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DRAFT: AN APPROACH TOWARDS GENERATING SURROGATE MODELS BY USING RBFN WITH A PRIORI BIAS

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ABSTRACT

In this paper, an approach to generate surrogate models constructed by radial basis function networks (RBFN) with a priori bias is presented. RBFN as a weighted combination of radial basis functions only, might become singular and no interpolation is found. The standard approach to avoid this is to add a polynomial bias, where the bias is defined by imposing orthogonality conditions between the weights of the radial basis functions and the polynomial basis functions. Here, in the proposed a priori approach, the regression coefficients of the polynomial bias are simply calculated by using the normal equation without any need of the extra orthogonality prerequisite. In addition to the simplicity of this approach, the method has also proven to predict the actual functions more accurately compared to the RBFN with a posteriori bias. Several test functions, including Rosenbrock, Branin-Hoo, Goldstein-Price functions and two mathematical functions (one large scale), are used to evaluate the performance of the proposed method by conducting a comparison study and error analysis between the RBFN with a priori and a posteriori known biases. Furthermore, the aforementioned approaches are applied to an engineering design problem, that is modeling of the material properties of a three phase spherical graphite iron (SGI) . The corresponding surrogate models are presented and compared.

1 INTRODUCTION

In result of increasing challenge of developing complex and successful products and the complexity of engineering applications, designer are attracted to simulation based designs. Designers are eager to predict the behaviour of their product before producing the cost expensive physical model, also creating an optimal product or system in sense of different objectives is a goal of every designer. Computer simulations will aid designers to fulfill the aforementioned requirements. However, simulation of physical systems are often computationally expensive, for instance in multidisciplinary design optimization (MDO) applications. The necessity of developing an inexpensive and accurate explicit function to represent the relation between input design variables and the corresponding responses in place of computer simulations which are often black boxes is essential. Therefore, metamodels or surrogates approaches are employed to substitute the original computationally expensive and complex computer simulations. The general concept of metamodeling is to obtain a global approximation function of a given set of data points and the corresponding responses, which adequately represents the original function over a defined design space.

Several metamodeling techniques have been reported in literatures; response surface methodology(RSM) or polynomial regression [1], kriging [2], radial basis function networks (RBFN) [3], support vector regression (SVR) [4] and neural networks [5].

Furthermore, a recent trend in developing metamodels which has begun to draw the attention of researchers is to combine different techniques in order to acquire the strength of each method, named as ensemble of metamodels or hybrid metamodeling. The comparative studies argue the superiority of the hybrid metamodeling over other individual techniques.

Despite the numerous studies investigating the accuracy and effectiveness of variouse surrogate models by performing comparison studies, there is no one joint belief in dominance of one method over others. Jin et al. [6], compared four different metamodeling technique: polynomial regression, kriging, multivariate adaptive regression splines and radial basis function networks using 14 mathematical and engineering test problems. They concluded that in overall RBFN performed the best for both large and small scale problems with high-order of non-linearity. Backlund et al. [7] studied the accuracy of RBFN, kriging and support vector regression with respect to their capability in approximating high-dimensional, non-linear and multi-modal functions. The conclusion of results can be summarized as kriging being the dominant method in its ability to approximate accurately with fewer or equivalent number of training points, while RBFN was the slowest in building the model with increasing number of training points. In contrast SVR was the fastest in large scale multi-modal problems. Fang et al. [8], studied RSM and RBFN to find the best method for modeling highly non-linear responses found in impact related problems. They also compared the RSM and RBFN models with a highly non-linear test function. Compromising the computation cost of RBFN, they concluded dominance of RBFN over RSM in such optimization problems. Mullur [9], compared his proposed metamodeling method name extended radial basis function (E-RBF) with three other approaches; RSM, RBFN and kriging. He introduced E-RBF as the superior method since it resulted in an accurate metamodel without the need of parameter setting and significant increase in computation time. Nevertheless, a number of parameters influence the choice of an accurate method such as non-linearity, number of variables, associated sampling technique, internal parameter setting of each method and number of objectives in optimization problems [10].

Researchers have been attracted to employ RBFN in engineering applications due to the good performance of this method in approximating highly non-linear responses with low computational cost. Several studies with applying RBFN in real world engineering applications are carried out for example: modelling the sensor for a space shuttle main engine [11], detection of structural damage in a helicopter rotor blade [12], optimization of a micro-electrical packaging system [13], design of turbo machinery and propulsion components [14], fitting the best approximation of wing weight data of subsonic transports [15], optimization of helicopter rotor blades [16], prediction of flank wear in drilling [17] and multi-objective optimization of a disc brake system [18].

