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Mixed kernel function support vector regression for global sensitivity analysis

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ABSTRACT

Global sensitivity analysis (GSA) plays an important role in exploring the respective effects of input variables on an assigned output response. Amongst the wide sensitivity analyses in literature, the Sobol indices have attracted much attention since they can provide accurate information for most models. In this paper, a mixed kernel function (MKF) based support vector regression (SVR) model is employed to evaluate the Sobol indices at low computational cost. By the proposed derivation, the estimation of the Sobol indices can be obtained by post-processing the coefficients of the SVR meta-model. The MKF is constituted by the orthogonal polynomials kernel function and Gaussian radial basis kernel function, thus the MKF possesses both the global characteristic advantage of the polynomials kernel function and the local characteristic advantage of the Gaussian radial basis kernel function. The proposed approach is suitable for high-dimensional and non-linear problems. Performance of the proposed approach is validated by various analytical functions and compared with the popular polynomial chaos expansion (PCE). Results demonstrate that the proposed approach is an efficient method for global sensitivity analysis.

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1. Introduction

As the complexity of modern models in physics, chemistry, economics, risk analysis and other areas keep increasing, the uncertainty of model structures and inputs is increasing rapidly. Dealing with uncertainty analysis (UA) has been recognized as an essential part of model application [1,2].

Sensitivity analysis (SA) has become a natural step in the UA framework in the past decades [3]. SA of a model aims at quantifying the relative importance of each input variable. Methods of SA are usually classified into two categories, i.e., the local SA [4] and the global SA [5,6]. Local SA is limited to examine effects of variations of the input variables in the vicinity of their nominal values [7]. Global sensitivity analysis (GSA) is also called uncertainty importance measure analysis [8]. It can provide more complete information by accounting for variations of the input variables in their entire domain, and then the priority level of the input variables can be determined in experiment or research. The ranking of the input variables resulting from the GSA can help designers to decide how to reduce the uncertain scope of response.

Over the last decade, GSA has gained considerable attention among practitioners, and many different global sensitivity analysis methods have been well developed. These methods include: nonparametric techniques [9]; variance-based sensitivity indices [10,11]; moment independent sensitivity indices [12], among which the Sobol variance-based sensitivity indices have a quite universal applicability because of their acknowledged features [13].

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The computation of the Sobol indices by the Monte Carlo or Quasi Monte Carlo simulation technique [14,15] usually leads to high computational burden. To reduce the computational cost, various surrogate-based methods have been proposed. Sudret [5] proposed to compute the Sobol indices by post-processing the coefficients of polynomial chaos expansion (PCE) meta-models. The key concept in PCE is to expand the model response onto a basis made of orthogonal multivariate polynomials in the input variables. The computational cost associated with Sobol indices essentially reduces to that of estimating the PCE coefficients. Unfortunately, the number of the expansion coefficients increases exponentially with the increasing dimensionality of the input variables, namely, the PCE faces the so-called "curse of dimensionality". To handle this issue, some sparse representations of PCE have been studied in Refs. [6,16,17], where only a small number of significant basis functions are retained in the response PCE approximation. This sparse PCE has been proved to be superior to the classic full PCE for GSA [6].

