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Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates

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Abstract

Global sensitivity indices for rather complex mathematical models can be efficiently computed by Monte Carlo (or quasi-Monte Carlo) methods. These indices are used for estimating the influence of individual variables or groups of variables on the model output.

Keywords: Sensitivity analysis; Monte Carlo method; Quasi-Monte Carlo method; Mathematical modelling

1. Introduction

Assume that the model under investigation is described by a function $u = f(x)$, where the input $x = (x_1, \ldots, x_n)$ is a point inside an n-dimensional box and u is a scalar output.

Let $u^* = f(x^*)$ be the required solution. In most papers, the sensitivity of the solution u^* with respect to x_k is considered. It is estimated by the partial derivative $(\partial u/\partial x_k)_{x=x^*}$. This approach to sensitivity is sometimes called local sensitivity.

The global sensitivity approach does not specify the input $x = x^*$, it considers the model $f(x)$ inside the box. Therefore, global sensitivity indices should be regarded as a tool for studying the mathematical model rather then its specified solution. Both approaches are represented in [3,8].

In this paper, I is the unit interval [0, 1], I^n the n-dimensional unit hypercube, and $x \in I^n$. All the integrals below are from 0 to 1 for each variable and $dx = dx_1 \cdots dx_n$.

2. ANOVA-representation

Consider an integrable function $f(x)$ defined in I^n. We shall study its representation in the form

$$f(x) = f_0 + \sum_{s=1}^{n} \sum_{i_1<\cdots<i_s}^{n} f_{i_1\cdots i_s}(x_{i_1}, \ldots, x_{i_s}), \tag{1}$$

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where $1 \le i_1 < \cdots < i_s \le n$. Formula (1) means that

$$f(x) = f_0 + \sum_i f_i(x_i) + \sum_{i<j} f_{ij}(x_i, x_j) + \cdots + f_{12\cdots n}(x_1, x_2, \ldots, x_n),$$

the total number of summands in (1) is 2^n.

Definition 1. Formula (1) is called ANOVA-representation of $f(x)$ if

$$\int_0^1 f_{i_1\cdots i_s}(x_{i_1}, \ldots, x_{i_s})\,\mathrm{d}x_k = 0 \quad \text{for} \quad k = i_1, \ldots, i_s. \tag{2}$$

It follows from (2) that the members in (1) are orthogonal and can be expressed as integrals of $f(x)$. Indeed,

$$\int f(x)\,\mathrm{d}x = f_0,$$

$$\int f(x) \prod_{k \ne i} \mathrm{d}x_k = f_0 + f_i(x_i),$$

$$\int f(x) \prod_{k \ne i,j} \mathrm{d}x_k = f_0 + f_i(x_i) + f_j(x_j) + f_{ij}(x_i, x_j),$$

and so on.

In my early papers, (1) with (2) was called decomposition into summands of different dimensions [11,12]. The term ANOVA comes from Analysis Of Variances [2].

Assume now that $f(x)$ is square integrable. Then all the $f_{i_1\cdots i_s}$ in (1) are square integrable also. Squaring (1) and integrating over I^n we get

$$\int f^2(x)\,\mathrm{d}x - f_0^2 = \sum_{s=1}^{n} \sum_{i_1<\cdots<i_s}^{n} \int f^2_{i_1\cdots i_s}\,\mathrm{d}x_{i_1} \cdots \mathrm{d}x_{i_s}.$$

The constants

$$D = \int f^2\,\mathrm{d}x - f_0^2, \qquad D_{i_1\cdots i_s} = \int f^2_{i_1\cdots i_s}\,\mathrm{d}x_{i_1} \cdots \mathrm{d}x_{i_s},$$

are called variances and

$$D = \sum_{s=1}^{n} \sum_{i_1<\cdots<i_s}^{n} D_{i_1\cdots i_s}.$$

The origin of this term is clear: if x were a random point uniformly distributed in I^n, then $f(x)$ and $f_{i_1\cdots i_s}(x_{i_1}, \ldots, x_{i_s})$ would be random variables with variances D and $D_{i_1\cdots i_s}$, respectively.

