

A general first-order global sensitivity analysis method

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Abstract

Fourier amplitude sensitivity test (FAST) is one of the most popular global sensitivity analysis techniques. The main mechanism of FAST is to assign each parameter with a characteristic frequency through a search function. Then, for a specific parameter, the variance contribution can be singled out of the model output by the characteristic frequency. Although FAST has been widely applied, there are two limitations: (1) the aliasing effect among parameters by using integer characteristic frequencies and (2) the suitability for only models with independent parameters. In this paper, we synthesize the improvement to overcome the aliasing effect limitation [Tarantola S, Gatelli D, Mara TA. Random balance designs for the estimation of first order global sensitivity indices. *Reliab Eng Syst Safety* 2006; 91(6):717–27] and the improvement to overcome the independence limitation [Xu C, Gertner G. Extending a global sensitivity analysis technique to models with correlated parameters. *Comput Stat Data Anal* 2007, accepted for publication]. In this way, FAST can be a general first-order global sensitivity analysis method for linear/nonlinear models with as many correlated/uncorrelated parameters as the user specifies. We apply the general FAST to four test cases with correlated parameters. The results show that the sensitivity indices derived by the general FAST are in good agreement with the sensitivity indices derived by the correlation ratio method, which is a non-parametric method for models with correlated parameters.

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1. Introduction

Identification and representation of uncertainty are recognized as essential components in model application [1–6]. In the study of uncertainty, we need to know how much uncertainty there is in the model output (uncertainty analysis) and where the uncertainty comes from (sensitivity analysis).

There are two groups of sensitivity analyses: local sensitivity analysis and global sensitivity analysis [7]. The local sensitivity analysis examines the local response of the output(s) by varying input parameters one at a time while holding other parameters at central values. The global sensitivity analysis examines the global response (averaged over the variation of all the parameters) of model output(s) by exploring a finite (or even an infinite) region. The local sensitivity analysis is easy to implement. However, local

sensitivity analysis can only inspect one point at a time and the sensitivity index of a specific parameter is dependent on the central values of the other parameters. Thus, more studies currently are using global sensitivity analysis methods instead of local sensitivity analysis.

Many global sensitivity analysis techniques are now available [7,8], such as Fourier Amplitude Sensitivity Test (FAST) [8–15]; the design of experiments method [16–20]; regression-based methods [5,21–24]; Sobol's method [25]; McKay's one-way ANOVA method [26]; and moment independent approaches [27–29]. One of the most popular global sensitivity analysis techniques is FAST. The theory of FAST was first proposed by Cukier et al. in 1970s [10–12,15]. The main mechanism of FAST is to assign each parameter with a characteristic frequency through a search function. Then, for a specific parameter, the variance contribution can be singled out of the model output by the characteristic integer frequency. Koda et al. [9] and McRae et al. [13] provided the computational codes for FAST. FAST is computationally efficient and can be used for

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nonlinear and non-monotonic models. Thus, it has been widely applied in sensitivity analysis of different models, such as chemical reaction models [10–12,14,15,30]; atmospheric models [31–33]; nuclear waste disposal models [34]; soil erosion models [35]; and hydrological models [36].

Although FAST has been widely applied, there are two limitations. First, there will be an aliasing effect among parameters when using integer characteristic frequencies. In order to avoid the aliasing effect, large sample sizes are needed when there are many candidate parameters. Second, FAST can only be applied for models with independent parameters [32]. However, in many cases, the parameters are correlated with one another. For example, in meteorology, the central pressure of the storm is correlated with the radius of the maximum wind [3].

Recently, there have been two improvements aimed at overcoming the aliasing and independency limitation. The aliasing effect limitation can be circumvented by using a random balance design [1]. For the independence limitation, it can be overcome by reordering [2]. In this paper, we propose to synthesize the two improvements using both a random balance design and reordering. In this way, FAST can be a general first-order global sensitivity analysis method for linear/nonlinear models with as many correlated/uncorrelated parameters as the user specifies.

