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A Novel Method for Ensemble of Surrogates Based on Global and Local Measures

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Abstract: Surrogate models are widely used in the community of engineering design and optimization to substitute computationally expensive simulations for efficient approximation of system behaviors. However, since the actual system behaviors are usually not known a priori, it is very challenging to select the most appropriate surrogate model for a specific application.To deal with this issue, an ensemble model that combines different surrogate models has been presented, and many efforts are devoted to the weight factor selection for the component surrogate models based on global measure and local measure respectively. In this paper, a novel ensemble of surrogate models is developed to take advantage of both global and local measures, and a unified strategy is conceived over the entire design space with proper tradeoff between these two measures. The effectiveness of the new ensemble model is tested on six mathematical benchmark examples with varying dimensionality. The results show that the proposed ensemble model has more desirable accuracy and robustness for a majority of test problems compared with the individual surrogate models and other ensemble models.

Keywords: Surrogate model, Metamodel, Ensemble, Global measure, Local measure.

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I. INTRODUCTION

High-fidelity computer simulations such as finite element analysis play an important role in the design and optimization of complex engineering systems.Despite the rapid development of computing technology, the need of getting more accurate and reliable simulation results with ever-increasing complexity of numerical models still makes engineering system analysis time-consuming. Hence, surrogate models (also known as metamodels) are widely used as the replacement of computationally expensive high-fidelity simulations for efficient estimation of system characteristics. Commonly used surrogate models in the engineering design and optimization include polynomial response surface (PRS) (Myers and Montgomery 2002), radial basis functions (RBF) (Fang and Horstemeyer 2006; Liu et al. 2006), Kriging (KRG) (Martin and Simpson 2005), and support vector regression (SVR) (Clarke et al. 2005). However, owing to the different characteristics of practical engineering applications, it is very difficult, if not impossible, to know a priori which surrogate model is most desirable for an unknown problem. Therefore, an ensemble of surrogate models has been recently developed by combing multiple surrogates through a weighted form to take advantage of the prediction ability of each individual surrogate. The weight factor of each individual surrogate is determined by the model accuracy. According to the measures of evaluating the weight factors, existing ensemble modeling methods can be generally classified as global measures and local measures. The weight factors evaluated by global measures keep constant over the entire design space. Goel et al. (2007) used a global metric called generalized mean square cross-validation error (GMSE) to calculate the weight factors of individual surrogate models in the ensemble. Acar and Rais-Rohani (2009) proposed an ensemble of surrogate models in which the optimized weight factors were obtained by minimizing GMSE or root mean square error (RMSE). As for local measures, weight factors of the individual surrogate are determined at each sampling point respectively. Acar (2010) proposed a spatial ensemble of surrogates using pointwise cross validation error with various approaches. Zhang et al. (2012a) developed adaptive hybrid functions with weight factors of each contributing surrogate model determined locally in a pertinent trust region. Liu et al. (2016) presented an optimal weighted pointwise ensemble by combining the RBF models of different basis functions. To make use of advantages of both global and local measures, Chen et al. (2018) proposed an ensemble model which hybridized a global measure and a local measure. However in this method, the design space has to be pre-divided into outer and inner regions as per each sample point, and different strategies for evaluating the weight factors are adopted accordingly. Motivated by the above analysis, this paper proposes a unified ensemble of surrogates (UES) based on the

integration of global and local measures. No division of the design space is needed, and a unified strategy is devised over the entire domain with the trade-off between global and local error metrics.

II. THE PROPOSED ENSEMBLE METHOD

The traditional technique of surrogate modeling is usually composed of constructing a number of different surrogates, selecting one with the best accuracy and discarding the rest candidates. Nevertheless, two major shortcomings exist. First, most of the resource spent on the construction of different surrogates is wasted. Second, the performances of different surrogates are dependent on the sample points, so there is no guarantee that the selected surrogate model will be accurate on a new data set. To overcome these drawbacks, an ensemble of surrogates rather than an individual one is proposed.An ensemble is a weighted average of several different surrogates. The resulting ensemble model is formulated as

$$\hat{y}_{ens}(x) = \sum_{i=1}^{N_s} w_i(x)\,\hat{y}_i(x) \tag{1}$$

where $\hat{y}_{ens}(x)$ is the prediction value of the ensemble, N_s is the number of surrogates used, and w_i is the weight factor for *i*th surrogate model $\hat{y}_i(x)$. The weight factors are calculated with the following requirement

$$\sum_{i=1}^{N_s} w_i(x) = 1 \tag{2}$$

To maximize the prediction accuracy of an ensemble, the weight factors are selected such that the component surrogate with higher accuracy will occupy a larger proportion in the ensemble model and vice versa. According to the measures of evaluating the weight factors, existing ensemble modeling methods can be generally classified as global measures and local measures.