3. Sensitivity indices

Definition 2. The ratios

$$S_{i_1\cdots i_s} = \frac{D_{i_1\cdots i_s}}{D} \tag{3}$$

are called global sensitivity indices.

The integer s is often called the order or the dimension of the index (3). All the $S_{i_1\cdots i_s}$ are nonnegative and their sum is

$$\sum_{s=1}^{n}\sum_{i_1<\cdots<i_s}^{n} S_{i_1\cdots i_s} = 1.$$

For a piecewise continuous function $f(x)$, the equality $S_{i_1\cdots i_s} = 0$ means that $f_{i_1\cdots i_s}(x_{i_1},\ldots,x_{i_s}) \equiv 0$. Thus the functional structure of $f(x)$ can be investigated by estimating numbers $S_{i_1\cdots i_s}$.

The introduction of $S_{i_1\cdots i_s}$ can be regarded as more or less evident. The main breakthrough in [12] is the computation algorithm that allows a direct estimation of global sensitivity indices using values of $f(x)$ only. And this is a Monte Carlo algorithm.

Three types of problems will be indicated below that can be studied with the aid of global sensitivity indices.

1. Ranking of variables in $f(x_1,\ldots,x_n)$.
2. Fixing unessential variables in $f(x_1,\ldots,x_n)$.
3. Deleting high order members in (1).

4. Ranking of input variables

The simplest approach is to estimate first order indices $S_1,\ldots,S_n$ and to order the variables according to these values. For this purpose several techniques were applied already in the eighties, e.g. FAST (Fourier Amplitude Sensitivity Test) [1,4]. However, such an approach is insufficient if the sum $S_1+\cdots+S_n$ is much less than 1.

As an example, consider a problem where x_i and x_j are amounts of two different chemical elements. It may happen that both S_i and S_j are much smaller than S_{ij}. This is an indication that an important role is played by chemicals that include both elements.

One can easily notice that $S_1+\cdots+S_n = 1$ means that $f(x)$ is a sum of one-dimensional functions

$$f(x) = f_0 + \sum_{i=1}^{n} f_i(x_i).$$

4.1. Numerical example

A function with separated variables was considered [9,10]

$$g = \prod_{i=1}^{n}\varphi_i(x_i),$$

where $\varphi_i(t) = (|4t-2| + a_i)/(1+a_i)$ depends on a nonnegative parameter a_i. If $a_i = 0$ the multiplier $\varphi_i(t)$ varies from 0 to 2 and the variable x_i is important. If $a_i = 3$ the $\varphi_i(t)$ varies from 0.75 to 1.25 and the corresponding x_i is unimportant.

$$\text{Let } n = 8,\ a_1 = a_2 = 0,\ a_3 = \cdots = a_8 = 3.$$

The importance of the first two variables can be seen from the indices: $S_1 = S_2 = 0.329$ while $S_3 = \cdots = S_8 = 0.021$. The second order indices are: $S_{12} = 0.110$; $S_{ij} = 0.007$ if one of the indices is 1 or 2; and $S_{ij} = 0.0004$ if both i and j correspond to unimportant variables. The largest third order indices are $S_{12k} = 0.002$ for $k \geq 3$; the other third order indices do not exceed 0.00014.

5. Sensitivity indices for subsets of variables

Consider an arbitrary set of m variables, $1 \leq m \leq n-1$, that will be denoted by one letter

$$y = (x_{k_1}, \dots, x_{k_m}), \qquad 1 \leq k_1 < \cdots < k_m \leq n,$$

and let z be the set of $n-m$ complementary variables. Thus $x = (y, z)$.

Let $K = (k_1, \dots, k_m)$. The variance corresponding to the subset y can be defined as

$$D_y = \sum_{s=1}^{m} \sum_{(i_1 < \cdots < i_s) \in K} D_{i_1 \cdots i_s} \tag{4}$$

The sum in (4) is extended over all groups $(i_1, \dots, i_s)$ where all the $i_1, \dots, i_s$ belong to K.

