}}{D},\quad S_y=\frac{D_y}{D},\quad S_y^{\mathrm{tot}}=\frac{D_y+D_{yz}}{D}.$$

From these definitions one can see that $S_z^{\mathrm{tot}}=1-S_y$, $S_y^{\mathrm{tot}}=1-S_z$.

Now an expression for $\delta(z_0)$ can be derived:

$$\begin{aligned}\delta(z_0)&=\frac{1}{D}\int\left[g_2(z)+g_{12}(x)-g_2(z_0)-g_{12}(y,z_0)\right]^2\mathrm{d}x\\&=\frac{1}{D}\int\left[g_2^2(z)+g_{12}^2(x)+g_2^2(z_0)+g_{12}^2(y,z_0)\right]\mathrm{d}x\\&=\frac{1}{D}\left[D_z+D_{yz}+g_2^2(z_0)+\int g_{12}^2(y,z_0)\,\mathrm{d}y\right].\end{aligned}$$

The final result is $\delta(z_0)=S_z^{\mathrm{tot}}+(1/D)[g_2^2(z_0)+\int g_{12}^2(y,z_0)\,\mathrm{d}y]$.

Both assertions of the theorem follow immediately: $\delta(z_0)\geqslant S_z^{\mathrm{tot}}$ and $\int\delta(z_0)\,\mathrm{d}z_0=2S_z^{\mathrm{tot}}$.

Proof of the Corollary. Consider a non-negative random variable $\eta=\delta(z_0)/S_z^{\mathrm{tot}}-1$. Clearly, $E\eta=1$. A well-known Chebyshev inequality for non-negative random variables with finite expectation can be applied: for an arbitrary $h>0$ the probability $P\{\eta\geqslant h\}\leqslant E\eta/h$.

We put $\varepsilon=1/h$ and turn to the opposite event: $P\{\eta<1/\varepsilon\}>1-\varepsilon$.

The last relation is equivalent to the assertion of the corollary.

3. Analytic example: the *g*-function

We illustrate the theorem by using the g-function of Sobol', which is often used as a benchmark for sensitivity analysis exercises (see e.g., [2]) as the exact analytical values can be easily calculated. The function is defined as

$$f=\prod_{i=1}^{n}g_i(x_i), \tag{3}$$

where n is the number of independent input factors and $g_{\mathrm{i}}(x_{\mathrm{i}})$ is

$$g_i(x_i)=\frac{|4x_i-2|+a_i}{1+a_i}, \tag{4}$$

for $0\leqslant x_i\leqslant 1$ and $a_i\geqslant 0$.

The parameter a_i is set to determine the importance of the input factor x_i, given that the range of variation of $g_i(x_i)$ depends exclusively on the value of a_i. If $a_i=0$, the corresponding factor x_i is important; if $a_i=1$, x_i is relatively important, while for $a_i=9$ it becomes non-important and for $a_i=99$ non-significant.

For the function (3) the first-order partial variances are $D_i=1/3(1+a_i)^2$, the higher order partial variances are products $D_{i_1\ldots i_s}=D_{i_1},\cdots,D_{i_s}$, and the total variance $D=\prod_{i=1}^{n}(D_i+1)-1$.

The group variances D_y, D_z, $D_y^{\mathrm{tot}}=D_y+D_{yz}$, $D_z^{\mathrm{tot}}=D_z+D_{yz}$ are sums of partial variances. However, integral representations for these variances allow direct numerical computation of their values [6,8].

Test 1. *We consider a model with eight input factors, where*

$$a_i=\{0,\quad 1,\quad 4.5,\quad 9,\quad 99,\quad 99,\quad 99,\quad 99\},$$

so that the eight factors are in decreasing order of importance. Table 1 contains total indices $S_i^{\text{tot}} = D_i^{\text{tot}}/D$ (the set contains one variable x_i).

Let us assume that one of the non-influential factors (e.g. x_4) is fixed at z_0. By substituting (3) into (1) we obtain the expression for $\delta(z_0)$:

$$\delta(z_0) = \frac{1}{D}\left[\frac{1}{(a_4+1)^2}(4/3+2a_4+a_4^2) - 2\frac{|4z_0-2|+a_4}{1+a_4} + \left(\frac{|4z_0-2|+a_4}{1+a_4}\right)^2\right]\prod_{\substack{i=1\\ i\neq 4}}^{8}\frac{1}{(1+a_i)^2}(4/3+2a_i+a_i^2).$$

The values of $\delta(x_4)$ are shown in Fig. 1.

