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A novel sequential exploration-exploitation sampling strategy for global metamodeling

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Abstract: Sampling strategy has direct impact on the accuracy of metamodel. In this paper,we propose a novel sequential exploration-exploitation sampling strategy for global metamodeling. A new criterion is proposed to focus on characteristic of output space. Space-filling requirement is treated as a constraint to avoid clustered sample points. The methodology developed in this paper is compared to existing methods using an analytic numerical case with two inputs. The results indicate that the proposed approach achieves the more desired accuracy of metamodel than the other approaches.

Keywords: metamodeling; optimal experiment design; sampling strategy; metamodel accuracy; characteristic of output space

1. INTRODUCTION

Simulation models have been widely used in engineering design of complex real world system (Myers et al. 2009). It may cause expensive computational cost directly using these simulation models for real system (Eason and Cremaschi 2014). To solve this problem, designers often use metamodels to replace simulation models. An important problem is how to build a high accurate metamodel with less number of sample points. In general, the sampling strategy has direct impact on the accuracy of metamodels.

A typical sampling strategy generate all sample points at one time, that is called one-stage approach. The existing one-stage method, such as Latin hypercube design (LHD) (Sudjianto et al. 1998), optimal Latin hypercube design (OLHD) (McKay et al. 2000) and orthogonal array (Zhang 2011), etc. only consider design space to make sample points distributed uniformly in the whole design space. The main disadvantage of one-stage approach is that too many sample points may have been evaluated to achieve the desired accuracy (oversampling) or too little sample points may have been evaluated (undersampling), in which case designer must completely restart the experiment to improve the initial design.

Another type of sampling strategy is called sequential sampling. The strategy select one or several points at one time until the accuracy of the metamodel or the total number of sample points achieve to the expected value. The most important issue in a sequential sampling strategy is how to choose a new sample point. Some sequential sampling approaches such as maximin distance approach (Johnson et al. 1990) only considers the distribution of sample points in design space. Some approaches such as Leave-one-out Cross-validation only focus on characteristics of output space. In general, there are smooth region and region where response values change sharply. Li et al. (2010) put forward a sequential sampling strategy to combine both the characteristics of the input space and output space, but it is difficult to determine the correlation coefficient. Yang et al. (2014) select new sample points based on a weighted sum of characteristics of input space and output space. However, this method is only suitable for Kriging model. Meanwhile, selection of the value of weighted factor is subjective.

In this paper, a new sampling strategy for global metamodeling using weighted accumulative error (WAE) is proposed. The proposed approach focus on characteristic of output space to make sample points distribute more reasonable. Meanwhile the input space-filling is considered in the selection process of sample points.

This paper is organized as the following. Section 2 gives the technical background of our study. The proposed WAE approach is introduced in details in section 3. After that, A numerical example is tested in section 4 to illustrate the proposed approach step by step.

2. TECHNICAL BACKGROUND

2.1 Kriging Method

Kriging metamodels is an interpolative Bayesian metamodeling technique. It was originated from geo-statistical and used by Sacks et al. (1989) for predicting the unknown response at sample points. Kriging treats the

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observed response as a combination of a global model and local deviations:

$$y(x) = f(x) + z(x) \tag{1}$$

where $y(x)$ is an unknown function of interest, $f(x)$ is an known approximation function, and $z(x)$ is the realization of a stochastic process with mean zero and nonzero covariance.

2.2 Optimal Latin Hypercube Design

Consider sample m points in a n-dimension space, LHD divide each dimension into m intervals uniformly. These levels are randomly combined to generate a $m \times n$ matrix that is called random Latin hypercube (each level of a dimension appears only once). OLHD swap the order of two levels in a column of the matrix to make the points spread as uniform as possible. In this paper, OLHD proposed by McKay et al. 2000 is used to generate initial sample set for the sequential sampling approach.