In this paper, the focus is on RBFN metamodelling method which an approach with a bias known a priori is compared to the approach with a posteriori known bias, commonly used in literature. First, the theoretical model of the two approaches are described and performance measures are defined. A set of six mathematical test functions and an engineering design application, followed by the comparison procedure is covered in the next section. Next, The preliminary results of the comparative study and the performance of the a priori approach is presented and discussed. Finally, the conclusion and the potential future studies are summarized.

2 RADIAL BASIS FUNCTION NETWORKS (RBFN)

Radial basis function networks were originally developed for solving multi-quadratic equations of topography based on coordinate data with interpolation [3]. Radial basis functions networks of a set of sampling points x_i can be shown as

$$f(\mathbf{x}) = \sum_{i=1}^{n} \lambda_i \phi_i(\mathbf{x}) + b, \tag{1}$$

where $f(\mathbf{x})$ is the approximation function, n is the number of sampling points, $\phi_i = \phi_i(\mathbf{x})$ is the radial basis function, λ_i is the weight for the i_{th} basis function, and b is a bias. Some of the most commonly used radial basis functions are

$$\begin{aligned}
\text{Linear:} \quad & \phi(r) = r, \\
\text{Cubic:} \quad & \phi(r) = r^3, \\
\text{Gaussian:} \quad & \phi(r) = e^{-\gamma r^2},\ 0 \le \gamma \le 1, \\
\text{Quadratic:} \quad & \phi(r) = \sqrt{r^2 + \gamma^2},\ 0 \le \gamma \le 1,
\end{aligned} \tag{2}$$

where γ is a positive shape parameter and

$$r = ||\boldsymbol{x} - \boldsymbol{c}_i||, \tag{3}$$

is the radial distance, where it is expressed in terms of the Euclidean distance of the sampling points $\boldsymbol{x}$ from a center point $\boldsymbol{c}_i$, which typically is taken to be the design variable $\hat{\boldsymbol{x}}_i$ at the i_{th} sampling point. Here, the bias in Eq. (1) is a polynomial function, formulated as

$$b = b(\mathbf{x}) = \sum_{i=1}^{m} \beta_i \eta_i(\mathbf{x}), \tag{4}$$

where $\eta_i = \eta_i(\mathbf{x})$ represents the polynomial basis functions and β_i are the unknown regression coefficients of the polynomial bi-

ases. Therefore, for a specific sampling point $\hat{\mathbf{x}}_\mathbf{j}$ the corresponding approximation function is

$$f(\hat{\mathbf{x}}_\mathbf{j}) = \sum_{i=1}^{n} \lambda_i A_{ji} + \sum_{i=1}^{m} \beta_i B_{ji}, \tag{5}$$

where $A_{ji} = \phi(\hat{\mathbf{x}}_\mathbf{j})$ and $B_{ji} = \eta_i(\hat{\mathbf{x}}_\mathbf{j})$.

Furthermore, by training the radial basis functions networks for a set of sampling points and their corresponding response values $\left[\hat{\mathbf{x}}_\mathbf{j}, \hat{f}_j\right]$ the latter equation can be compactly formulated as

$$\hat{\mathbf{f}} = \mathbf{A}\boldsymbol{\lambda} + \mathbf{B}\boldsymbol{\beta}, \tag{6}$$

where $\boldsymbol{\lambda} = [\lambda_1, \lambda_2 ... \lambda_n]^T$, $\boldsymbol{\beta} = [\beta_1, \beta_2 ... \beta_m]^T$, and $\hat{\mathbf{f}} = \left[\hat{f}_1, \hat{f}_2 ... \hat{f}_n\right]^T$.

The bias in Eq. (1) is augmented to the classic form of RBFN in order to improve the performance of the classic RBFN in linear problems. Also, the RBFN without any augmented bias might become singular and no interpolation is found. This bias is considered to be known either a priori or a posteriori. However, in literature the bias is regarded as unknown a priori.

Therefore, the unknown parameters are more than the number of equations in Eq. (6), the equation is undetermined and can not be solved. This is overcome by imposing the following orthogonality condition

$$\sum_{i=1}^{n} \lambda_i \eta_j(\mathbf{c}_\mathbf{i}) = 0 \quad \text{for } j = 1, 2 ... m. \tag{7}$$

Combining equations (6) and (7) will lead to the matrix form of

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B^T} & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \boldsymbol{\lambda} \\ \boldsymbol{\beta} \end{Bmatrix} = \begin{Bmatrix} \hat{\mathbf{f}} \\ \mathbf{0} \end{Bmatrix}. \tag{8}$$

The unknown coefficients $\boldsymbol{\lambda}$ and $\boldsymbol{\beta}$ of the RBFN will be obtained by solving Eq. (8).