Similarly, the variance D_z can be introduced. Then the total variance corresponding to the subset y is

$$D_y^{\text{tot}} = D - D_z.$$

One can notice that D_y^{tot} is also a sum of $S_{i_1 \cdots i_s}$; but it is extended over all groups $(i_1, \dots, i_s)$ where at least one $i_l \in K$. Here $1 \leq s \leq n$.

Two global sensitivity indices for the subset y are introduced [5,12].

Definition 3.

$$S_y = \frac{D_y}{D}, \qquad S_y^{\text{tot}} = \frac{D_y^{\text{tot}}}{D}.$$

Clearly, $S_y^{\text{tot}} = 1 - S_z$ and always $0 \leq S_y \leq S_y^{\text{tot}} \leq 1$. The most informative are the extreme situations:

$$S_y = S_y^{\text{tot}} = 0 \text{ means that } f(x) \text{ does not depend on } y,$$

$$S_y = S_y^{\text{tot}} = 1 \text{ means that } f(x) \text{ depends on } y \text{ only.}$$

Example 1. Assume that $n = 3$ and consider two subsets of variables:

1. $y = (x_1)$. Then $z = (x_2, x_3)$ and

$$S_{(1)} = S_1,$$

$$S_{(1)}^{\text{tot}} = S_1 + S_{12} + S_{13} + S_{123} = 1 - S_{(2,3)}.$$

2. $y = (x_1, x_2)$. Then $z = (x_3)$ and

$$S_{(1,2)} = S_1 + S_2 + S_{12},$$

$$S_{(1,2)}^{\text{tot}} = S_1 + S_2 + S_{12} + S_{13} + S_{23} + S_{123} = 1 - S_3.$$

6. Model approximation error

Let $h(x)$ be a square integrable function regarded as an approximation to $f(x)$. We shall use the scaled L_2 distance for estimating the approximation error:

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

If the crudest approximations $h(x) \equiv$ const are considered, the best result is obtained at $h(x) \equiv f_0$; then $\delta(f, f_0) = 1$. Hence, good approximations are the ones with $\delta(f,h) \ll 1$.

7. Fixing unessential variables

Assume that $S_z^{\mathrm{tot}} \ll 1$. In this case, $f(x)$ depends mainly on y and an approximation $h = f(y, z_0)$ with some fixed $z_0 \in I^{n-m}$ can be suggested. The following theorem [12,13] shows that the approximation error $\delta(f,h) \equiv \delta(z_0)$ depends on S_z^{tot}.

Theorem 1. *For an arbitrary $z_0 \in I^{n-m}$*

$$\delta(z_0) \geq S_z^{\mathrm{tot}}.$$

But if z_0 is a random point uniformly distributed in I^{n-m} then for an arbitrary $\varepsilon > 0$

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

For example, selecting $\varepsilon = 1/2$ we conclude that the probability that $\delta(z_0) < 3S_z^{\mathrm{tot}}$ exceeds 0.5.

8. A Monte Carlo approach

Theorem 2. *Subset's variance D_y is equal to*

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

Proof. The integral in (5) can be transformed:

$$\int f(x)f(y,z')\,\mathrm{d}x\,\mathrm{d}z' = \int \mathrm{d}y \int f(y,z)\,\mathrm{d}z \int f(y,z')\,\mathrm{d}z' = \int \mathrm{d}y \left[\int f(y,z)\,\mathrm{d}z\right]^2.$$

Applying (1) we conclude that

$$\int f(y,z)\,\mathrm{d}z = f_0 + \sum_{s=1}^{m} \sum_{(i_1<\cdots<i_s)\in K} f_{i_1\cdots i_s}(x_{i_1},\ldots,x_{i_s}).$$