In this paper, the support vector regression (SVR) technique is proposed to evaluate the Sobol indices. SVR is based on strictly justified statistical learning theory. It maps data from sampling space to a higher dimensional characteristic space by the kernel function and converts a nonlinear problem into linear divisible problem to get an optimum surrogate [18,19]. The most important part of SVR is the kernel function. There are two different groups of kernels: global kernels and local kernels [20,21]. Global kernels have stronger extrapolation ability and local kernels have stronger interpolation ability. Standard kernels that can simultaneously extrapolate and interpolate are to some degree inaccurate [20]. Thus, a mixed kernel function (MKF) is used to build the SVR meta-model in this paper. The MKF here consists of orthogonal polynomials kernel function and Gaussian radial basis kernel function (RBF), therefore it combines the advantages of both the polynomial kernel and the RBF kernel. To obtain a high performance meta-model by the MKF-SVR, the hyper-parameters of MKF-SVR model are determined by the chaotic particle swarm optimization (CPSO) algorithm [22–24]. After the meta-model is established by the MKF-SVR technique, the Sobol indices can be obtained analytically by post-processing the coefficients of MKF-SVR model and the detailed derivation is proposed in Section 4. As a classification and regression method where the underlying structural risk minimization inference rule is employed, MKF-SVR has excellent learning ability with a small amount of information and good capability of generalization over the complete data. Thus the proposed method could reduce the computational cost of the sensitivity analysis tremendously.

The remainder of the paper is organized as follows: the methodology of MKF-SVR and the CPSO algorithm are reviewed in Section 2. Section 3 gives a brief description of the Sobol decomposition algorithm for GSA. Section 4 deduces the Sobol indices based on the meta-model built by MKF-SVR. Several numerical examples and engineering application are used to demonstrate the advantage of the proposed method in Section 5. The conclusion comes in Section 6.

2. Review on support vector regression

2.1. SVR network model

In the early 1990s, a support-vector machine (SVM) was developed based on statistical learning theory [25,26]. SVM can be divided into a class support-vector machine and a regression support vector machine. The former is primarily used for classification problem, and the latter is primarily used for parameter prediction, which is usually called as a support-vector machine for regression (SVR). SVM is known for its good generalization performance and its ability to handle nonlinear problems.

SVM uses the adaptive margin-based loss functions (Fig. 1c) and projects the learning data (linearly or non-linearly) into higher dimensional feature space (Fig. 1). It finds the best decision rule that has good generalization ability. The final SVR model takes the form:

$$Y = f(\boldsymbol{x}) = \sum_{i=1}^{N}(\alpha_i - \alpha_i^*)k(\boldsymbol{x}_i, \boldsymbol{x}) + b = \sum_{i=1}^{N} w_i k(\boldsymbol{x}_i, \boldsymbol{x}) + b \tag{1}$$

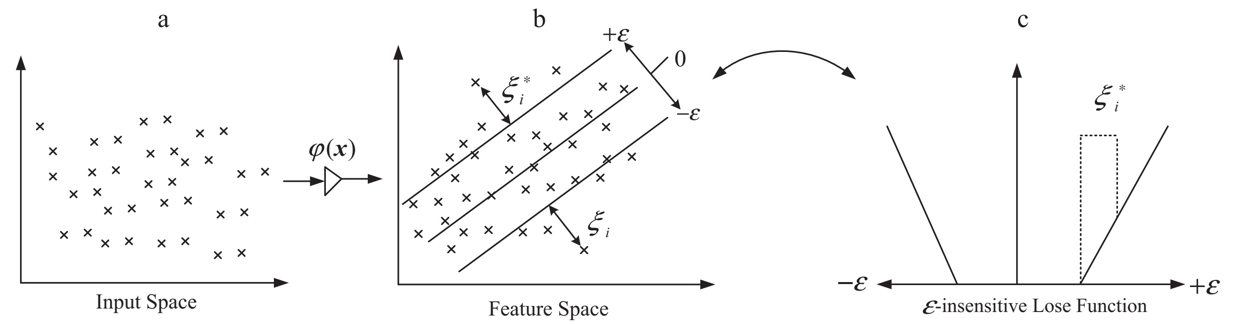

Fig. 1. Transformation process illustration of a SVR model. A nonlinear mapping function $\varphi(\boldsymbol{x})$ defined to convert a nonlinear problem in the original (low dimensional) data input space (a) to linear problem in a (higher dimensional) feature space (b). The points lying on or outside the ε-tube of the decision function are support vectors; (c) the ε-insensitive loss function is shown in which the slope is determined by C.

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