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Extended Radial Basis Functions: More Flexible and Effective Metamodeling

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Economic competitiveness is driving industry to new frontiers of engineering design. Robustness and reliability-based design, multidisciplinary-simulation-based design, increased complexity and sophistication of our design, and optimization-aided design are four such areas that are seriously challenging our ability to keep pace with the need to adequately model the systems we seek to design—in spite of the exponential growth of computing power. An emerging consensus within the community is that the effective development of computationally benign models (metamodels) will help us navigate the challenging road ahead. The process of constructing metamodels for computationally expensive models, such as finite element, aerodynamic, and heat-transfer models, is representative of the tasks we must address. Among the available metamodeling techniques, radial basis functions (RBFs) have recently generated much interest for their effectiveness and versatility. Radial basis functions offer numerous advantages over the traditional response surface methodology, including their ability to effectively generate multidimensional interpolative approximations. However, we show how the typical RBF approach lacks the critical flexibility required to handle the wide variety of complex models arising from the use of advanced techniques, such as uncertainty handling and multiobjective optimization, often encountered in modern design. Furthermore, in this paper we propose a novel approach—the extended radial basis function (E-RBF) approach—that provides the designer with significant flexibility and freedom in the metamodeling process, compared to conventional RBFs. Examples are provided that demonstrate the effectiveness of the new approach and explore its potential superiority to traditional RBF and response surface methodologies. Initial investigation indicates that the E-RBF possesses unique and novel properties not available in any other single method.

Nomenclature

$f(x)$	=	computationally expensive analysis [Eq. (2)]
$\tilde{f}(x)$	=	computationally benign metamodel of $f(x)$ [Eq. (1)]
m	=	number of design variables (dimension of the problem) [Eq. (1)]
n	=	order of monomial in nonradial basis functions (Table 1)
n_p	=	number of data points evaluated [Eq. (2)]
r	=	radial distance from a given data point [Eq. (3)]
x	=	generic point in the design space [Eq. (4)]
x_j	=	jth element of the vector x [Eq. (1)]
x^i	=	ith design configuration, or data point [Eq. (1)]
γ	=	smoothness parameter in nonradial basis functions (Table 1)
ξ_j^i	=	jth element of vector ξ^i [Eq. (11)]
ξ^i	=	coordinate vector of point x relative to data point x^i [Eq. (10)]
$\phi(\xi)$	=	nonradial basis function developed in the paper [Eq. (10)]
$\psi(r)$	=	typical radial basis function [Eq. (3)]

I. Introduction

A. Metamodeling: Industry Needs

MOTIVATED by the increasing challenge of developing commercially successful products and systems, designers are taking simulation based design to new levels that are well beyond today's computing capabilities, unless traditional modeling methods also keep pace. The need to quantify the economic and engineering performance of complex products under uncertainty leads to highly complex and computationally expensive models. Such complexity, although unavoidable, can prove to be prohibitive in an optimization environment and can severely limit comprehensive exploration of design alternatives. Models of such complexity are not uncommon, especially within a multidisciplinary design optimization (MDO) framework, which can form an integral component of concurrent engineering and design. For example, a single crash testing simulation can require 10 to 15 h even when performed in a parallel processing environment.[1] Other analyses such as computational fluid dynamics and heat transfer can also require prohibitively large amounts of computation time. Unfortunately, the state-of-the-art practice is 1) to degrade the model for the sake of computational savings by ignoring important physical behaviors or 2) to unduly limit design space exploration.

To meet the challenge of increasing model complexity, the process of building approximate models, or metamodeling, has gained wide acceptance from the design community. Such approximation techniques have been successfully applied to several MDO problems.[2–4] Metamodels of complex analysis codes significantly reduce the design cycle time—by reducing the number of times the complex code is evaluated—and ultimately result in the increased effectiveness of the design process.

B. Response Surface Methodology

The literature shows a wide variety of metamodeling techniques used within various MDO environments. The response surface methodology (RSM) is a statistical tool,[5,6] primarily developed for experimental design, and subsequently adapted for approximating expensive computer simulations. The response surface methodology falls under the broad category of parametric metamodeling, a class of metamodeling techniques that typically assumes a specific form, such as polynomial, for the approximation function.[7] The most popular form of the RSM involves fitting second-order polynomial functions using least-squares regression over a set of sampled data points. The response surface methodology presently enjoys a popular status in the design community because of the

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well-established literature and successful implementation for several MDO applications, such as high-speed civil transport,[3,8] aircraft concept sizing and autonomous hovercraft application,[9] and collaborative optimization.[10]

C. Nonparametric Metamodeling

Several recent publications,[7,11–13] however, recognize that polynomial regression techniques, such as the RSM, might not be adequate for handling the level of complexity typically encountered in engineering applications. The response surface methodology, being a regression technique, is more appropriate within the realm of physical experiments because it typically smooths out the random error present in the experiment. In the case of deterministic computer experiments, it is instead more appropriate to use a technique that produces an exact (interpolative) fit through all of the computed data points, rather than one that produces a least-squares fit.[14] The challenge of exact fitting has led researchers to explore the so-called nonparametric metamodeling techniques,[7] which provide an interpolating surface through all sampled data points. The term nonparametric can be misleading, as it does not imply that the methods are parameterless. It simply means that these techniques do not assume any specific form (such as polynomial) for the overall approximation function. Instead, these methods typically involve a collection of functions, each associated with individual data points.

Nonparametric metamodeling techniques offer important advantages over the traditional RSM, such as ease of extending to higher dimensions and greater accuracy for topographically complex models. Kriging,[15–17] neural networks,[14,18,19] radial basis functions,[7,13,14,20] and multivariate adaptive regression splines[21,22] have been previously proposed as nonparametric metamodeling techniques.