After squaring and integrating over $\mathrm{d}y = \mathrm{d}x_{k_1}\cdots\mathrm{d}x_{k_m}$ we obtain

$$\int f(x)f(y,z')\,\mathrm{d}x\,\mathrm{d}z' = f_0^2 + \sum_{s=1}^{m}\sum_{(i_1<\cdots<i_s)\in K} D_{i_1\ldots i_s} = f_0^2 + D_y.$$

And this is equivalent to (5). □

A formula similar to (5) can be written for D_z:

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

Thus, for computing S_y and $S_y^{\mathrm{tot}} = 1 - S_z$ one has to estimate four integrals:

$$\int f(x)\,\mathrm{d}x, \quad \int f^2(x)\,\mathrm{d}x, \quad \int f(x)f(y,z')\,\mathrm{d}x\,\mathrm{d}z' \quad \text{and} \quad \int f(x)f(y',z)\,\mathrm{d}x\,\mathrm{d}y'.$$

Now a Monte Carlo method can be constructed. Consider two independent random points ξ and ξ' uniformly distributed in I^n and let $\xi = (\eta, \zeta)$, $\xi' = (\eta', \zeta')$. Each Monte Carlo trial requires three computations of the model: $f(\xi) \equiv f(\eta,\zeta)$, $f(\eta, \zeta')$ and $f(\eta', \zeta)$. After N trials, crude Monte Carlo estimates are obtained:

$$\frac{1}{N}\sum_{j=1}^{N} f(\xi_j) \xrightarrow{P} f_0, \qquad \frac{1}{N}\sum_{j=1}^{N} f(\xi_j)f(\eta_j,\zeta_j') \xrightarrow{P} D_y + f_0^2,$$
$$\frac{1}{N}\sum_{j=1}^{N} f^2(\xi_j) \xrightarrow{P} D + f_0^2, \qquad \frac{1}{N}\sum_{j=1}^{N} f(\xi_j)f(\eta_j',\zeta_j) \xrightarrow{P} D_z + f_0^2. \tag{6}$$

The stochastic convergence $\xrightarrow{P}$ in (6) is implied by absolute convergence of the four integrals that follows from the square integrability of $f(x)$.

9. On computation algorithms

1. A Monte Carlo algorithm corresponding to (6) can be easily defined: for the jth trial, $2n$ standard random numbers $\gamma_1^j, \ldots, \gamma_{2n}^j$ are generated; then

   $$\xi_j = (\gamma_1^j, \ldots, \gamma_n^j), \qquad \xi_j' = (\gamma_{n+1}^j, \ldots, \gamma_{2n}^j),$$

   and $j = 1, 2, \ldots, N$.
2. A quasi-Monte Carlo algorithm can be defined similarly [14]. Let $Q_1, Q_2, \ldots$ be a low discrepancy sequence of points in I^{2n} (sometimes it is called quasi-random sequence). For the jth trial the point $Q_j = (q_1^j, \ldots, q_{2n}^j)$ is generated and

   $$\xi_j = (q_1^j, \ldots, q_n^j), \qquad \xi_j' = (q_{n+1}^j, \ldots, q_{2n}^j).$$

   As a rule, quasi-Monte Carlo implementations of (6) converge faster than ordinary Monte Carlo. Quite often LP_τ-sequences (also called (t, s)-sequences in base 2 or Sobol sequences) are used [2].

3. The computation of variances from (6) may proceed with a loss of accuracy if the mean value f_0 is large. Therefore it was suggested in [12] to find a crude approximate value $c_0 \approx f_0$ and to introduce a new model function $f(x) - c_0$ rather than $f(x)$. For the new model function the constant term in (1) will be small: $f_0 - c_0$.
4. It must be mentioned that several variance reducing techniques (importance sampling, weighted uniform sampling, variance reducing multipliers) are inefficient if a vanishing integral is evaluated. Therefore in [15] an attempt was made to use variance reduction in integrations of $f^2(x)$, $f(x)f(y, z')$ and $f(x)f(y', z)$ while $f(x)$ was integrated by crude Monte Carlo. In these experiments quasi-Monte Carlo outplayed Monte Carlo with variance reduction.
5. Monte Carlo estimates (6) can be applied for evaluating all the indices $S_{i_1 \cdots i_s}$.

