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A Bayesian Monte Carlo-based method for efficient computation of global sensitivity indices

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Global sensitivity analysis, such as Sobol' indices, plays an important role for quantifying the relative importance of random inputs to the response of complex model, and the estimation of Sobol' indices is a challenging problem. In this paper, Bayesian Monte Carlo method is employed for developing a new technique to estimate the Sobol' indices with low computational cost. In the developing technique, the output response is expanded as the sum of different order components accurately, then the posterior predictors of all order components are analytically derived by use of the Bayesian inference, on which an analytical predictor of Sobol' index can be derived conveniently for input following any arbitrary distributions. In all analytical derivations, only the hyperparameters which are used to obtain a posterior predictor of output need to be estimated by the input-output samples, and the number of the hyperparameters grows linearly with the dimension of the input, thus the efficiency of the newly developing method is very high. The advantages of the proposed method are demonstrated through applications to several examples. The results show that the newly developing technique is comparable to the sparse polynomial chaos expansion and Quasi-Monte Carlo method.

1. Introduction

Since the early work of Sobol [1], sensitivity analysis has received a lot of attention in the computer code experiments community. Sensitivity analysis is a valuable tool in model calibration, development, and validation, since it can be used to identify how a model can be improved by obtaining more input information. In general, there are two types for sensitivity analysis. One is the local sensitivity analysis, local sensitivity analysis is often carried out in the form of derivative of the model output with respect to the input parameters. The other is global sensitivity analysis (GSA), GSA explores the whole space of the input factors, thus it is more informative and robust than the local sensitivity analysis (LSA). Several kinds of GSA techniques also known as importance measures have been proposed by researchers for different purposes [2–6].

The Sobol' variance-based GSA is a powerful and versatile approach, and it can be also applicable to nonlinear and non-monotonic models [7]. Thus, we concern this GSA in this paper. The main idea of variance-based GSA is to evaluate the variance contribution components from all of the individual or groups of input variables. Sobol made a breakthrough by deriving a first-order sensitivity index and decomposing a performance function into a sum of terms with increasing dimensionality [1]. Furthermore, Homma and Saltelli introduced the total sensitivity index [8] and discussed its properties as well. The variance-based GSA depends on the assumption that the variance is sufficient to describe output uncertainty. Distribution based sensitivity indices [3,6,9] and their solutions were proposed to measure the effect of selected input on the probability

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density function (PDF) or the cumulative distribution function (CDF) of the response. However, distribution based indices are relatively less easy to implement than variance based ones, mainly because their computation requires the knowledge of many conditional PDFs and CDFs, and distribution estimation suffers from the curse of dimensionality [5,10].

The estimation of the Sobol' variance-based sensitivity indices requires solving multidimensional integrals over the input space. Thus, standard numerical integration methods, e.g., multidimensional quadrature and Quasi Monte Carlo (QMC) simulation are difficult to be directly applied because of the high computational burden. This problem has been tackled by various surrogate modeling methods. Sudret et al. [11–14] estimated the Sobol' indices using polynomial chaos expansion (PCE). PCE is used to approximate the variance components needed for the calculation of sensitivity indices. Benefitting from the orthogonal polynomial basis, the Sobol' indices can be calculated directly by post-processing the coefficients of the PCE surrogate model. Cheng et al. [15] approximated the spatial model output using a proper orthogonal decomposition whose kernel functions are modeled by support vector regression; Furthermore, the high dimensional model representations (HDMR) [16] were developed to provide a straightforward approach based on orthogonal polynomial basis functions to explore the input-output behavior of high dimensional systems. HDMR needs a large number of samples to estimate the decomposition coefficients and is only used for compute first and second order Sobol' indices. Song et al. [17] proposed a modified group method of data handling-neural network algorithm to reduce the amount of computation cost in HDMR procedure for calculating Sobol' indices. In these surrogate model-based methods, PCE performs very well.