Here in this paper, an approach based on a priori known bias is used to solve the RBFN. The a priori known bias can be expressed as

$$\boldsymbol{\beta} = \hat{\boldsymbol{\beta}}, \tag{9}$$

where in this study $\hat{\boldsymbol{\beta}}$ the regression coefficient of the bias is defined a priori by using the optimal regression coefficient

$$\hat{\boldsymbol{\beta}} = (\mathbf{B^T B})^{-1} (\mathbf{B^T} \hat{\mathbf{f}}), \tag{10}$$

which is resulted from a parabolic or quadratic response surface formulated by

$$\begin{aligned} f(\mathbf{x}) &= \beta_0 + \sum_{i=1}^{n} \beta_i x_i + \sum_{i=1}^{n} \beta_{ii} x_i^2, \\ f(\mathbf{x}) &= \beta_0 + \sum_{i=1}^{n} \beta_i x_i + \sum_{i=1}^{n} \beta_{ii} x_i^2 + \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \beta_{ij} x_i x_j. \end{aligned} \tag{11}$$

The radial basis functions networks is trained to fit the given set of data $\left[\hat{\mathbf{x}}_\mathbf{j}, \hat{f}_j\right]$, by minimizing the error

$$\boldsymbol{\varepsilon} = \mathbf{f} - \hat{\mathbf{f}}, \tag{12}$$

in the least square sense, which is done by solving the following minimization problem

$$\min \quad \frac{1}{2} \left(\mathbf{A}\boldsymbol{\lambda} - (\hat{\mathbf{f}} - \mathbf{B}\hat{\boldsymbol{\beta}}) \right)^{\mathbf{T}} \left(\mathbf{A}\boldsymbol{\lambda} - (\hat{\mathbf{f}} - \mathbf{B}\hat{\boldsymbol{\beta}}) \right). \tag{13}$$

The solution to this problem is determined by the normal equation as

$$\hat{\boldsymbol{\lambda}} = (\mathbf{A^T A})^{-1} \mathbf{A^T} (\hat{\mathbf{f}} - \mathbf{B}\hat{\boldsymbol{\beta}}). \tag{14}$$

Further on in the present paper, RBFN the bias known a posteriori is briefly called a *posteriori RBFN* and abbreviated by $RBFN_{pos}$, and radial basis functions networks with bias known a priori is called *a priori RBFN* and abbreviated by $RBFN_{pri}$. The proposed a priori RBFN method eliminates any need of imposing the extra orthogonality condition in Eqn. (7).

The overall performance of the metamodels is evaluated using the standard statistical error analysis. The two standard performance metrics are applied to the off-design test points: (i)Root Mean Squared Error (RMSE), and (ii) Maximum Absolute Error (MAE).

The RMSE is expressed as

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n} \left(\hat{f}_i - f_i \right)^2}{n}}, \tag{15}$$

and MAE is given by

$$\text{MAE} = max|\hat{f}_i - f_i|, \tag{16}$$

where n is the number of test points selected to evaluate the model, $\hat{f}_i$ is the exact function value at the i_{th} test point and f_i represents the corresponding predicted function value. RMSE and MAE are typically on the same order of the actual function values. These error measure will not indicate the relative performance quality of the surrogates across different functions independently. Therefore, to compare the performance measures of the two approaches over test functions the normalized values of the two errors, NRMSE and NMAE by using the actual function values are calculated by

$$\text{NRMSE} = \sqrt{\frac{\sum_{i=1}^{n}\left(\hat{f}_i - f_i\right)^2}{\sum_{i=1}^{n}\left(\hat{f}_i\right)^2}}, \tag{17}$$

$$\text{NMAE} = \frac{max|\hat{f}_i - f_i|}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\hat{f}_i - \bar{f}_i\right)^2}}, \tag{18}$$

where $\bar{f}$ denotes the mean of the actual function values at the test points.

In addition, the NRMSE and NMAE of a priori RBFN is compared to the a posteriori RBFN approach by defining the corresponding relative differences. The relative difference in NRMSE (D^{NRMSE}) of a posteriori RBFN is given by

$$D^{NRMSE}_{RBF_{pos}} = \frac{NRMSE_{RBF_{pos}} - NRMSE_{RBF_{pri}}}{NRMSE_{RBF_{pri}}} \times 100\%, \tag{19}$$

and the relative difference in NMAE (D^{NMAE}) of a posteriori RBFN is defined by

$$D^{NMAE}_{RBF_{pos}} = \frac{NMAE_{RBF_{pos}} - NMAE_{RBF_{pri}}}{NMAE_{RBF_{pri}}} \times 100\%, \tag{20}$$

where NRMSE and NMAE values of the RBF_{pos} approach are referred by $NRMSE_{RBF_{pos}}$ and $NMAE_{RBF_{pos}}$; and $NRMSE_{RBF_{pri}}$ and $NMAE_{RBF_{pri}}$ are the corresponding NRMSE and NMAE values of the RBF_{pri} approach.