A first order index S_i is estimated directly because $S_i = S_{(i)}$ — the index of a set consisting of one variable x_i.

A second order index S_{ij} is defined from the relation $S_{(ij)} = S_i + S_j + S_{ij}$ where $S_{(ij)}$ is estimated directly: it is the index of the set $y = (x_i, x_j)$. And so on.

Clearly, the estimation of high order indices can be spoilt by a loss of accuracy. However, the most interesting are the largest indices and for them the loss of accuracy is not so harmful.

10. An alternative Monte Carlo approach

The following integral representation of D_y^{tot} is a slight generalization of formulas used in [6] and [16].

Theorem 3. *Subset's total variance D_y^{tot} is equal to*

$$D_y^{\text{tot}} = \frac{1}{2}\int [f(y, z) - f(y', z)]^2 \mathrm{d}x\, \mathrm{d}y'. \tag{7}$$

$$\begin{aligned} &\frac{1}{2}\int [f(y, z) - f(y', z)]^2 \mathrm{d}y\, \mathrm{d}z\, \mathrm{d}y' \\ &\quad = \frac{1}{2}\int f^2(x)\, \mathrm{d}x + \frac{1}{2}\int f^2(y', z)\, \mathrm{d}y'\, \mathrm{d}z - \int f(x) f(y', z)\, \mathrm{d}x\, \mathrm{d}y' \\ &\quad = \int f^2(x)\, \mathrm{d}x - (D_z + f_0^2) = D - D_z = D_y^{\text{tot}}. \end{aligned} \qquad \square$$

Proof. An expression similar to (7) can be written for D_z^{tot}. Therefore the last two Monte Carlo estimates in (6) can be replaced by estimates

$$\frac{1}{2N}\sum_{j=1}^{N} \left[f(\xi_j) - f(\eta_j, \zeta'_j)\right]^2 \xrightarrow{P} D_z^{\text{tot}}, \qquad \frac{1}{2N}\sum_{j=1}^{N} \left[f(\xi_j) - f(\eta'_j, \zeta_j)\right]^2 \xrightarrow{P} D_y^{\text{tot}}, \tag{8}$$

with a subsequent computation of $D_y = D - D_z^{\text{tot}}$, $D_z = D - D_y^{\text{tot}}$. $\square$

11. Comparison of variances

Consider the estimators from Section 8:

$$\mu = f(\xi) f(\eta, \zeta')$$

and

$$\mu^{\text{tot}} = f^2(\xi) - f(\xi) f(\eta', \zeta).$$

Their expectations are $\boldsymbol{E}(\mu) = D_y + f_0^2$, $\boldsymbol{E}(\mu^{\text{tot}}) = D_y^{\text{tot}}$.

The corresponding estimators from Section 10 are

$$\lambda = f^2(\xi) - \tfrac{1}{2}[f(\xi) - f(\eta, \zeta')]^2$$

and

$$\lambda^{\text{tot}} = \tfrac{1}{2}[f(\xi) - f(\eta', \zeta)]^2$$

with expectations $\boldsymbol{E}(\lambda) = D_y + f_0^2$, $\boldsymbol{E}(\lambda^{\text{tot}}) = D_y^{\text{tot}}$.

Theorem 4. *The variances of μ, λ, μ^{tot}, λ^{tot} satisfy inequalities*

$$\text{var}(\mu) \le \text{var}(\lambda), \qquad \text{var}(\mu^{\text{tot}}) \ge \text{var}(\lambda^{\text{tot}}). \tag{9}$$