D. Radial Basis Functions: Effective Metamodeling

In this paper, we explore the radial basis function (RBF) approach as an effective and powerful metamodeling technique. RBF approaches are among the most effective multidimensional approximation methods whose performances—to an extent—are independent of the dimensionality (number of design variables) of the problem.[23] RBFs have recently generated significant interest as an approximation technique because of a combination of desirable attributes. These include 1) their ability to accurately model arbitrary functions, 2) their ability to handle scattered data points in multiple dimensions, and 3) their relatively simple implementation compared to kriging and neural networks. These benefits make RBFs more desirable than other interpolation techniques, such as 1) spline-based methods, because of difficulties in extending to higher dimensions,[13,23] 2) neural networks, because of the trial and error associated with their use,[22] and 3) kriging, because of the lack of readily available software.[14]

E. Extended Radial Basis Functions: Novel and Powerful Extension

Unfortunately, the potential benefits of using RBFs have not translated into their widespread use within the engineering community in the MDO context. In this paper, we explore the drawbacks of the typical RBF approach, which might be limiting its use as a metamodeling technique in the context of MDO, and we propose a novel extension to the RBF approach that successfully overcomes its current shortcomings.

The MDO environment presents a wide variety of complex models, such as computational fluid dynamics (CFD) analyses and crash simulations. Advanced optimization techniques, such as multiobjective optimization and robust design optimization, are often used in conjunction with such complex models. The metamodeling requirements for such disparate situations can be considerably different. For example, a designer might prefer a metamodel that is convex or might require one that is unimodal (that is, not containing local minima), when the underlying data possess such convexity or unimodality properties. The introduction of computationally acquired spurious local minima, for example, can pose a serious hindrance to gradient-based optimization. In their typical form, RBFs do not provide sufficient flexibility to cater to such requirements or to the freedom to incorporate designer-specified requirements. More specifically, RBFs yield an interpolating surface that is unique with respect to a given set of prescribed data points. The interpolating surface is a result of solving a square system of linear equations. This feature of "unique solvability" is interestingly occasionally quoted as a potential advantage of RBFs.[23] In this paper, however, we strongly caution that within the MDO environment this feature can severely restrict their use. Our total inability to avoid resulting spurious local minima is a notable glaring deficiency.

Several researchers have proposed modifications to the typical RBF approach to overcome some of its limitations. In 1987, Powell[24] proposed the concept of improving the performance of RBFs by augmenting them with a set of polynomial functions and imposing constraints, which leads to a system of linear equations. Krishnamurthy[13] explores the concept of adding local support to RBFs. Although these modifications improve the performance of RBFs, they do not result in an increased flexibility in the model building process.

There have been important recent advances in constructing metamodels with smoothing properties. Girosi[25] presents the support vector machine (SVM) technique from the context of data interpolation. The SVM technique allows for smoothness constraints to be incorporated in the model building process. Craven and Wahba[26] discuss smoothing capabilities of splines, while Juttler[27] develops convex approximations using tensor product splines. In the present paper, however, we restrict our discussion to the RBF approach, and present an effective way to incorporate smoothing capabilities.

To realize the significant potential that RBFs offer and to make the approach more adaptable to the diverse and complex engineering applications encountered in MDO, there is a need to make the metamodeling process more flexible from the point of view of the designer. In this paper, we explore the novel idea of developing a method called the extended radial basis function (E-RBF) approach, which in fact deliberately avoids the notion of unique solvability. The E-RBF approach results in an underdetermined system of linear equations, which yields a family of solutions. This new technique allows the designer more freedom in building metamodels and ultimately results in more accurate and effective metamodels.

The remainder of this paper is structured as follows. Section II provides a synopsis of the typical RBF approach to metamodeling and briefly describes its potential shortcomings. Section III presents the development of a new class of basis functions—the nonradial basis functions (N-RBFs), which will form an integral component of the newly developed E-RBF approach. In Sec. IV, we describe the new extended radial basis function approach. Examples are provided in Sec. V, and Sec. VI concludes the paper.

II. Metamodeling Using Radial Basis Functions

In this section, we present some requisite mathematical preliminaries for metamodeling in general and introduce the terminology used in the paper. We then present a brief description of the typical RBF approach and discuss potential deficiencies associated with its use. The general metamodeling problem is stated as follows: Given a set of data points $x^i \in \mathbb{R}^m$, $i = 1, \ldots, n_p$, and the corresponding expensive function values $f(x^i)$, obtain a global approximation function $\tilde{f}(x)$ that accurately represents the original function over a given design domain.

In this paper, we consider metamodels that are accurate over the entire design domain, rather than locally valid approximations. Polynomial-based techniques, such as the RSM, are generally inadequate in providing such globally accurate metamodels because of their typical restrictive use of quadratic approximation functions, as follows:

$$\tilde{f}(x) = a_0 + \sum_{i=1}^{m} a_i x_i + \sum_{i=1}^{m} a_{ii} x_i^2 + \sum_{i=1}^{m} \sum_{\substack{j=1 \\ j \neq i}}^{m} a_{ij} x_i x_j \tag{1}$$

where the a are unknown coefficients determined by the least-squares approach. Interpolating metamodels,[7,12,22] on the other hand, are capable of yielding globally accurate response surfaces.

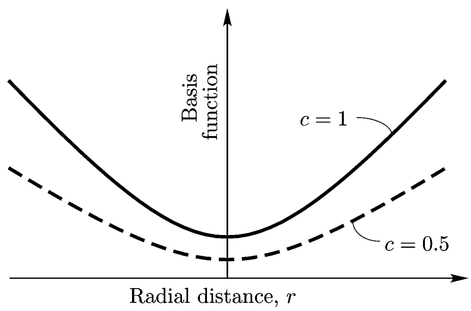


Fig. 1 Multiquadric radial basis function.

An interpolating metamodel typically satisfies the following set of conditions:

$$\tilde{f}(x^k) = f(x^k), \qquad k = 1, \ldots, n_p \tag{2}$$

which indicate that the function and the approximation are equal at all of the prescribed data points. In this paper, we define a metamodel that satisfies the conditions in Eq. (2) as one that provides an interpolative solution. Interpolating approximations can be typically obtained by using nonparametric metamodeling techniques, such as the RBF approach discussed next.