In the following sections, the performance $RBFN_{pos}$ and $RBFN_{pri}$ approaches are compared by using several test problems and aforementioned accuracy measures.

3 NUMERICAL EXAMPLES

This section defines the test problems and the approach used to compare the performance of the a priori RBFN, developed in this paper, with the a posteriori RBFN. Six test functions and an engineering design problem are used for the comparison study.

3.1 Test Functions

The comparison is based on the following five analytical benchmark problems for unconstrained global optimization chosen from literatures:

1. Branin-Hoo Function [19]

$$f_1 = (x_2 - \frac{5.1x_1^2}{4\pi^2} + \frac{5x_1}{\pi} - 6)\ 2 + 10(1 - \frac{1}{8\pi})\cos(x_1) + 10. \tag{21}$$

2. Goldstein-Price Function [20]

$$\begin{aligned} f_2 = {} & [1 + (x_1 + x_2 + 1)^2 \\ & \times (19 - 14x_1 + 3x_1^2] - 14x_2 + 6x_1x_2 + 3x_2^2)] \\ & \times [30 + (2 * x_1 - 3x_2)^2 \\ & \times (18 - 32x_1 + 12x_1^2 + 48x_2 - 36x_1x_2 + 27x_2^2)]. \end{aligned} \tag{22}$$

3. Rosenbrock Function [21]

$$f_3, f_4 = \sum_{n=1}^{N-1}[100(x_{n+1} - x_n^2)^2 + (x_n - 1)^2]. \tag{23}$$

Two versions of this test function are used based on the number of design variables, (i) Rosenbrock-2 with two design variables, and (ii) Rosenbrock-10 with ten input design variables.

4. Math1 (A 10-variable Mathematical Function) [22]

$$f_5 = \sum_{m=1}^{10}\left[\frac{3}{10} + \sin(\frac{16}{15}x_m - 1) + \sin(\frac{16}{15}x_m - 1)^2\right]. \tag{24}$$

5. Math2 (A 16-variable Mathematical Function) [23]

$$f_6 = \sum_{m=1}^{16}\sum_{n=1}^{16} a_{mn}(x_m^2 + x_m + 1)(x_n^2 + x_n + 1), \tag{25}$$

where a is defined in [23].

3.2 SGI Micro Structural Material Model

In this study the RBF_{pri} approach is used to accurately approximate the material properties (cauchy stress σ and strain ε) of Spherical Graphite Iron (SGI) based on the micro structure of the material. The material behavior is obtained for the three phases in Pearlitic-Ferritic SGI, *i.e.* Graphite, Ferrite and Pearlite by using a micro-mechanical finite element model. The micro structural image of SGI including the three phases and the nodule used a a template is shown in Fig. 1. For simplicity the

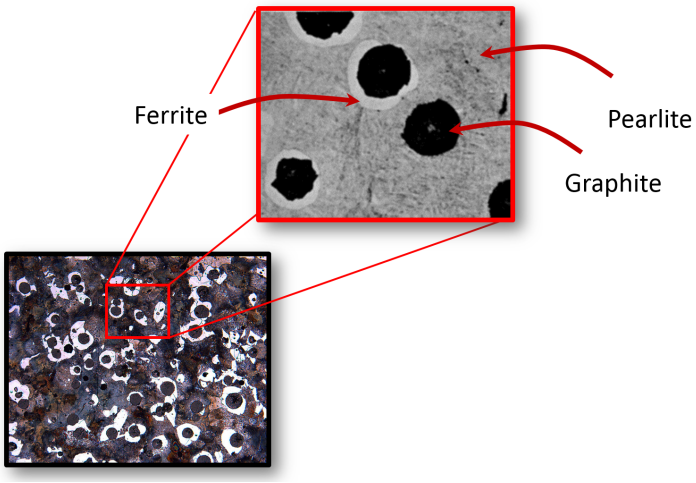
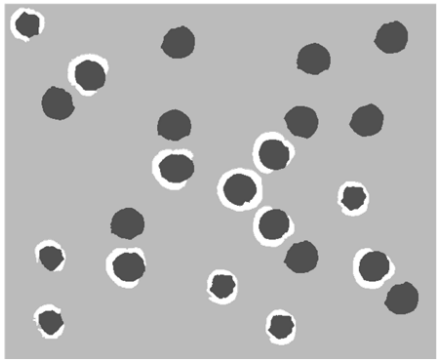
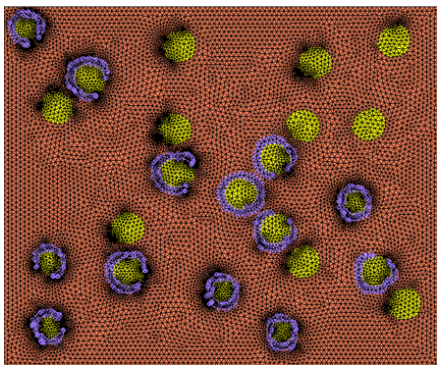


FIGURE 1: THE MICRO STRUCTURE AND THE THREE PHASES OF SGI USED AS A TEMPLATE FOR THE INDIVIDUAL NODULES.