Goel et al. (2007) proposed an ensemble of surrogates based on global measures in which GMSE was used to select the weight factors from a heuristic formulation

$$\begin{aligned} w_i &= \frac{w_i^*}{\sum_{j=1}^{N_s} w_j^*} \\ w_i^* &= (E_i + \alpha\bar{E})^{\beta} \\ \bar{E} &= \frac{1}{N_s}\sum_{i=1}^{N_s} E_i \end{aligned} \tag{3}$$

where E_i is the GMSE of the ith surrogate model evaluated from

$$E_i = \frac{1}{n}\sum_{k=1}^{n}\left(y(x_k) - \hat{y}_i^{(-k)}(x_k)\right)^2 \tag{4}$$

where *n* is the number of sample points, x_k is the *k*th sampling point, y(x_k) is the true response value at x_k, and $\hat{y}_i^{(-k)}(x_k)$ is the corresponding prediction value of the *i*th surrogate model constructed using all except the *k*th sampling point. two parameters α = 0.05 and β =−1 were recommended by Goel et al. (2007).

As an alternative to using prediction variance, Acar (2010) proposed a spatial model in which the pointwise cross validation error was selected as the localerror measure.

$$\begin{aligned} w_i &= \frac{w_i^*}{\sum_{j=1}^{N_s} w_j^*} \\ w_i^* &= \sum_{k=1}^{n} W_{ik}\, I_k(x) \\ I_k(x) &= \frac{1}{d_k^2(x)} \\ d_k(x) &= \|x - x_k\| \end{aligned} \tag{5}$$

where W_{ik} is the pointwise weight factor of the *i*th surrogate model at the *k*th sample point. The 0−1 weighting strategy is adopted: W_{ik} equals one for the surrogate model with the smallest cross validation error, and zero for all other individual surrogates. $I_k(x)$is the spatial location metric, $w_i^* = W_{ik}$ is used when $d_k(x) = 0$.

An ensemble of surrogates constructed solely with global measures or local measures both have pros and cons. Global measures are relatively straightforward, computationally inexpensive, and generally accurate from the global perspective of view, but they may not reflectthe diversity of each component surrogate. On the other hand, the ensemble model by using local measures are more flexible but less robust, because local error fluctuation may heavily deteriorate the model accuracy. In this paper, global measuredeveloped by Goel et

al.(2007) and local measureproposed by Acar (2010) are integrated for ensemble modeling with a unified formulation over the entire design space. Taking advantage of multiple kinds of error metrics, the accuracy and robustness of the proposed unified ensemble of surrogates (UES) are enhanced with modeling efficiency nearly the same with other ensemble of surrogates.

To evaluate the accuracy of an ensemble surrogate, the commonly used error measures are cross-validation error, prediction variance and mean square error (or root mean square error) (Zhou et al. 2011). As no additional test (validation) points are required for error evaluation, the cross-validation error is selected to construct the UES model in this article. Cross-validation error, also known as leave-one-out cross-validation error, is the prediction error at each sample point while the surrogate model is built with the other (n−1) sample points. For ensemble modeling, the cross-validation error of the *i*th surrogate at the *k*th sample point is formulated as

$$e_{ik} = y(x_k) - \hat{y}_i^{(-k)}(x_k) \tag{6}$$

To have a fair comparison and to reduce the computational cost as well, the same error matrix is adopted to construct all ensemble surrogates. And the weight factors can be obtained as follows

$$\begin{cases} \mathcal{L}^G(e^{CV}) \Rightarrow w^G \\ \mathcal{L}^L(e^{CV}) \Rightarrow w^L \end{cases} \tag{7}$$