A. Radial Basis Functions

The idea of using RBFs as approximation functions was first proposed by Hardy[28] in 1971, when he used the multiquadric RBFs [Fig. 1, Eq. (3)] to fit irregular topographical data. Since then, several researchers have successfully used RBFs for several applications that require fitting global approximations to multidimensional scattered data. It is only recently that RBFs have gained increased consideration in metamodeling activities in the context of MDO.[7,14,22]

RBFs are expressed in terms of the Euclidean distance, $r = \|x - x^i\|$, of a point x from a given data point x^i. Perhaps one of the most effective forms is the multiquadric function,[7,24,29] which is shown in Fig. 1, and mathematically defined as

$$\psi(r) = \sqrt{r^2 + c^2} \tag{3}$$

where $c > 0$ is a prescribed parameter. The final approximation function is a linear combination of these basis functions across all data points, as given by

$$\tilde{f}(x) = \sum_{i=1}^{n_p} \sigma_i \psi(\|x - x^i\|) \tag{4}$$

where σ_i are unknown coefficients to be determined and n_p denotes the number of prescribed data points. To calculate the coefficients, we enforce the constraints given in Eq. (2), which yields an interpolative approximation function. This results in the linear system of equations

$$\sum_{i=1}^{n_p} \sigma_i \psi(\|x^k - x^i\|) = f(x^k), \qquad k = 1, \ldots, n_p \tag{5}$$

The preceding equations can be written in matrix form as

$$[A]\{\sigma\} = \{F\} \tag{6}$$

where

$$A_{ik} = \psi(\|x^k - x^i\|), \qquad i = 1, \ldots, n_p, \qquad k = 1, \ldots, n_p \tag{7}$$

$$\{\sigma\} = \begin{bmatrix}\sigma_1 & \sigma_2 \ldots \sigma_{n_p}\end{bmatrix}^T \tag{8}$$

$$\{F\} = [f(x^1) \quad f(x^2) \ldots f(x^{n_p})]^T \tag{9}$$

Solving the preceding system of equations uniquely defines the vector $\{\sigma\}$, following which Eq. (4) can be used to estimate the function value at any generic point x in the design domain. An appealing property of the approximation hypersurface defined by $\tilde{f}$ in Eq. (4) is that it passes through all data points used in its construction.

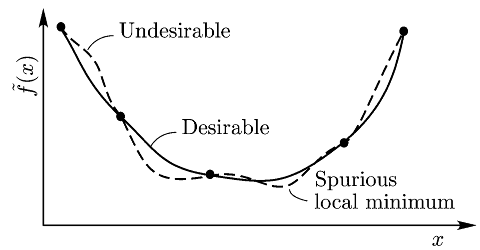


Fig. 2 Distinct metamodels.

B. Unique Solvability of RBFs: A Potential Drawback

Because the system of equations in Eq. (6) is square (that is, equal number of equations and unknowns), there generally exists a unique set of coefficients $\{\sigma\}$ that solves the linear system. As stated earlier, some mathematically oriented publications[23,24] maintain that this unique solvability is a desirable feature of RBFs. In this paper, we propose the notion that within the MDO framework this unique solvability could in fact hinder the prospects of effectively using RBFs because it does not provide the designer with adequate freedom in the metamodel building process. Under the typical RBF approach, the designer cannot impose any requirement regarding the shape of the final metamodel because such a metamodel is fully prescribed by a unique problem formulation. Fictitious local minima typify associated deficiencies.

To further explain, consider Fig. 2. The design variable value is shown on the horizontal axis and the metamodel value on the vertical axis. The solid dots represent the prescribed data points. We show two arbitrary but distinct metamodels that are interpolative solutions. That is, they pass through all of the data points. We importantly note that there exists an infinite set of such metamodels, of differing desirabilities. Specifically, the metamodel shown as a solid line is likely to be more desirable to a designer than the one shown as a dashed line. In particular, the latter contains several spuriously introduced local minima, which could cause serious difficulties—particularly for gradient-based optimization techniques (Fig. 2). The typical RBF approach does not provide the capability of generating a metamodel of choice.

Thus, the two main aspects of the preceding discussion can be summarized as follows: 1) the typical RBF approach provides only a unique interpolative solution to the metamodeling problem, and 2) the typical RBF approach does not provide a means for the designer to express desirable properties for the metamodels. These shortcomings could be detrimental from the point of view of the design process and could potentially result in far-from-optimal design configurations.

In this paper, we present a novel metamodeling method based on RBFs, called the extended radial basis function (E-RBF) approach. The latter allows the designer to impose certain constraints during the metamodel building process, which leads to more effective metamodels, and ultimately better and more competitive designs. We now introduce the notion of the so-called nonradial basis functions (N-RBFs), which provide more freedom and flexibility to the existing multiquadric RBFs. As we shall see in Secs. IV and V, when used in conjunction with RBFs under the E-RBF approach, N-RBFs provide a useful technique that can accurately model a wide range of topographically complex functions.

III. Nonradial Basis Functions

In this section, we present a new class of basis functions, termed nonradial basis functions (N-RBF). Following their development, we discuss some of their important properties, such as convexity. In Sec. IV, we discuss a novel metamodeling approach that uses N-RBFs in conjunction with RBFs.

A. Mathematical Development

The multiquadric RBF is perhaps one of the most effective basis functions among the available RBFs. This observation was the motivation for embedding some of its characteristics within the newly developed N-RBFs, which (as will be seen) yielded highly favorable results in the development of our new metamodel.

Nonradial basis functions, as the name suggests, are not functions of the Euclidean distance r (as defined earlier). Instead, they are functions of the individual coordinates of generic points x relative to a given data point x^i, in each dimension separately. We define the coordinate vector as $\xi^i = x - x^i$, which is a vector of m elements, each corresponding to a single coordinate dimension. Thus, ξ_j^i is the coordinate of any point x relative to the data point x^i along the jth dimension. Figure 3 depicts the difference between the Euclidean distance r used in RBFs and the relative coordinates ξ used for N-RBFs for a two-dimensional case.

The N-RBF for the ith data point and the jth dimension is denoted by ϕ_{ij}. It is composed of three distinct components:

$$\phi_{ij}\left(\xi_j^i\right) = \alpha_{ij}^L \phi^L\left(\xi_j^i\right) + \alpha_{ij}^R \phi^R\left(\xi_j^i\right) + \beta_{ij}\phi^\beta\left(\xi_j^i\right) \tag{10}$$

where α_{ij}^L, α_{ij}^R, and β_{ij} are coefficients to be determined for given problems; and the superscripts L and R indicate left and right, respectively. Figure 4 depicts a generic basis function along one of the dimensions for arbitrary values of α^L, α^R, and β. Note that for the sake of clarity we have not shown the subscripts i, j in the figure. The functions ϕ^L, ϕ^R, and ϕ^β are defined in Table 1. Four distinct regions (I–IV) are depicted in Fig. 4, each corresponding to a row in Table 1.

