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Radial basis functions with a priori bias as surrogate models: A comparative study

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ABSTRACT

Radial basis functions are augmented with a posteriori bias in order to perform robustly when used as metamodels. Recently, it has been proposed that the bias can simply be set a priori by using the normal equation, i.e., the bias becomes the corresponding regression model. In this study, we demonstrate the performance of the suggested approach (RBF_{pri}) with four other well-known metamodeling methods; Kriging, support vector regression, neural network and multivariate adaptive regression. The performance of the five methods is investigated by a comparative study, using 19 mathematical test functions, with five different degrees of dimensionality and sampling size for each function. The performance is evaluated by root mean squared error representing the accuracy, rank error representing the suitability of metamodels when coupled with evolutionary optimization algorithms, training time representing the efficiency and variation of root mean squared error representing the robustness. Furthermore, a rigorous statistical analysis of performance metrics is performed. The results show that the proposed radial basis function with a priori bias achieved the best performance in most of the experiments in terms of all three metrics. When considering the statistical analysis results, the proposed approach again behaved the best, while Kriging was relatively as accurate and support vector regression was almost as fast as RBF_{pri}. The proposed RBF is proven to be the most suitable method in predicting the ranking among pairs of solutions utilized in evolutionary algorithms. Finally, the comparison study is carried out on a real-world engineering optimization problem.

1. Introduction

Nowadays, the role of simulation codes and software is inevitably crucial in the initial stages of product design, to analyze the design alternatives, especially in multidisciplinary design optimization (MDO). A designer can create an optimized design with respect to multiple objectives and several input variables, without creating a physical prototype. This will reduce the cost of the product development phase which leads to designing products with higher efficiency and performance. However, the computational cost of the complex and high fidelity computer simulations is a drawback in simulation-based design optimization. Although the computational power increases exponentially, the complexity and accuracy of simulations and the related software is expanding proportionately. One strategy is to approximate the complex and expensive simulations with fast and accurate models often called surrogate models or metamodels. In addition to predicting the response of a computationally expensive simulation-based model, metamodels develop a relation between the input variables and their corresponding responses.

Many metamodeling methods have been developed for metamodel-based design optimization problems. Response surface methodology (RSM) or polynomial regression (Box and Wilson, 1951), Kriging (KG) (Sacks et al., 1989), radial basis functions (RBF) (Hardy, 1971), support vector regression (SVR) (Vapnik et al., 1996) and neural networks (NN) (Haykin, 1998) are some of the most well-known and extensively studied methods. Several studies (Forrester and Keane, 2009; Simpson et al., 2001a, b; Wang and Shan, 2007) reviewed different metamodeling methods and their applications. Several studies comparing various surrogate models, in terms of accuracy, robustness, efficiency and effectiveness, can be found in the literature. However, in reviewing all the literature, one can conclude that there is no proof of obvious dominance of one particular method over other techniques, with regards to all the performance criteria.

A systematic comparison study of polynomial regression, KG, multivariate adaptive regression splines (MARS) and RBF under different modeling criteria was initiated by Jin et al. (2001) on a set of 14 mathematical and engineering test problems. They considered three modeling criteria, i.e., nonlinearity of problem (low and high), sample

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size (scarce, small and large), noise behavior (smooth and noisy), and five evaluation measures, i.e., accuracy, robustness, efficiency, transparency and conceptual simplicity. The results concluded that RBF performance excelled in both large and small scale problems with a high order of nonlinearity. Mullur and Messac (2006), compared their proposed metamodeling method, extended radial basis function (E-RBF), with three other approaches; RSM, RBF and KG. A number of modeling criteria including problem dimension (low and high), sampling technique (Latin hypercube, Hammersely, and Random) and sample size (low, medium and high) were considered. They employed the accuracy as the performance metric to identify the E-RBF as the superior method, since the parameter setting was not needed in their proposed method. Kim et al. (2009) performed a comparative study of four metamodeling techniques, i.e., moving least square (MLS), KG, RBF and SVR, using six mathematical functions, one modeling criterion i.e., problem dimension, and one evaluation criterion, i.e., accuracy. Kriging and MLS showed promising results in that study. In a research study (Zhao and Xue, 2010), quantitative measures considering accuracy, confidence, robustness and efficiency were employed to compare multivariate polynomial, RBF, KG and Bayesian NN. They also included three sample merits which influence the metamodeling performance, such as sample size, uniformity and noise, in their study. Another systematic comparison study by Li et al. (2010) analyzed the strengths and weaknesses of NN, RBF, SVR, KG, and MARS, in terms of three quantitative metrics, namely, accuracy, robustness and efficiency, and three qualitative measures including software availability, parameter tuning and interpretation of the model. The study was based on four deterministic mathematical simulation problems. The results concluded that SVR was the most accurate and robust method. Backlund et al. (2012) studied the scalability of RBF, KG and SVR by applying them on three distinct test functions, i.e., kernel density function, Rosenbrock, and modified Rosenbrock test function, with the dimension ranging from 15 to 50 independent variables. Kriging appeared to be the dominant method in its ability to approximate accurately with fewer or an equivalent number of training points. Furthermore, in Kriging parameter setting was done automatically during the training process. RBF was found to be the slowest in building the model with a large number of training points, while SVR was the fastest in large scale multi-modal problems. Han and Zheng (2012) compared RSM, MARS, RBF, Kriging and SVR, in terms of robustness, as well as global and local accuracy. They included several modeling criteria, such as complexity and nonlinearity of problems and as well as scale and distribution of samples. Recently, a study (Bandaru and Ng, 2015) compared ten different metamodels, with respect to their accuracy and training time, by using a simple stochastic simulation model. They considered two modeling criteria, i.e., sample size and number of variables (problem dimension). RBF and elastic net were the most accurate in predicting the response. However, RBF, elastic net, random forest and boosted tree ensemble were the best choices in using the metamodels in evolutionary algorithm optimization methods. Díaz-Manríquez et al. (2017) compared four metamodeling techniques: polynomial RSM, KG, RBF, and SVR by utilizing six scalable test functions to evaluate their suitability for optimization algorithms and low budget of computational time. They found RBF and SVR the most efficient approach and selected RBF as the most robust and scalable approach.