2.3 Characteristics of Output Space

A one-dimensional function is used to illustrate the characteristics of output space. The range of input variable is [-8 8]. The Characteristic of output space is shown in Fig. 1. It can be seen in Fig. 1 that the function values change sharply in the range [-3 3] but is smooth in the other ranges. The highly nonlinear region is marked with dotted box. In order to obtain a metamodel with high accuracy, It should select more sample points in highly nonlinear region but less in smooth region .

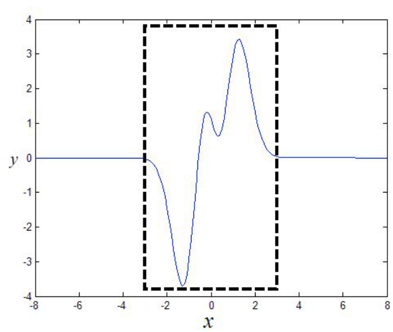

Fig. 1 The highly nonlinear region and the smooth region

3. PROPOSED APPROACH

3.1 Leave-one-out Cross-validation Error

leave-one-out cross-validation error (Li et al. 2010; Meckesheimer et al. 2002) is often used to metamodel accuracy evaluation.The advantage of this approach is that no new sample points are needed in order to save computational cost. The approach begins by leaving out an sample point from a existing sample set **D** and build a metamodel with the rest of the sample points in **D**. Then, metamodel was used to predict the response value of the sample point leaved out. Finally, it calculates the error between predicted value and the real response value. The error is called leave-one-out (LOO) error. The LOO error for x_i ($e_{LOO}^{x_i}$) can be expressed as :

$$e_{LOO}^{x_i} = \left| \hat{y}_{-i}(x_i) - y(x_i) \right| \tag{2}$$

Where $y(x_i)$ is real response of point x_i ; $\hat{y}_{-i}(x_i)$ is the predicted response of point x_i using metamodel built with remain points in **D**. Leave-one-out cross-validation error is used to predict the error of a new point (Jin et al. 2002). The error on x is predicted by average LOO error:

$$e(x) = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\hat{y}_{-i}(x) - \hat{y}(x))^2} \tag{3}$$

Where $\hat{y}(x)$ is the predicted response on x based on metamodel built with all points in **D**; $\hat{y}_{-i}(x)$ is the predicted response on x based on metamodel built with remain points in **D** (with point x_i leaved out). A point with maximum average LOO error $e(x)$ was chosen to be the new points.

3.2 WAE Approach

In the LOO approach, a point with maximum average LOO error is chosen as the new sample points. But the new point tend to be close to an existing point in some cases, this can lead to an accumulation of sample points. Another point is that when we select a new point using LOO approach, existing points have equal influence on the prediction error of x . This can be known from Eq.(3). In fact,the point closer to x has a larger influence on the prediction error of x than the point which is farther to x .

3.2.1 Criterion of Selecting New sample Point

The proposed WAE approach is based on leave-one-out cross-validation prediction error and a single-objective optimization problem. The prediction error of WAE approach can be expressed as:

$$e_{WAE}(x) = \sqrt{\sum_{i=1}^{n} \mathrm{w}_i (\hat{y}_{-i}(x) - \hat{y}(x))^2} \tag{4}$$

Where the definition of $\hat{y}_{-i}(x)$ and $\hat{y}(x)$ are the same as that in Eq.(3). w_i (i=1,2,...,n) are the weight of each error.The value of w_i reflects the influence of different sample points on the error on x . The value of w_i is lager when point x_i is closer to x . We define the weight w_i as:

$$w_i = \exp(-\|x - x_i\|) / \sum_{i=1}^{n} \exp(-\|x - x_i\|) \tag{5}$$

From Eq.(5), we can see that the value of w_i only related to the distance between x and other sample points. The closer x is to x_i , the lager the value of w_i is, and $\sum_{i=1}^{n} w_i = 1$. Consider the phenomenon of clustering, WAE approach