The proposed N-RBF takes different forms in different regions. It is an nth-order monomial $\alpha\xi^n$ ($n \geq 2$ is an even integer) supplemented by a linear component or tilt ($\beta\xi$) in the central regions between $\xi = -\gamma$ and $\xi = +\gamma$ (regions II and III). Beyond these regions on either side (regions I and IV), the function is linear, such that the function and its first derivative are continuous at $\xi = \pm\gamma$. A small value of γ would result in a smaller curved portion surrounding $\xi = 0$. Thus, γ can be viewed as a smoothness parameter. The parameters γ and n are prescribed. Figure 4a represents the case where the coefficient $\beta = 0$ (no tilt), whereas Fig. 4b depicts the case where $\beta \neq 0$. Specifically, the parameters used to plot Fig. 4 are as follows: $n = 2$, $\gamma = 2.5$, $\alpha^L = 2$, $\alpha^R = 5$, and $\beta = 4$.

For most real-life problems, values of $n = 2$ or 4 are recommended. There is no obvious advantage in terms of performance gain for higher values of n. Suitable values for γ will depend on the magnitudes of the design variables (refer to Sec. V for more details regarding the selection of the γ parameter). However, normalization of the design space, say between 0 and 1, might preclude the need for the designer to choose a value for γ. In general, one would select a high value of γ for better smoothing properties of the metamodels. From our preliminary investigation, however, we observed that the accuracy of the metamodel is not overly sensitive to γ within the range discussed in Sec. V.

Figure 5 shows a plot of the N-RBF in two dimensions. The complete N-RBF for the ith data point is defined as the sum of the individual basis functions in each dimension as

$$\phi_i(\xi^i) = \sum_{j=1}^{m} \phi_{ij}\left(\xi_j^i\right) \tag{11}$$

Table 1 Nonradial basis function

Region	Range of ξ_j^i	ϕ^L	ϕ^R	ϕ^β
I	$\xi_j^i \leq -\gamma$	$(-n\gamma^{n-1})\xi_j^i + \gamma^n(1-n)$	0	ξ_j^i
II	$-\gamma \leq \xi_j^i \leq 0$	$\left(\xi_j^i\right)^n$	0	ξ_j^i
III	$0 \leq \xi_j^i \leq \gamma$	0	$\left(\xi_j^i\right)^n$	ξ_j^i
IV	$\xi_j^i \geq \gamma$	0	$(n\gamma^{n-1})\xi_j^i + \gamma^n(1-n)$	ξ_j^i

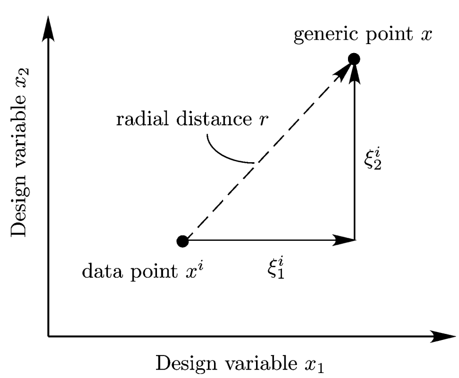


Fig. 3 Definition of coordinate ξ.

B. Necessity of the Tilt Component ϕ^β

We now comment on the critical merit of adding the tilt. Figure 6 shows a simple linear function, $f(x) = 0.5x_1 + 2$, approximated using three techniques: 1) the RBF (Fig. 6a); 2) the E-RBF without tilt, that is, $\phi^\beta = 0$ in Eq. (10) (Fig. 6b); and 3) the E-RBF with tilt (Fig. 6c). The solid dots represent the evaluated data points. We importantly observe that the typical RBF approach, as well as the E-RBF approach without tilt, fail to accurately model the linear

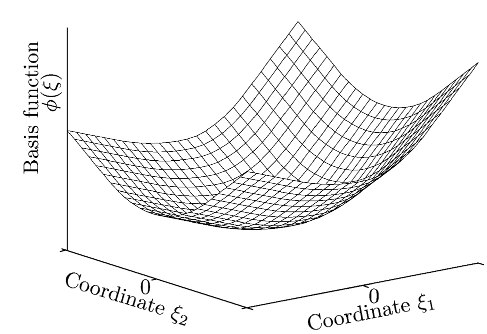
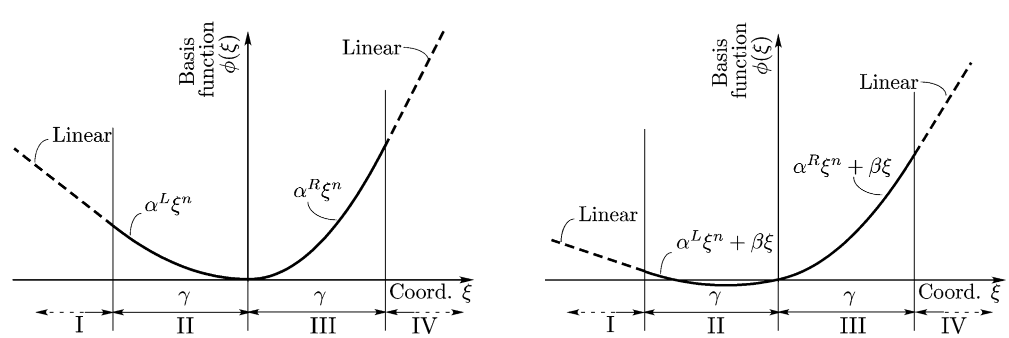
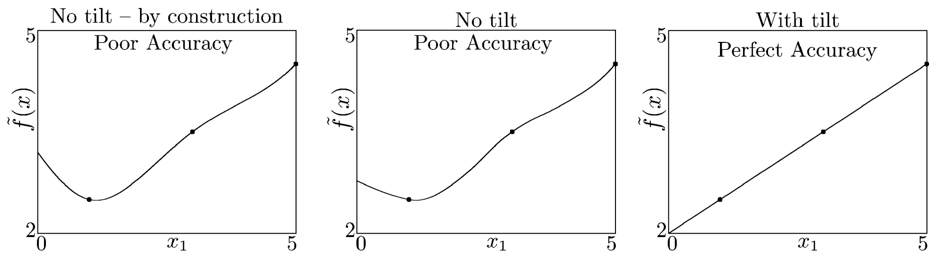