(a) Micro Structure



(b) Finite Element Mesh

FIGURE 2: THE MICRO STRUCTURE AND FINITE ELEMENT MESH OF THE MICRO STRUCTURE OF SGI.

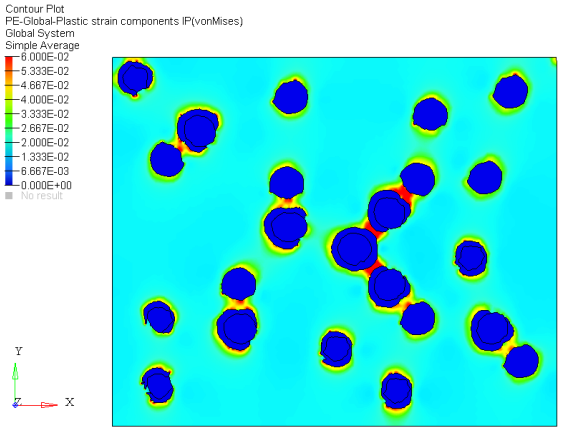


FIGURE 3: THE STRESS DISTRIBUTION OBTAINED FROM ONE FINITE ELEMENT ANALYSIS WITH RANDOMLY SELECTED PARAMETERS.

three phases *i.e.* Graphite, Ferrite and Pearlite, are considered to be separated by defined boundaries, and both Graphite and Fearite are assumed to be elastic. A finite element model of SGI's meshed micro structure predicts the behaviour of Pearlite in the material, which is approximated by the Ramberg-Osgood approximation model expressed by

$$E\varepsilon = \sigma + \alpha(\frac{|\sigma|}{\sigma_y})^{n-1}\sigma, \tag{26}$$

where E is the Young's modulus, ε is the strain, σ represents the Cauchy stress, σ_y is the Yield stress and α and n are material constants. Figure 2 illustrates the micro structure of the SGI and the finite element mesh of the micro structure. Parameters σ_y, α and n are to be determined by minimizing the difference between simulation and experimental data. Consequently, the objective function is a function of three variables σ_y, α and n, such that

$$f(\sigma_y,\alpha,n) = \frac{1}{W_i}\sum_{i}^{k}||\sigma_i^{sim} - \sigma_i^{exp})||, \tag{27}$$

where k is the number of data points, $||*||$ denotes the $L_2 - norm$, W_i, σ_i^{sim} and σ_i^{exp} are weight, simulated homogenized stress for the top boundary and experimental stress data for i_{th} data point, respectively. Surrogate models are generated and compared to approximate the simulated homogenized stress obtained from the FE simulation, by using RBF_{pri} and RBF_{pos} approaches. The result of finite element analysis with randomly selected parameters showing the stress distribution in the SGI micro structure is depicted in Fig. 3.

TABLE 1: NUMERICAL SET-UP FOR TEST PROBLEMS.

Function	Function name	No. of variables	Design range(s)	No. of DoE	No. of test points
f_1	Branin-Hoo	2	$x_1 : [-5, 10]$	36	500
			$x_2 : [0, 15]$	36	500
f_2	Goldstein-Price	2	$x_1, x_2 : [-2, 2]$	36	500
f_3	Rosenbrock-2	2	$x_1, x_2 : [-5, 10]$	12	500
f_4	Rosenbrock-10	10	$x_1, x_2 : [-5, 10]$	330	500
f_5	Math 1	10	$x_1, x_2 : [-1, 1]$	396	500
f_6	Math 2	16	$x_1, x_2 : [-1, 1]$	459	500
f_7	SGI material	3	$\sigma_y : [5E-3, 2E-4]$	200	3
	model		$\alpha : [0.05, 0.5] n : [3, 7]$		

Table 1 illustrates a summary on the properties of the test problems including number of design variables, design range, number of design of experiments and number of off-design test points.

3.3 Comparison Procedure

The approach for performing the comparison study of the two surrogate modeling methods, defined in the previous sections, is described in a six step procedure as follows:

Step 1: The number of design of experiments (DoE) for each test problem is chosen. The selection is with regards to the dimension of each function. However, the number of coefficients $k = (n+1)(n+2)/2$ in a second order polynomial with n number of variables is used as a reference. For all the test functions the number of DoE is chosen as a coefficient of k.