In this paper, in Bayesian Monte Carlo (BMC) framework [18], a novel method is developed to estimating Sobol' indices. The BMC was exploited successfully to the estimation of small failure probability in engineering practices [19]. The application was motivated by the strategy of transforming the integral evaluation to a Bayesian inference problem.

In the proposed BMC, a Gaussian process prior with squared exponential covariance function is assigned for model output, and the posterior of output can be inferred by combing some observations. In the Bayesian inference, the prior is taken to represent our prior beliefs over the kinds of target functions to be concerned before any data is given. In principle, Gaussian process with an exponential covariance may not be best choice of the prior. If sufficiently informative data are observed, the prior will be overwhelmed by the data and the posterior will be hardly influenced by the prior. Thus, posterior performances are not always sensitive to the prior [20].

By observing data and updating this prior, the posterior can be obtained. Gaussian process is not a parametric model. Thus, when the assumption of prior is Gaussian process, we do not have to worry about whether it is possible for the model to fit the data [21]. Another attraction of using Gaussian process with an exponential covariance function as a prior is that it makes posterior model of output smooth and stationary [21]. Thus, compared with GSA methods which employ the orthogonal polynomial as basis, the proposed method is more suitable for high non-linear problems.

The starting of our proposed approach is to approximate a computationally expensive output function by a fully Bayesian model. Then, the problem of estimating Sobol' indices using a limited number of output evaluations is transformed into a Bayesian inference problem. Compared with previous Gaussian process-based Sobol' indices estimation method [22], the appealing feature of the approach is that it has a closed-form analytical expression not only for main indices, but also for total indices. Thus, the computational efficiency of the proposed approach is quite high. Further, rather than restricting the distribution type of input to Gaussian [19], the proposed method generalizes BMC algorithm and is applicable to input following any distribution types.

The rest of this paper is organized as follows. Section 2 reviews the work of ANOVA-representation and Sobol' global sensitivity indices. Section 3 discusses the general procedure of a meta-model with BMC method where the derivation of the Sobol' indices is given in detail. In Section 4 we demonstrate the proposed method by application to a set of numerical and engineering modelling examples. Section 6 presents conclusions.

2. Global sensitivity analysis and Sobol' decomposition

Let consider a square integrable scalar response mode $Y = g(\boldsymbol{X})$ with n-dimensional independent input vector $\boldsymbol{X} = \{X_1, \dots, X_n\}$. The joint PDF of $\boldsymbol{X}$ is $f_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{i=1}^{n} f_{X_i}(\boldsymbol{x}_i)$, where $f_{X_i}(x_i)$ is the PDF of X_i. Then high dimensional model representation (HDMR) of $Y = g(\boldsymbol{x})$ has the following form [23]:

$$g(\boldsymbol{x}) = g_0 + \sum_{i=1}^{n} g_i(x_i) + \sum_{1 \leqslant i \leqslant j \leqslant n} g_{i,j}(x_i, x_j) + \dots + g_{1,\dots,n}(x_1, \dots, x_n) \tag{1}$$

where g_0 is the mean value of Y. And the components in Eq. (1) can be expressed as integrals of $g(\boldsymbol{x})$ as follows,

$$\begin{aligned}
g_i(x_i) &= \int g(\boldsymbol{x}) \prod_{j \neq i}^{n} \left(f_{X_j}(x_j) dx_j \right) - g_0 \\
g_{i,j}(x_i, x_j) &= \int g(\boldsymbol{x}) \prod_{k \neq i,j}^{n} \left(f_{X_k}(x_k) dx_k \right) - g_i(x_i) - g_j(x_j) - g_0 \\
&\cdots \\
g_{i_1,\dots,i_s}(x_{i_1}, \dots, x_{i_s}) &= \int g(\boldsymbol{x}) \prod_{j \neq i_1,\dots,i_s}^{n} \left(f_{X_j}(x_j) dx_j \right) - \sum_{k=1}^{s-1} \sum_{j_1,\dots,j_k \in (i_1,\dots,i_s)} g_{j_1,\dots,j_k}(x_{j_1}, \dots, x_{j_k}) - g_0
\end{aligned} \tag{2}$$