Fig. 5 Nonradial basis function in two dimensions.



a) Without tilt: $\beta = 0$ **b) With tilt: $\beta \neq 0$**

Fig. 4 Development of nonradial basis functions.



a) RBF b) E-RBF, $\phi^\beta = 0$ c) E-RBF, $\phi^\beta \neq 0$

Fig. 6 Critical value of tilt.

function because of the lack of polynomial terms in the approximation function. On the other hand, the E-RBF approach with tilt provides a perfect fit to the linear function. For this simple one-dimensional example, the values of the coefficients are obtained by solving a linear program that constrains the metamodel to be convex. The coefficient values obtained are $\alpha^L = 0$, $\alpha^R = 0$, and $\beta = \{0.4339 \;\; 1.3823 \;\; -1.3161\}^T$. These coefficients are defined in Eq. (10). We discuss the linear programming approach in detail in Sec. IV of this paper.

Thus, by introducing the tilting component ϕ^β we can significantly improve the accuracy of the metamodels for regions of the actual function that are largely linear in nature. As will be seen, the existence of the tilt is but one of the novel features of the E-RBF. Other unique features include the fundamental departure from the Euclidean distance as the argument of the approximating function and the flexibility afforded by the nonuniqueness of the solution process, which is judiciously exploited.

C. Differences Between the Multiquadric and Nonradial Basis Functions

At this stage, it is important to understand the critical differences that make N-RBFs more flexible than the multiquadrics. The following differences are presented with the aid of Figs. 1 and 4:

1) The radial basis functions ψ [Eq. (3)] are characterized by a single coefficient σ, whereas the N-RBFs [Eq. (10)] are characterized by three distinct coefficients α^L, α^R, and β in each dimension. Thus, for an m-dimensional problem, each N-RBF is characterized by $3m$ coefficients, rather than a single one.

2) The multiquadric function [Eq. (3)] is symmetrical about the data point ($r = 0$), whereas in the case of N-RBFs the function is not necessarily symmetrical about $\xi = 0, \alpha^L \neq \alpha^R$ in general. Stated differently, the artificial constraint of radial symmetry in the RBF is not present in the N-RBF.

3) The multiquadric functions do not provide any tilt. The N-RBFs provide additional flexibility in the form of a linear component $\beta\xi$, as shown in Fig. 4b. The no-tilt option is a special case of the E-RBF, where $\beta = 0$.

4) The N-RBFs are uncoupled in terms of the design variables, unlike RBFs. That is, a N-RBF along a given dimension j is independent of the basis function along any other dimensions. Stated differently, the RBF approach imposes constant values circumferentially, while the N-RBF does not. No artificial constraint is imposed by the form of the assumed function. The behavior of the approximation function is governed by the data being interpolated.

The N-RBFs are not a replacement to the typical RBFs: they are instead combined with the conventional RBFs, as discussed in Sec. IV, to yield benefits that neither alone possesses.

D. Convexity of Nonradial Basis Functions

It is important to derive the conditions for the convexity of the N-RBFs defined in Eq. (10) and Table 1. Later in Sec. IV, we use these important properties to impose convexity constraints on the metamodels—when the underlying data allow. One can easily show that if α_{ij}^L and α_{ij}^R are nonnegative, then $\phi_{ij}(\xi_j^i)$ is a convex function of x. (Recall that the prescribed parameter n in the definition of the N-RBFs is an even integer.) Also, because a nonnegative linear combination of convex functions is a convex function, we can conclude that $\phi_i(\xi^i)$, defined in Eq. (11), is convex for all x, if $\alpha_{ij}^L, \alpha_{ij}^R \geq 0$. We also make the observation that the multiquadric function in Eq. 3 is convex for all x. In the next section, we present the E-RBF metamodeling approach, which uses these convexity conditions in obtaining the coefficients.

IV. Metamodeling Using the E-RBF Approach

In this section, we present a metamodeling approach that uses a combination of radial and nonradial basis functions. We term this approach the E-RBF approach. This novel concept possesses the appealing properties of both types of basis functions: the effectiveness of the multiquadric RBFs together with the flexibility of the N-RBFs. We also present a linear-programming-based approach that imposes convexity constraints on the metamodels, when appropriate.

A. Combining Radial and Nonradial Basis Functions

As discussed earlier, the E-RBF approach advances the notion of using more than one basis function for each data point. Specifically, we propose the novel concept of appending the N-RBFs developed in Sec. III to the multiquadric RBFs. Using these two distinct basis functions, we formally define the following approximation function as

$$\tilde{f}(x) = \sum_{i=1}^{n_p} \sigma_i \psi(\|x - x^i\|) + \sum_{i=1}^{n_p} \phi_i(x - x^i) \tag{12}$$

where $\psi(\|x - x^i\|)$ and $\phi_i(x - x^i)$ are defined in Eqs. (3) and (11), respectively. Note that every data point x^i is associated with two distinct but complementary basis functions: 1) the typical RBF defined in Eq. (3) and 2) the basis function defined in Eq. (11). We use the definition of N-RBFs provided in Eqs. (10) and (11) to obtain

$$\tilde{f}(x) = \sum_{i=1}^{n_p} \sigma_i \psi(\|x - x^i\|) + \sum_{i=1}^{n_p} \sum_{j=1}^{m} \left[\alpha_{ij}^L \phi^L\left(\xi_j^i\right) + \alpha_{ij}^R \phi^R\left(\xi_j^i\right) + \beta_{ij} \phi^\beta\left(\xi_j^i\right)\right] \tag{13}$$

where ϕ^L, ϕ^R, and ϕ^β are defined in Table 1. We define the following coefficient vectors and their sizes as

$$\alpha^L = \left\{\alpha_{11}^L \quad \alpha_{12}^L \quad \cdots \quad \alpha_{1m}^L \quad \cdots \quad \alpha_{(n_p)(m)}^L\right\}_{(mn_p)\times(1)}^T \tag{14}$$

$$\alpha^R = \left\{\alpha_{11}^R \quad \alpha_{12}^R \quad \cdots \quad \alpha_{1m}^R \quad \cdots \quad \alpha_{(n_p)(m)}^R\right\}_{(mn_p)\times(1)}^T \tag{15}$$

$$\beta = \left\{\beta_{11} \quad \beta_{12} \quad \cdots \quad \beta_{1m} \quad \cdots \quad \beta_{(n_p)(m)}\right\}_{(mn_p)\times(1)}^T \tag{16}$$