Step 2: In order to avoid scaling errors because of divers magnitudes of the design variables, the design domains are mapped between 0 and 1. The surrogate models are fitted using the mapped variables, while the performance measurement is carried out in the original space.

Step 3: To avoid any probable sensitivity of metamodels to a specific DoE, 100 distinctive sample sets are generated for each sample size of step 1 (except the SGI material model problem), using the Iterative Latin hypercube sampling method. The MATLAB Latin hypercube function(LHSDESIGN) using maximin (maximize minimum distance between points) with 20 iterations is employed in this step.

Step 4: Metamodels are constructed using the two RBFN approaches (RBF_{pri} and RBF_{pos}) with each of the four different radial basis functions (linear, cubic, guassian and quadratic) to be compared for each set of DoE. Therefore, for each test function 800 (100 set of DoE$\times$2 RBFN approaches$\times$4 radial basis functions) surrogate models are constructed.

Step 5: 500 sample points are randomly selected within the design space. The exact function value $\hat{f}_i$ and the predicted function value f_i at each test point is calculated. RMSE, MAE, NRMSE and NMAE are computed for each sample set and radial basis function using equations 15 to 18. The average of NMAE and NRMSE ($NRMSE_{mean}, NMAE_{mean}$) is calculated across the 100 set of samples. Finally, the relative difference measures of the computed average errors, $NRMSE_{mean}$ and $NMAE_{mean}$ for RBF_{pos} are calculated by using equations 19 and 20.

Step 6: The procedure from step 1 to 5 is repeated for all test problems. The mean error measures, $NRMSE_{mean}$ and $NMAE_{mean}$, are computed for the surrogate approaches and each radial basis function across all problems.

In the comparison study of the SGI material model, due to computational cost of the FE model there are some modification in the above steps . First, only one set of DoE with the sample size mentioned in table 1 (200 design points) is created. Secondly, 3 of the sampling points are randomly chosen as test points. The surrogate models are fitted at the other 197 remaining DoE, and the performance measures RMSE, MAE, NRMSE and NMAE is calculated at the 3 sampling test points. To avoid any probable sensitivity of metamodel to a specific DoE, the above procedure is repeated 100 times, for each run 3 different test points, consequently 197 training points are randomly selected and the errors are calculated. Finally, the average of all 100 sets of errors and the relative difference in the averaged errors are computed for comparison.

In result of including step 2 in the comparison procedure, which is mapping the variables to a unit hypercube, the parameters can be set without considering the magnitude of the design variables. Therefore, the parameter γ used in the radial basis functions in Eq. 2 is set to one ($\gamma = 1$). Also, in the SGI problem we have chosen the Young's modulus $E = 90GPa$ and the Poison ratio $\nu = 0.3$ as the inputs to the finite element model.

4 RESULTS AND DISCUSSION

In this section, the results obtained from performing the comparison study of a priori and a posteriori RBFN, by following the comparison procedure defined in the previous section, is presented and discussed.

The average RMSE and MAE of all test problems corresponding to each radial basis function by using the RBF_{pri} and RBF_{pos} are summarized in Tab 2. The highlighted values illustrate the lowest errors of each test problem among the different radial basis functions. It can be observed that, the cubic basis function generate the best fitted surrogate model for test problems f_1, f_3, f_4 and f_6. Test function 2 and 5 are best fitted by using the quadratic radial basis function and the SGI material model problem (f_7) has the best approximation by using the lin-

TABLE 2: RMSE AND MAE SUMMARY OF THE A PRIORI AND A POSTERIOR RBFN BY USING DIFFERENT RADIAL BASIS FUNCTIONS ACROSS THE TEST PROBLEMS.

Test Problems	RBF Approach	Linear		Cubic		Gaussian		Quadratic	
		$RMSE_{mean}$	MAE_{mean}	$RMSE_{mean}$	MAE_{mean}	$RMSE_{mean}$	MAE_{mean}	$RMSE_{mean}$	MAE_{mean}
f_1	RBF_{pri}	12.105	78.587	**6.789**	**41.293**	26.212	228.123	8.200	60.043
	RBF_{pos}	13.341	96.976	**6.925**	**46.228**	29.151	263.235	8.077	60.416
f_2	RBF_{pri}	53266	407422	39643	310873	24632	204426	**23305**	**173584**
	RBF_{pos}	56991	459249	40952	326382	25905	225865	**23572**	**175875**
f_3	RBF_{pri}	69485.3	305412	**52358.2**	**241511**	81650.6	329664	66934.7	318879
	RBF_{pos}	92006.1	459130	**59384.4**	**318219**	145268	547187	85312.8	448168
f_4	RBF_{pri}	232155	842508	**225503**	**827567**	235359	924701	226385	842481
	RBF_{pos}	257040	1076576	**226315**	**873849**	252397	1010650	232746	914767
f_5	RBF_{pri}	0.2358	0.7845	0.2172	0.7460	0.2217	0.8067	**0.2114**	**0.7566**
	RBF_{pos}	0.2229	0.7357	0.2152	0.7505	0.1994	0.7063	**0.2063**	**0.7230**
f_6	RBF_{pri}	2.1602	9.5950	**1.9795**	**7.4934**	2.1945	10.0124	2.0637	8.4291
	RBF_{pos}	3.7575	22.4872	**2.1690**	**11.2378**	3.8974	24.2357	2.6166	15.7370
f_7	RBF_{pri}	**3.75E-05**	**5.22E-05**	4.74E-05	6.83E-05	1.22E-03	1.98E-03	2.43E-04	3.84E-04
	RBF_{pos}	**3.97E-05**	**5.73E-05**	4.89E-05	7.12E-05	1.21E-03	1.96E-03	2.59E-04	4.13E-04