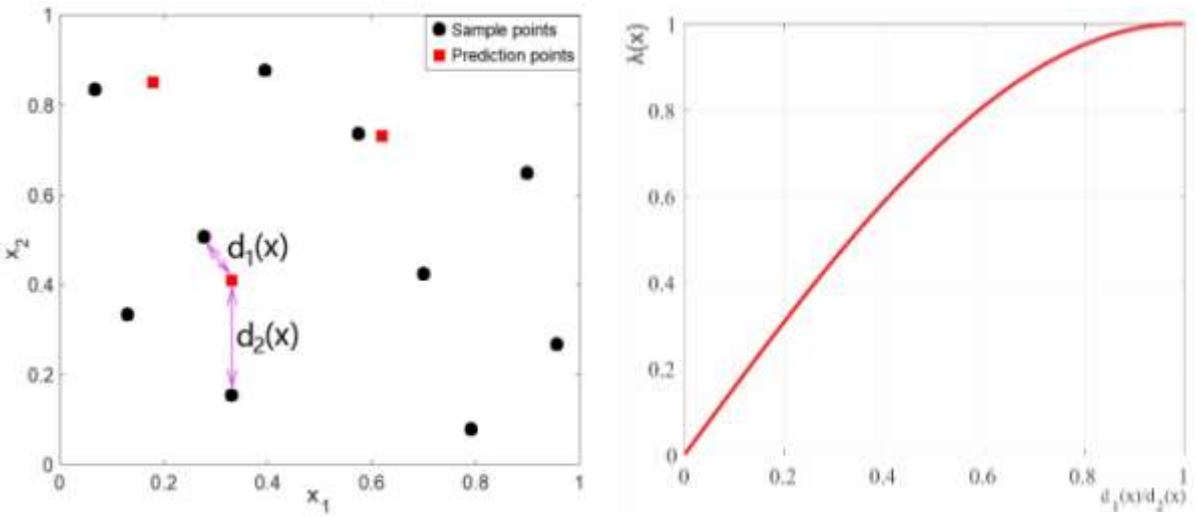
where e^{CV} denotes the error matrix computed from cross-validation error, $\mathcal{L}^G(.)$ and $\mathcal{L}^L(.)$ represent the strategies of calculating the weight factor by using global measure (w^G, named global weight factor) and the weight factor by using local measure (w^L, named local weight factor) respectively.

Global measures evaluate the weight factors of individual surrogates with an overall model accuracy from the entire error matrix. Local measures regard weight factors as the diversity indicator of component surrogates at different locations in the design space, so the weight factors at a prediction point are severely affected by the adjacent sample points. Therefore, local measures dominate in the evaluation of weight factors when the prediction point is near to the sample points, while global measures are more suitable for prediction points far from the sample points. To this end, a unifiedensemble of surrogates (UES) with global measure and local measure is proposed to define the weight factors for the entire design space as:

$$\begin{aligned} w_i &= \frac{w_i^*}{\sum_{j=1}^{N_s} w_j^*} \\ w_i^* &= w_i^G \lambda(x) + w_i^L \big(1 - \lambda(x)\big) \end{aligned} \tag{8}$$

where w_i^G and w_i^L are respectively global weight factor and local weight factor for the *i*th surrogate model. $\lambda(x)$ is the coefficient of measure impact to control the influence regions of global and local measures on calculating the weight factors at the prediction point *x*.the coefficient $\lambda(x)$ must satisfy the following conditions:`

$$\begin{aligned} &\lim_{d_1(x)\to 0} \lambda(x) = 0 \\ &\lim_{d_1(x)\to d_2(x)} \lambda(x) = 1 \end{aligned} \tag{9}$$



(a) (b)

Figure 1:(a)A 2D illustration of sample and prediction points for deriving the coefficient of measure impact; (b)Coefficient function λ(x);

where, as shown in Figure.1(a), $d_1(x)$ is the distance between the prediction point x and its nearest sample point, $d_2(x)$ is the distance between x and its second-nearest sample point. In this study, the Sine function, as shown in Figure.1(b), were selected as candidate coefficient functions.

$$\lambda(x) = \sin\left\{\frac{\pi}{2}\left(\frac{d_1(x)}{d_2(x)}\right)\right\} \tag{10}$$

III. EXAMPLE PROBLEMS

Six well-known mathematical benchmark problems varying from 2-D to 12-D are chosen to test the characteristics of the UES models: (1) Branin-Hoo function (2-D); (2) and (3) are Hartman functions (3-D and 6-D, denoted as Hartman-3 and Hartman-6 respectively); (4) Dette and Pepelyshev function (8-D); (5) Griewank function (8-D) and (6) Dixon-Price function (12-D). Detailed information on these functions can be found in Table1.