If we calculate $E[\delta(z_0)]$ we obtain 0.020, which is twice the total index of factor 4. It means that when fixing factor 4, we commit an average error corresponding to 2% of the variance of the original g-function.

We have selected 100 values $x_4 = 0.01(k-0.5)$, $1 \leqslant k \leqslant 100$, and computed the corresponding errors $\delta(x_4)$. The average of these 100 errors was 0.020—in full agreement with the analysis above. The graph in Fig. 1 is rather sophisticated, with two minimum values, and depends strongly on the behavior of $f(x)$.

Test 2. *Consider the factor x_8. We have selected 100 values of x_8 and calculated the corresponding errors $\delta(x_8)$. The behavior of $\delta(x_8)$ is similar to $\delta(x_4)$ in Fig. 1 but the numerical values are completely different and the average of these 100 errors was 0.00021 which is twice S_8^{tot}.*

Table 1
Total indices

Factor	Total index
1	0.787
2	0.242
3	0.034
4	0.010
5	1.05e-04
6	1.05e-04
7	1.05e-04
8	1.05e-04

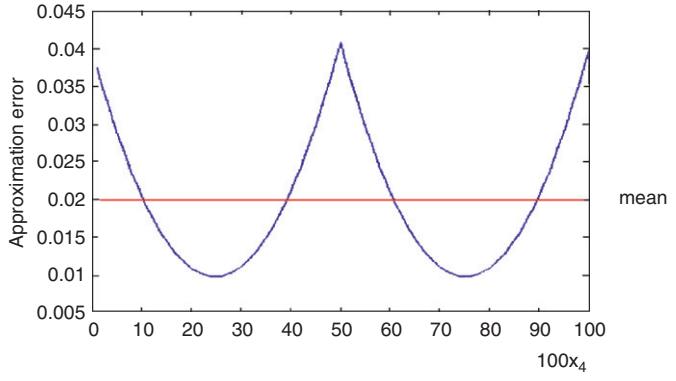

Fig. 1. Approximation error $\delta(x_4)$ versus x_4.

Test 3. *We now illustrate the theorem in the case where a group of factors is fixed; this is particularly useful for models with a high number of factors.*

One characteristic of variance-based methods is in fact the capability of treating grouped factors as if they were single factors. This property of synthesis is essential for the agility of the interpretation of results (see [4] for applications).

We consider the five non-important factors (from 4 to 8) as a single group z, and the remaining three in another group y. We fix group z at z_0.

Estimating $E[\delta(z_0)]$, we obtain 0.022 which is twice the total index of group z: $S_z^{\text{tot}} = 0.011$.

It is worth noticing that by fixing all the factors of group z, the approximation error is 2.2% of the variance of the g-function, i.e. only 0.2% more than when fixing factor 4 alone.

Remark. The analytical values from Table 1 were reproduced numerically by the Monte Carlo method. The sample size was $N = 7 \times 10^4$.

4. On the numerical estimation of small sensitivity indices

According to [6], the integral representation,

$$D_y = \int f(x)f(y,z')\,dx\,dz' - f_0^2, \tag{5}$$

was used for defining a Monte Carlo algorithm for the estimation of $S_y = D_y/D$. For the kth Monte Carlo trial two independent random points $x_{(k)}$ and $x'_{(k)}$ are used, $1 \leqslant k \leqslant N$. If the number of trials N is sufficiently large, then

$$f_0 \approx \frac{1}{N}\sum_{k=1}^{N} f(x_{(k)}), \tag{6}$$

$$D + f_0^2 \approx \frac{1}{N}\sum_{k=1}^{N} f^2(x_{(k)}), \tag{7}$$

$$D_y + f_0^2 \approx \frac{1}{N}\sum_{k=1}^{N} f(x_{(k)})f(y_{(k)}, z'_{(k)}). \tag{8}$$

However in the case when $D_y \ll f_0^2$, the computation of D_y from (8) is spoilt by a loss of accuracy.