TABLE 3: COMPARISON OF THE PERFORMANCE OF THE TWO APPROACHES BY USING RMSE.

Test	RBF_{pri}		RBF_{pos}	
Problems	$RMSE_{mean}$	$NRMSE_{mean}$	$RMSE_{mean}$	$NRMSE_{mean}$
f_1	**6.7888**	**0.0966**	6.9249	0.0985
f_2	**23304.9**	**0.1679**	23572.2	0.1698
f_3	**52358.2**	**0.2225**	59384.4	0.2643
f_4	**225503**	**0.1718**	226314	0.1724
f_5	0.2114	0.1079	**0.2063**	**0.1053**
f_6	**1.9795**	**0.0217**	2.1690	0.0238
f_7	**3.74E-05**	**0.2258**	3.97E-05	0.2419

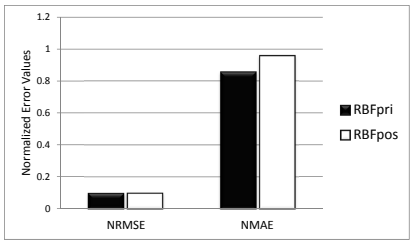
TABLE 4: COMPARISON OF THE PERFORMANCE OF THE TWO APPROACHES BY USING MAE.

Test	RBF_{pri}		RBF_{pos}	
Problems	MAE_{mean}	$NMAE_{mean}$	MAE_{mean}	$NMAE_{mean}$
f_1	**41.2931**	**0.85590**	46.2278	0.95818
f_2	**173584**	**1.34564**	175875	1.3634
f_3	**329664**	**1.54175**	547187	2.5591
f_4	**827567**	**1.281071**	873849	1.35272
f_5	0.75659	2.62218	**0.72300**	**2.50576**
f_6	**7.49343**	**0.34508**	11.2377	0.51751
f_7	**5.22E-05**	**2.90777**	5.73E-05	3.12578

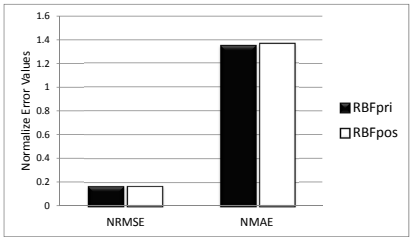
ear basis function. However, by studying the performance measures of the cubic basis function column in Tab. 2 for all the test problems, it can be seen that the difference of errors between the cubic and the best basis function is not considerable. Therefore, one could conclude that in case of lack of any data on the response surface, cubic basis function can be a robust and accurate choice for generating surrogate models of black boxes. However, there is a need in a more thorough and detailed comparison study of selecting the best radial basis function for the RBF_{pri}.

In order to perform the comparison study accurately, the performance measures of the most accurate radial basis function corresponding to each of the two surrogate approaches are extracted for all test problems. Table 3 presents the average of and normalized RMSE for the seven test problems obtained from RBF_{pri} and RBF_{pos}. As it can be observed from the table, the proposed approach has the lower RMSE and NRMSE compared to the RBF_{pos} method for all test problems except f_5. Similarly, the average of MAE and normalized MAE values corresponding to each method for all test problems are shown in Tab. 4. The MAE and NMAE errors in this table also have the lower values (bold faced) in the RBF_{pri} column compared to the a posteriori RBFN for all problems except the Math 1 test function (f_5), which indicate the better performance of our proposed approach. On the other hand, by focusing on the error values of test function 5 (f_5) in Tab. 3 and Tab. 4, one could recognize that the superiority of RBF_{pos} in f_5 is minor due to the small differences between the performance measures of RBF_{pri} and RBF_{pos}.