Recently, an approach for generating RBF with the bias known a priori (RBF_{pri}) adjacent to the classic augmented RBF with the bias known a posteriori (the RBF studied in several literature papers) has been proposed (Amouzgar and Strömberg, 2016). A detailed and comprehensive comparison study on the performance of the proposed RBF_{pri} with the classical augmented RBF (RBF with a posteriori bias, RBF_{pos}) has also been conducted (Amouzgar and Strömberg, 2016; Amouzgar et al., 2015). The factors that are present during the construction of a metamodel (modeling criteria), including the dimension of the problem, the type of radial basis functions used in RBF, the sampling technique and sample size were considered, and their effects were explored. The results demonstrated the promising potentials of RBF with a priori bias, in addition to the simplicity and straightforward use of the approach. Furthermore, the proposed method was applied on an engineering application, i.e., multi-objective optimization of a disk brake system (Amouzgar et al., 2013). However, there is no evidence that the RBF_{pri} has advantages over other metamodeling methods. Thus, in this paper, we focus on investigating the performance of the proposed approach in comparison to other well-known techniques. Kriging, SVR, NN and MARS are the methods chosen for this purpose. In addition to the traditional accuracy and computational efficiency metrics, we put emphasis on the behavior of the methods when employed in evolutionary algorithms (EA) by using a ranking metric.

This paper is structured by defining the a priori RBF approach and the other four surrogate modeling methods in Section 2. Thereafter, in Section 3 the comparison procedure, including the employed test functions, replications and data sampling, parameter tuning as well as the performance metrics, are described. The results are presented in Section 4 by discussing the accuracy under dimension and sampling size. The overall accuracy, suitability of the methods when coupled with EA, computational efficiency and robustness are explained in the same section. Furthermore, a statistical analysis of the performance metrics is carried out in Section 4. This is followed by a comparison study on a real-world engineering optimization problem in Section 5. Finally, the conclusion of this study is summarized.

2. Metamodeling methods

In this section, the recently proposed RBF approach, and the other four methods are described. There are a number of parameters in each surrogate modeling method that requires to be predefined by the user. These parameters have a noticeable impact on the accuracy of each method. Hence, for the sake of a fair comparison the parameter setting procedure described in Section 3.3 is followed for all metamodeling methods.

2.1. Radial basis functions networks

Radial basis functions were first used by Hardy (1971) for multivariate data interpolation. He proposed RBFs as approximation functions by solving multi-quadratic equations of topography based on coordinate data with interpolation. A radial basis function network of ingoing variables x_i collected in $\boldsymbol{x}$ can be written as

$$f(\boldsymbol{x}) = \sum_{i=1}^{N_\Phi} \Phi_i(\boldsymbol{x})\alpha_i + b(\boldsymbol{x}), \tag{1}$$

where $f = f(\boldsymbol{x})$ is the outgoing response of the network, $\Phi_i = \Phi_i(\boldsymbol{x})$ represents the radial basis functions, N_Φ is the number of radial basis functions, α_i are weights and $b = b(\boldsymbol{x})$ is a bias. The number of radial basis functions is set equal to the number of ingoing variables.

Examples of popular radial basis functions are

$$\begin{aligned} \text{Linear:}\quad & \Phi_i(r) = r, \\ \text{Cubic:}\quad & \Phi_i(r) = r^3, \\ \text{Gaussian:}\quad & \Phi_i(r) = e^{-\eta_i r^2}, \\ \text{Quadratic:}\quad & \Phi_i(r) = \sqrt{r^2 + \eta_i^2}, \end{aligned} \tag{2}$$

where η_i represents the shape parameters and

$$r(\boldsymbol{x}) = \sqrt{(\boldsymbol{x} - \boldsymbol{c}_i)^T(\boldsymbol{x} - \boldsymbol{c}_i)} \tag{3}$$

is the radial distance. In physical interpretation, the shape parameters control the width of the radial basis functions. A radial basis function with a small value of η_i gives a narrower effect on the surrounding region. In other words, the nearby points of an unknown point will affect the prediction of the response on that point. In this case, the risk of overfitting will occur, which means the sample points will influence only on