For improving the situation, Saltelli [1] proposed a direct estimation of f_0^2. From the identity

$$f_0^2 = \int f(x)f(x')\,dx\,dx', \tag{9}$$

the approximation

$$f_0^2 \approx \frac{1}{N}\sum_{k=1}^{N} f(x_{(k)})f(x'_{(k)}), \tag{10}$$

can be derived. Despite the fact that the statistical error produced by (10) is larger than the statistical error of (6), the use of (8) and (10) reduces the loss of accuracy in the computation of D_y.

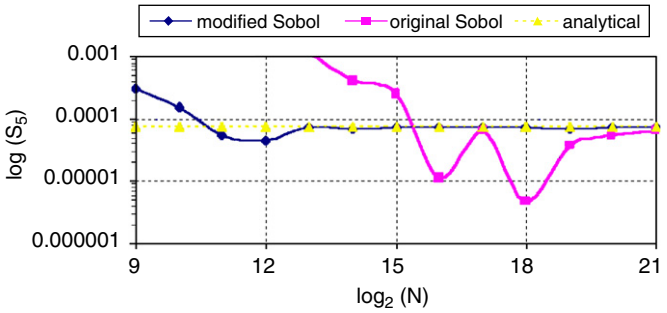

Fig. 2. Numerical evaluation of S_5 using modified and original formulas.

We made a further step in this direction: substituting (9) into (5) we obtained a new integral representation for D_y:

$$D_y = \int f(x)[f(y,z') - f(x')]\,\mathrm{d}x\,\mathrm{d}x', \tag{11}$$

and the corresponding approximation

$$D_y \approx \frac{1}{N}\sum_{k=1}^{N} f(x_{(k)})\left[f(y_{(k)}, z'_{(k)}) - f(x'_{(k)})\right], \tag{12}$$

which is a combination of (8) and (10).

Despite the fact that the dimension of the integral in (11) is higher than the dimension of the integral in (5), the modified Monte Carlo algorithm (6)+(7)+(12) is less sensitive to the loss of accuracy and allows to reduce the number of trials N.

Fig. 2 shows the numerical evaluation of S_5 for the g-function at different N using both Monte Carlo algorithms. The performance of the modified algorithm (6)+(7)+(12) is much more stable than that of the original algorithm (6)+(7)+(8). The exact value is $S_5 = 7.15 \times 10^{-5}$.

The representation (11) makes possible a standard statistical error evaluation for the approximation (12).

Remark 1. In [1] instead of (5) the representation $D_y = \int f(x')f(y',z)\,\mathrm{d}z\,\mathrm{d}x'$ was used. In this case our modification can be applied also.

Remark 2. In [5], another way to deal with loss of accuracy was proposed: to choose a constant $c \approx f_0$ and to carry out the calculations with $f(x)-c$ instead of $f(x)$.

5. Conclusions

This work shows how to estimate the approximation error committed when fixing non-important factors.

In our example the sensitivity indices were estimated both analytically and numerically; in general, they can be computed numerically.

The proposed theorem can be easily applied to global sensitivity methods that provide estimates of total indices; we have shown the applicability of the procedure also in cases where factors are treated by groups.

For numerical computation of small sensitivity indices a modified Monte Carlo algorithm was studied that reduces the loss of accuracy.

References

[1] Saltelli A. Making best use of model evaluations to compute sensitivity indices. Comput Phys Commun 2002;145:280–97.
[2] Saltelli A, Sobol' IM. About the use of rank transformation in sensitivity analysis of model output. Reliab Eng Syst Safety 1995; 50(3):225–39.
[3] Saltelli A, Chan K, Scott M, editors. Sensitivity analysis. London: Wiley; 2000.
[4] Saltelli A, Tarantola S, Campolongo F, Ratto M, editors. Sensitivity analysis in practice. London: Wiley; 2004.
[5] Sobol' IM. Sensitivity estimates for nonlinear mathematical models. Mat Modelirovanie 1990;2(1):112–8 [in Russian]. English translation: Math Modelling Comput Exp 1993;1(4):407–14.
[6] Sobol' IM. Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates. Math Comput Simul 2001; 55(1–3):271–80.
[7] Sobol' IM. Theorems and examples on high dimensional model representation. Reliab Eng Syst Safety 2003;79:187–93.
[8] Sobol' IM, Kucherenko SS. Global sensitivity indices for nonlinear mathematical models. Rev Wilmott Mag 2005(1):56–61.