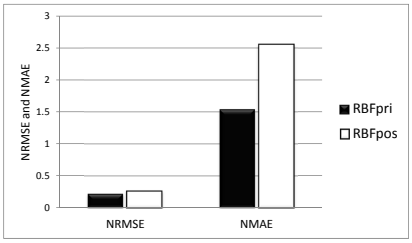
The comparison of the performance RBF_{pos} and RBF_{pri} by using NRMSE and NMAE is illustrated through bar diagrams in Fig.4. The comparison of two approaches are also presented as the relative differences in NRMSE and NMAE in Tab. 5. The positive values in the table represent the degree of the superiority of RBF_{pri} in percentage for each test function, and the only negative percentage value shows the extent which the RBF_{pos} performed better. The charts and the relative difference table



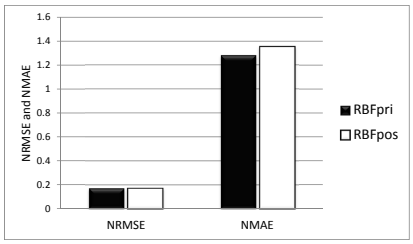
(a) f_1:Branin-Hoo



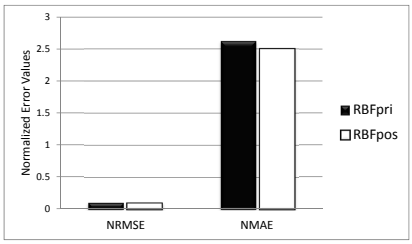
(b) f_2:Goldstein-Price



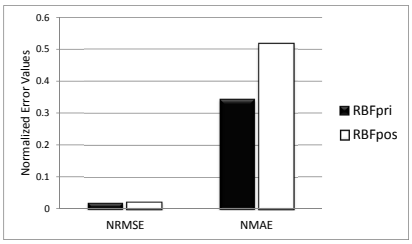
(c) f_3:Rosenbrock-2



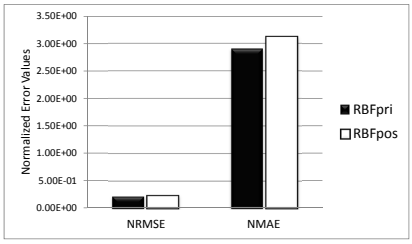
(d) f_4:Rosenbrock-10



(e) f_5:Math 1



(f) f_6:Math 2



(g) f_7:SGI Test Problem

FIGURE 4: COMPARISON OF THE PERFORMANCE OF RBF_{pri} AND RBF_{pos} IN EACH TEST FUNCTION.

demonstrate a clear view of the differences between the performance of the two approaches, and again the superior performance of a priori approach can be seen. Also, from Tab. 5, we observe that the RBF_{pri} method yields to a better NMAE, which is indicative of local deviations, compared to RMSE, which provides a global error measure. Specially in Math 2 test function, that is a large scale test function with 16 input variables, the a posteriori RBFN generates a maximum absolute error of near 50% more than a priori RBFN. Also by looking at the error charts in Fig. 4c and Fig. 4d corresponding to f_3 and f_4, which are the same functions (Rosenbrock) with different number of variables, we can detect the lower error values obtained from both approaches in the function with the higher number of variables. This can be the effect of the sampling size on the performance of the surrogate models.

5 CONCLUDING REMARKS

The comparative study presented in this paper has indicated that the RBFN with a priori known bias approach has a better performance than the a posteriori known bias RBFN, which is commonly used in literature as the approach to generate radial basis

TABLE 5: RELATIVE DIFFERENCE OF NRMSE AND NMAE COMAPRING RBF_{Pri} TO THE OTHER SURROGATE APPROACH $RBF_{\mathbf{Pos}}$.

Test Problems	$RBF_{\mathbf{pos}}$	
	$D_{\mathbf{NRMSE}}(\%)$	$D_{\mathbf{NMAE}}(\%)$
f_1	2.00	11.95
f_2	1.15	1.32
f_3	18.79	31.76
f_4	0.36	5.59
f_5	-2.39	-4.44
f_6	9.57	49.97
f_7	7.14	7.50

functions networks surrogates. A set of six test functions with different degrees of dimensionality, and an engineering design problem in approximating the material properties of SGI (spherical graphite iron) was used to compare the approaches. The best radial basis function among the four used in this study (linear, cubic, Gaussian and quadratic) was chosen for each test problem by performing a separate comparison. The study showed the robustness of cubic radial basis function, although other basis functions illustrated lower errors. The evaluation of various performance measures, including RMSE, MAE and their normalized values also the percentage of relative differences, justified the superiority of RBF_{pri} over RBF_{pos} for most of the test problems, except one test function which the difference was small.

In future, the proposed approach can be compared to other metamodeling methods such as RSM, Kriging, SVR, extended RBF and the recent hybrid methods. Furthermore, the effect of different modelling criteria i.e. sampling technique, sample size and problem dimensionality can be investigated for the proposed approach.

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