In addition to these vectors, the coefficient vector σ is defined in Eq. (8). The vectors α^R, α^L, and β, just defined, contain mn_p elements each, and the vector σ contains n_p coefficients. Thus, the total number of coefficients to be determined in order to fully define the metamodel in Eq. (13) is given by $n_u = (3m + 1)n_p$.

As we shall see in the following subsection, the E-RBF approach results in an underdetermined system of equations, the resulting freedom of which will be judiciously exploited.

Table 2 Type of linear system of equations for various metamodeling techniques

Method	No. of equations	No. of unknowns	Type of system	Interpolative solutions	Solution approach
RSM[a]	n_p	$(m+1)(m+2)/2$	Overdetermined	None/Unique	Least squares
RBF	n_p	n_p	Square	Unique	Matrix inverse
E-RBF	n_p	$(3m+1)n_p$	Underdetermined	Family	Linear programming

[a]Assuming second-order response surfaces.

B. Exploring the Determinacy of the Resulting Equations

Consider the approximation function in Eq. (13). We are interested in a metamodel that interpolates all of the data points. Accordingly, we force the approximation to be exact at the data points, or $\tilde{f}(x^k) = f(x^k)$, $k = 1, \ldots, n_p$. Thus, the number of independent equations is equal to n_p. We welcome the fact that these equations are linear in the unknowns σ_i, α_{ij}^L, α_{ij}^R, and β_{ij}, $(i = 1, \ldots, n_p,\ j = 1, \ldots, m)$. The number of unknown coefficients is $n_u = (3m+1)n_p$. Because the number of unknowns is more than the number of equations, we have an underdetermined system of linear equations.

It is important at this stage to compare the metamodeling techniques discussed so far in terms of their respective resulting sets of equations. Table 2 makes these differences clear. The column labeled "interpolative solutions" denotes the number of possible metamodels that the method provides (such that each metamodel passes through all of the data points).

The response surface methodology generally results in an overdetermined system because there are usually more equations than unknowns. The least-squares approach is used to solve for the polynomial coefficients [Eq. (1)], and in most cases, it is not an interpolative solution. Metamodeling using typical RBFs [Eq. (4)] requires calculating n_p unknown coefficients: $\sigma_i (i = 1, \ldots, n_p)$, thus resulting in a square system of equations. The E-RBF approach, in contrast, results in an underdetermined system of linear equations, which yields a family of interpolative solutions.

The underdetermined system goes a step beyond the typical RBF approach. Not only does it provide an interpolative solution, but it is also capable of yielding the most desirable solution by imposing appropriate constraints while solving for the unknown coefficients. An underdetermined system can be solved using several approaches. We discuss a solution approach based on linear programming in Sec. IV.C, which allows for the imposition of important convexity constraints.

Before discussing the solution approach, we formulate the system of equations under the E-RBF approach by casting it into a matrix form similar to the typical RBF approach in Eq. (6). To begin, we satisfy the condition of Eq. (13) as

$$\tilde{f}(x^k) = f(x^k), \qquad k = 1, \ldots, n_p \tag{17}$$

Substituting the expression for $\tilde{f}$ from Eq. (13), the preceding conditions lead to

$$\sum_{i=1}^{n_p} \sigma_i \psi(\|x^k - x^i\|) + \sum_{i=1}^{n_p}\sum_{j=1}^{m} \Big[\alpha_{ij}^L \phi^L\big(x_j^k - x_j^i\big) + \alpha_{ij}^R \phi^R\big(x_j^k - x_j^i\big) + \beta_{ij}\phi^\beta\big(x_j^k - x_j^i\big)\Big] = f(x^k), \qquad k = 1, \ldots, n_p \tag{18}$$

In matrix notation, the preceding system of equations can be written as

$$[A]\{\sigma\} + [B]\{(\alpha^L)^T \quad (\alpha^R)^T \quad \beta^T\}^T = \{F\} \tag{19}$$

where $[A]$, $\{\sigma\}$, and $\{F\}$ are defined in Eq. (6), and the coefficient vectors $\{\alpha^L\}$, $\{\alpha^R\}$, and $\{\beta\}$ are defined in Eqs. (14–16). The kth row of matrix B in Eq. (19) is given by

$$B^k = \{B^{Lk} \quad B^{Rk} \quad B^{\beta k}\}_{(1)\times(3mn_p)} \tag{20}$$

where

$$B^{Lk} = \Big[\phi^L\big(x_1^k - x_1^1\big) \quad \phi^L\big(x_2^k - x_2^1\big) \quad \cdots \quad \phi^L\big(x_m^k - x_m^1\big) \cdots \quad \phi^L\big(x_m^k - x_m^{n_p}\big)\Big]_{(1)\times(mn_p)} \tag{21}$$

The vectors B^{Rk} and $B^{\beta k}$ can be obtained from the preceding equation by simply replacing L with R and β, respectively. Equation (19) can now be compactly written in matrix form as

$$[\bar{A}]\{\bar{\alpha}\} = \{F\} \tag{22}$$

where $[\bar{A}] = [A \quad B]$, and

$$\bar{\alpha} = \{\sigma^T \quad (\alpha^L)^T \quad (\alpha^R)^T \quad \beta^T\}^T \tag{23}$$

To contrast the RBF and N-RBF approaches, we compare their systems of equations in Eqs. (6) and (22). In Eq. (6), matrix A is of size $(n_p) \times (n_p)$, σ is a vector of n_p coefficients, and F is a vector of n_p function values. In contrast, in Eq. (22), matrix $\bar{A}$ is of size $(n_p) \times [n_p(3m+1)]$, and $\bar{\alpha}$ is a vector of $n_p(3m+1)$ coefficients. Thus in Eq. (22), there is ample freedom to be exploited. We now discuss a strategy for solving this underdetermined system of equations, which exploits these degrees of freedom to impose convexity constraints on the metamodels, when the underlying data allow.