Table 1: Summary of benchmark problems

Function	Dimension	Formulation	Definition domain
(1)	2	$f(x) = \left(x_2 - \frac{5.1x_1^2}{4\pi^2} + \frac{5x_1}{\pi} - 6\right)^2 + 10\left(1 - \frac{1}{8\pi}\right)\cos x_1 + 10$	[-5,10; 0,15]^D
(2)	3	$f(x) = -\sum_{i=1}^{4} c_i exp\left[-\sum_{i=1}^{3} a_{ij}\left(x_j - p_{ij}\right)^2\right]$	$[0,1]^D$
(3)	6	$f(x) = -\sum_{i=1}^{4} c_i exp\left[-\sum_{i=1}^{6} a_{ij}\left(x_j - p_{ij}\right)^2\right]$	$[0,1]^D$
(4)	8	$f(x) = 4(x_1 - 2 + 8x_2 - 8x_2^2) + (3 - 4x_2^2)^2$ $+16\sqrt{(x_3+1)}(2x_3-1)^2 + \sum_{i=4}^{8} iln(1+x_i)$	$[0,1]^D$
(5)	8	$f(x) = \frac{1}{4000}\sum_{i=1}^{8} x_i^2 - \prod_{i=1}^{8}\cos\left(\frac{x_i}{\sqrt{i}}\right) + 1$	$[0,1]^D$
(6)	12	$f(x) = (x_1 - 1)^2 + \sum_{i=2}^{12} i(2x_i^2 - x_{i-1})^2$	$[0,10]^D$

For the design of experiments (DOE) of all benchmark problems, Latin hypercube sampling (LHS) technique is employed to select the locations of the training and test points. Table 2 presents the summary of training sets, sample points and test points for all benchmark problems.

Table 2: Summary of the training and test point sets used in the benchmark problems

Function	Dimension	Training sets	Sample points	Test points
(1)	2	1000	12	1000
(2)	3	500	20	1000
(3)	6	100	56	1000
(4)	8	30	90	1000
(5)	8	30	90	1000
(6)	12	15	182	1000

To have an exhaustive study on the proposed UES models, and also to make a comprehensive comparison with the existing ensemble models, two kinds of error metrics are selected: Coefficient of determination R^2, Normalised Maximum Absolute Error (NMAE).

$$R^2 = 1 - \frac{\sum_{i=1}^{N_{test}} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{N_{test}} (y_i - \bar{y})^2}$$

$$NMAE = max|y_i - \hat{y}_i| \Big/ \sqrt{\frac{1}{N_{test}} \sum_{i=1}^{N_{test}} (y_i - \hat{y}_i)^2} \quad (11)$$

Where N_{test} is the number of test points, std denotes the standard deviation of samples and mean is the mean value, $y_i$is the true value calculated by the benchmark functions, $\hat{y}_i$is the corresponding prediction value of the surrogate model and $\bar{y}$is the meanvalue of y_i.The value of R^2 iscloser to 1 and the value of $NMAE$ iscloser to 0, the closer the predictionsurrogate model is to the real benchmark function.

The accuracy and robustness of the UES models are compared with two existing ensemble models, namely: (i) the heuristic algorithm developed by Goel et al. (2007) (labeled by EG), (ii) the spatial model proposed by Acar (2010) (labeled by SP). Three representative surrogate models, polynomial response surface (PRS), radial basis functions (RBF), Kriging (KRG), are used as the component surrogates for all ensemble models and are also compared with the ensemble models. The results are shown in the following figure.