The inequalities (9) suggest a somewhat unexpected conclusion: it may be expedient to apply simultaneously (6) for estimating D_y and (8) for estimating D_y^{tot} with subsequent computation of

$$D_z = D - D_y^{\text{tot}}, \qquad D_z^{\text{tot}} = D - D_y.$$

Proof of the theorem. We shall compare expectations of squares. First, consider $\boldsymbol{E}(\lambda^2)$:

$$\begin{aligned}\boldsymbol{E}(\lambda^2) &= \int \left\{ f(x) f(y, z') + \frac{1}{2}[f^2(x) - f^2(y, z')] \right\}^2 \mathrm{d}x\, \mathrm{d}z' \\ &= \int f^2(x) f^2(y, z')\, \mathrm{d}x\, \mathrm{d}z' + \frac{1}{4} \int [f^2(x) - f^2(y, z')]^2 \mathrm{d}x\, \mathrm{d}z' \\ &\quad + \int [f^3(x) f(y, z') - f(x) f^3(y, z')]\, \mathrm{d}x\, \mathrm{d}z'.\end{aligned}$$

The last integral vanishes:

$$\int \mathrm{d}y \int f^3(y, z)\, \mathrm{d}z \int f(y, z')\, \mathrm{d}z - \int \mathrm{d}y \int f(y, z)\, \mathrm{d}z \int f^3(y, z')\, \mathrm{d}z' = 0.$$

The second integral is nonnegative. Hence

$$\boldsymbol{E}(\lambda^2) \ge \int [f(x) f(y, z')]^2 \mathrm{d}x\, \mathrm{d}z' = \boldsymbol{E}(\mu^2)$$

and $\text{var}(\lambda) \ge \text{var}(\mu)$.

Second, consider the expectation of $(\lambda^{\text{tot}})^2$:

$$\boldsymbol{E}[(\lambda^{\text{tot}})^2] = \frac{1}{4}\int [f(x) - f(y', z)]^4 \,\mathrm{d}x\,\mathrm{d}y'.$$

Denote by R the nonnegative function

$$R = [f(y, z) - f(y', z)]^2$$

that is symmetric in y and y'. Then

$$\begin{aligned}\boldsymbol{E}[(\lambda^{\text{tot}})^2] &= \frac{1}{4}\int [f(y, z) - f(y', z)]^2 R\,\mathrm{d}y\,\mathrm{d}y'\,\mathrm{d}z \le \frac{1}{4}\int [2f^2(y, z) + 2f^2(y', z)] R\,\mathrm{d}y\,\mathrm{d}y'\,\mathrm{d}z \\ &= \int f^2(x) R\,\mathrm{d}y\,\mathrm{d}y'\,\mathrm{d}z = \boldsymbol{E}[(\mu^{\text{tot}})^2].\end{aligned}$$

Hence $\mathrm{var}(\lambda^{\text{tot}}) \le \mathrm{var}(\mu^{\text{tot}})$. □

12. Deleting high order members in (1)

Recently, Prof. H. Rabitz [7] has suggested that quite often in mathematical models the low order interactions of input variables have the main impact upon the output. For such models the following approximation can be used:

$$h_L(x) = f_0 + \sum_{s=1}^{L} \sum_{i_1<\cdots<i_s}^{n} f_{i_1\cdots i_s}(x_{i_1}, \ldots, x_{i_s}) \tag{10}$$

with $L \ll n$.

Theorem 5. *If the model f(x) is approximated by* (10) *then the approximation error is*

$$\delta(f, h_L) = 1 - \sum_{s=1}^{L} \sum_{i_1<\cdots<i_s}^{n} S_{i_1\cdots i_s}. \tag{11}$$

Proof. From (1) and (10)

$$f(x) - h_L(x) = \sum_{s=L+1}^{n} \sum_{i_1<\cdots<i_s}^{n} f_{i_1\cdots i_s}(x_{i_1}, \ldots, x_{i_s})$$

and all the members on the right-hand side are orthogonal. Squaring, integrating over I^n and dividing by D, we obtain

$$\delta(f, h_L) = \sum_{s=L+1}^{n} \sum_{i_1<\cdots<i_s}^{n} S_{i_1\cdots i_s}$$

and this is equivalent to (11). □

Relation (11) shows that estimating low order sensitivity indices (with $s \leq L$) one can verify the suggestion of Prof. Rabitz.

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