C. Solving the Underdetermined System of Equations

As just discussed, the proposed solution approach exploits the several extra degrees of freedom available in Eq. (22). Matrix $\bar{A}$ contains more columns than rows, and Eq. (22) possesses a family of interpolative solutions. Under the E-RBF approach, the solution to the underdetermined system of equations results in a metamodel with the desirable properties discussed earlier.

In this paper, we pay special attention to the desirable notion of convexity, as it ensures that the metamodel does not contain spurious local optima that could be a hindrance to the optimization process. We develop a solution approach that can potentially produce convex metamodels, when the underlying data allow. It can be easily shown that the metamodel in Eq. (13) is convex for all x if the coefficients $\{\sigma\}$, $\{\alpha^L\}$, and $\{\alpha^R\}$ are nonnegative. Although these conditions guarantee convexity, there could exist convex metamodels that do not satisfy these nonnegativity constraints. Future research in this area could explore the possibility of discovering less stringent convexity conditions. The preceding nonnegativity constraints can be easily incorporated in a linear-programming problem formulation in the determination of the metamodel as follows:

$$\min_{\{\bar{\alpha}\}} \quad [b^T]\begin{Bmatrix}\sigma \\ \alpha^L \\ \alpha^R\end{Bmatrix} \tag{24}$$

s.t.

$$[\bar{A}]\{\bar{\alpha}\} = \{F\} \tag{25}$$

$$\{\sigma\}, \{\alpha^L\}, \{\alpha^R\} \geq 0 \tag{26}$$

Note that we do not impose any constraints on $\{\beta\}$ [Eq. (16)], which contains the coefficients of the linear component ϕ^β within the N-RBFs. Hence, the vector b, which helps define the objective function, consists of $(2m+1)n_p$ elements. In this work, we have considered b to be a vector of ones. Note that we have chosen to minimize the coefficients because extensive experimentation has shown that doing so yields well-behaved hypersurfaces. Future studies could further explore the structure of the objective function. Accordingly, the preceding linear program minimizes the sum of the nonnegative coefficients, while ensuring that the metamodel remains convex [Eq. (26)] and that it interpolates all data points [Eq. (25)]. In contrast, the typical RBF approach fails to provide any capability to impose such constraints.

D. Alternative Approach to Evaluating Coefficients

In some cases (even if the original function is convex), it is possible that the preceding linear program might not yield a feasible solution. One of the reasons for this infeasibility is our use of conservative convexity conditions [Eq. (26)]. It might be possible for the metamodel to be convex even if some of the coefficients $(\alpha^L, \alpha^R, \sigma)$ are negative. The task of deriving conditions under which the preceding linear program will yield a feasible solution is an interesting one and should be the subject of further investigation.

When the preceding linear program does not yield a feasible solution, we propose using the pseudo-inverse approach to solve the underdetermined system of equations [Eq. (22)] as

$$\{\bar{\alpha}\} = [\bar{A}]^{+}\{F\} \tag{27}$$

where $[\bar{A}]^{+}$ denotes the pseudo-inverse of $[\bar{A}]$. Recall that in the case of underdetermined systems, the pseudo-inverse yields a solution $\bar{\alpha}$, such that $\|\bar{\alpha}\|$ is minimum, that is, $\bar{\alpha}$ is the minimum norm solution. Importantly, we note that we have an interpolating hypersurface, even when we use Eq. (27) to evaluate the coefficients.

After obtaining the coefficients $\bar{\alpha}$ using one of the preceding approaches, one can evaluate the metamodels using Eq. (13). The resulting metamodel is one that is guaranteed to be convex and highly accurate if the linear program [Eqs. (24–26)] yields a feasible solution. In other cases, the pesudo-inverse approach will simply yield a solution that is generally better or comparable in performance to the original RBF approach. In the following section, we present a series of mathematical examples that demonstrate the effectiveness of the E-RBF approach.

V. Numerical Examples

In this section, we compare the performance of three metamodeling techniques: 1) the RSM using a quadratic fit, 2) the typical RBF, and 3) the E-RBF approach developed in this paper. Note that we consider only quadratic polynomials for the RSM because, in general, the analytical form of the actual function would not be available to us to select a polynomial with an appropriate order. Rather, we typically construct metamodels for black-box functions with little or no knowledge of their behavior. Thus, we choose quadratic polynomials in accordance with their wide use in the literature. Also, by keeping the order of the polynomial fixed for all of the following example functions, we ensure that a reasonable comparison can be made across the three metamodeling techniques.

For comparison purposes, we use seven representative mathematical functions (Table 3). Functions 1 and 2 are simple polynomials in two variables constructed by the authors, function 3 is from Hussain et al.,[7] functions 4 and 7 are from Jin et al.,[22] and functions 5 and 6 are from Giunta and Watson.[12] Table 3 also notes the degree of nonlinearity present in the functions and the number of data points used to build the metamodels. The constants $t_j (j = 1, \ldots, 10)$ in the definition of function 7 are as follows: $-6.089, -17.164, -34.054, -5.914, -24.721, -14.986, -24.100, -10.708, -26.662$, and -22.179.

A. Sampling Strategies

For functions 1 and 2, we use a random design sample of 10 points over the design domain. For functions 3 and 4, we use 8×8 and 7×7 grids, respectively, and for functions 5 to 7, we generate a Latin hypercube sample using the LHSDESIGN function in MATLAB®.

B. Selection of Parameters

For the RBF approach, we set $c = 0.9$ [which is a prescribed parameter for the multiquadric functions, Eq. (3)] for all of the examples. Note that the solutions were not sensitive to the value of c. For the E-RBF approach, the parameter γ is set equal to approximately $\frac{1}{3}$ of the average domain size. For instance, for function 1 the domain size is 10, which yields $\gamma \approx 3$. Our preliminary investigations, however, reveal that the E-RBF results are not unduly sensitive to γ. The parameter n is set equal to 2 for all of the functions.