Section 2.1 is a brief review of the traditional FAST method. We introduce the improvement to overcome the independence limitation in Section 2.2 and the improvement to overcome the aliasing effect limitation in Section 2.3. In Section 2.4, we propose to synthesize the two improvements described in Sections 2.2 and 2.3. We introduce a general rule to select the maximum harmonic order for the synthesized method in Section 2.5 and provide a detailed procedure for the proposed method in Section 2.6. Then, we provide four test cases in Section 3. In Section 4, we discuss the random error effect which is introduced by the random balance design and compare our proposed method with other sensitivity analysis methods for models with correlated parameters. Finally, we summarize the main contribution of this paper in Section 5.

2. Method

2.1. Review of FAST

The main idea of FAST is to introduce for all parameters a search function with a characteristic integer frequency. Through the search functions, the model output becomes a periodic function. Fourier analysis is then performed on the model outputs to derive the Fourier spectrum. Finally, the first-order sensitivity index of each parameter is derived from the Fourier spectrum based on the characteristic frequency.

We consider a computer model $Y = f(x_1, x_2, \dots, x_n)$, where n is the number of independent parameters and the

domain of independent parameters is the hypercube

$$\Omega_n = (X | x_i^{(\text{Min})} < x_i < x_i^{(\text{Max})}; i = 1, \dots, n), \quad (1)$$

where $x_i^{(\text{Min})}$ and $x_i^{(\text{Max})}$ is the minimum and maximum value for x_i . In FAST, a search function is introduced for each parameter to explore the space Ω_n :

$$x_i = F_i^{-1} \left(\frac{1}{2} + \frac{1}{\pi} \arcsin(\sin(\omega_i s)) \right), \quad -\pi \leq s \leq \pi, \quad (2)$$

where ω_i is the characteristic frequency for x_i and F_i^{-1} is the inverse cumulative distribution function (ICDF) for x_i [34]. s is the common variable for all parameters. The search function aims to sample the parameter space according to an expected probability density function and lets the parameter x_i to oscillate periodically at the corresponding frequency ω_i . Consequently the model output is a periodic function of s . If the ω_i 's are positive integers, the period T is 2π [15]. Thus, we can expand the model output with a Fourier series

$$\begin{aligned} Y &= f(x_1, x_2, \dots, x_n) \\ &= f(s) = A_0 + \sum_{k=1}^{+\infty} \{A_k \cos(ks) + B_k \sin(ks)\}, \end{aligned} \quad (3)$$

where the Fourier coefficients A_k and B_k are defined as

$$\begin{aligned} A_0 &= \frac{1}{2\pi} \int_{-\pi}^{\pi} f(s) ds, \\ A_k &= \frac{1}{\pi} \int_{-\pi}^{\pi} f(s) \cos(ks) ds, \\ B_k &= \frac{1}{\pi} \int_{-\pi}^{\pi} f(s) \sin(ks) ds, \end{aligned} \quad (4)$$

where $k \in Z = \{1, \dots, +\infty\}$.

For real problems, we need to use discrete sampling to get the Fourier coefficients of Eq. (4). We denote the sample for s as

$$S = \{s_1, s_2, \dots, s_j, \dots, s_N\}, \quad (5)$$

where $s_j = -\pi + \pi/N + (2\pi/N)(j - 1), \forall j = 1, 2, \dots, N$. The search function of Eq. (2) is then applied to each sample element from S to get the sampled values for each parameter:

$$\mathfrak{N}_i = \{x_{i1}, x_{i2}, \dots, x_{ij}, \dots, x_{iN}\}, \quad (6)$$

where $x_{ij} = F_i^{-1}(\frac{1}{2} + (1/\pi) \arcsin(\sin(\omega_i s_j)))$. Then the model is run N times on sample values for each parameter. Finally, through the sample S , the discretized Fourier coefficients can be calculated as follows:

$$\begin{aligned} A_0 &= \frac{1}{N} \sum_{j=1}^N f(s_j), \\ A_k &= \frac{2}{N} \sum_{j=1}^N f(s_j) \cos(s_j k), \\ B_k &= \frac{2}{N} \sum_{j=1}^N f(s_j) \sin(s_j k), \end{aligned} \quad (7)$$

where A_0 is equal to the sample mean of Y .

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