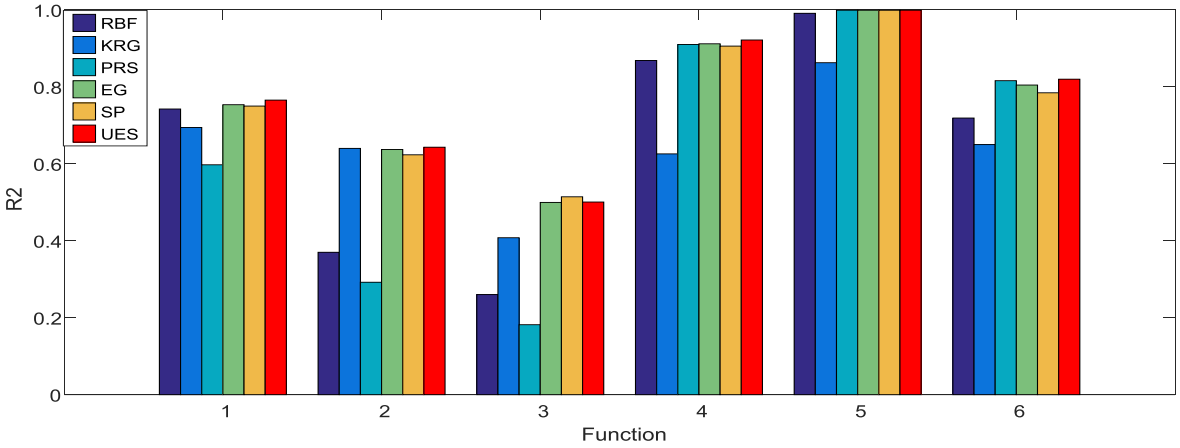


Figure 2:$R^2$of ensemble and individual surrogate models

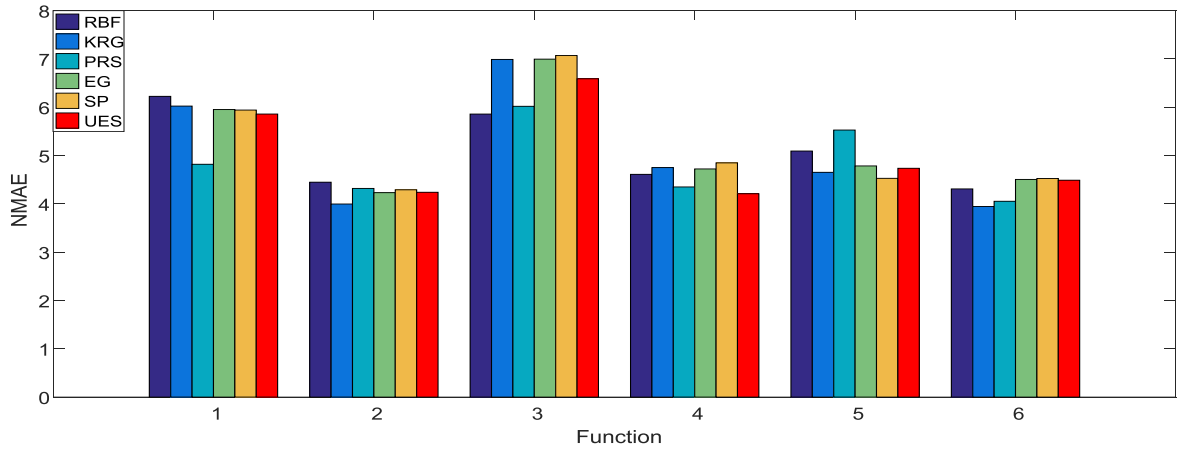


Figure 3:NMAE of ensemble and individual surrogate models

IV. CONCLUSION

It can be found fromfigure 2-3 that no individual surrogate model has always the best accuracy for all the benchmark functions. According to the test results, PRS is relatively better for high-dimensional (8-Dand 12-D) problems while KRG and RBF are more accurate for low-dimensional (2-D, 3-D and 6-D) examples. However in most scenarios, most of the ensemble methods perform better than the individual surrogatemodels. The proposed UES models surpass almost all of the individual surrogate models and other ensemble models in the vast majority of error metrics for all benchmark examples. In the future, we will focus on investigating more

individual surrogate models and selecting the appropriate baseline models to be included for the UES ensemble model.

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