C. Solution Approach

Under the E-RBF approach, we first solve the linear program in Eqs. (24–26), which is expected to yield a convex approximation surface when the actual function is convex (functions 1 and 2). In the case of nonconvex functions (functions 3–7), we use the pseudo-inverse approach given in Eq. (27). For the typical RBF approach, we simply solve the square system of linear equations given in Eq. (6), which yields a unique solution. In the case of the RSM, we fit a simple quadratic model [Eq. (1)] using least-squares regression.

D. Metamodel Accuracy Measures

To measure the accuracy of the resulting metamodels, we use the standard error measure: root-mean-squared error (RMSE).[7,22] Small values of the RMSE are desired. An RMSE value of 0 indicates a perfect fit. The error measure is defined as

$$\mathrm{RMSE} = \left\{ \frac{1}{K} \sum_{k=1}^{K} [f(x^k) - \tilde{f}(x^k)]^2 \right\}^{\frac{1}{2}} \tag{28}$$

where $f(x^k)$ denotes the exact function value for point x^k and $\tilde{f}(x^k)$ is the metamodel value for point x^k. The K additional data points are

Table 3 Function list

No.	Function $f(x)$	m[a]	Design domain	Nonlinearity	n_p[b]
1	$5x_1 - 10x_2$	2	$0 \le x_j \le 10$	None	10
2	$0.5x_1^3 + x_2^2 - x_1x_2 - 7x_1 - 7x_2$	2	$5 \le x_j \le 10$	Low	10
3	$x_1 \sin(x_2) + x_2 \sin(x_1)$	2	$-2\pi \le x_j \le 2\pi$	High	64
4	$[30 + x_1 \sin(x_1)] * \left[4 + \exp\left(-x_2^2\right)\right]$	2	$0 \le x_1 \le 10$ $0 \le x_2 \le 6$	High	49
5	$\sum_{j=1}^{5} \left[\frac{3}{10} + \sin\left(\frac{16}{15}x_j - 1\right) + \sin^2\left(\frac{16}{15}x_j - 1\right) \right]$	5	$-1 \le x_j \le 1$	High	80
6	$\sum_{j=1}^{10} \left[\frac{3}{10} + \sin\left(\frac{16}{15}x_j - 1\right) + \sin^2\left(\frac{16}{15}x_j - 1\right) \right]$	10	$-1 \le x_j \le 1$	High	100
7	$\sum_{j=1}^{10} x_j \left(t_j + \ln \frac{x_j}{x_1 + \cdots + x_{10}} \right)$	10	$0.5 \le x_j \le 10$	Low	200

[a]m = no. of variables. [b]n_p = no. of data points.

randomly sampled in the design space. We use 1000 points for the two-variable problems (functions 1 to 4), 3125 points for the five-variable problem (function 5), and 5000 points for the 10-variable problems (functions 6 and 7).

In addition to the preceding RMSE, we also calculate the normalized root-mean-squared error (NRMSE) as follows:

$$\text{NRMSE} = \left\{ \frac{\sum_{k=1}^{K}[f(x^k) - \tilde{f}(x^k)]^2}{\sum_{k=1}^{K}[f(x^k)]^2} \right\}^{\frac{1}{2}} \times 100 \tag{29}$$

The normalized RMSE allows comparison of the metamodel error values across different functions. The preceding error measure represents the percent error in the metamodel. A value of NRMSE = 0 indicates a perfect fit, whereas a high value of NRMSE indicates a poor fit.

The metamodel error values and the NRMSE values are provided in Table 4. The least RMSE and NRMSE values for each function are shown in boldface in Table 4. Figures 7–10 show the plots of the actual function and of the associated metamodels using the preceding three techniques (for the two-variable functions).

E. Results and Discussion

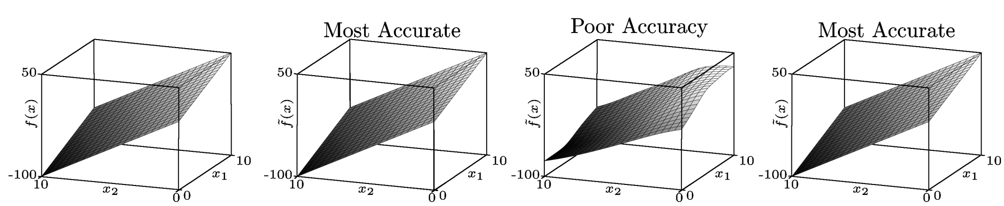
1. Functions 1 and 2

Referring to Fig. 7 and the error measures in Table 4, we can see that the E-RBFs result in a perfect fit to the linear function (function 1). This is a result of solving the linear-programming problem [Eqs. (24–26)], which ensures convexity of the metamodel over the entire design domain. The radial basis functions, on the other hand, yield an imperfect metamodel and one that is not convex over the design domain. The error is particularly evident by examining the top right and bottom left of Fig. 7c. In addition, the RBF approach does not provide any flexibility to correct such an error.

The convexity of the metamodel using the E-RBF approach ensures that the resulting metamodel is devoid of spurious local

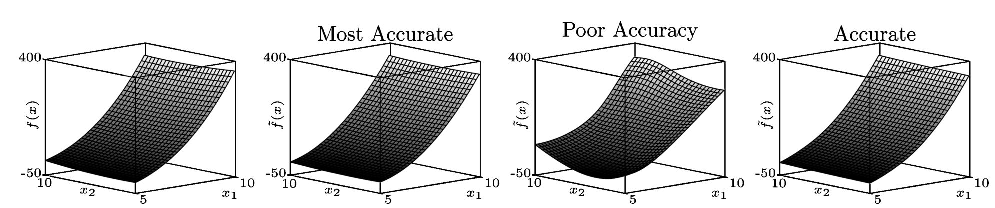
Table 4 Metamodel accuracy results for functions 1–7

Function	No. of vars.	RSM RMSE	RSM NRMSE	RBF RMSE	RBF NRMSE	E-RBF RMSE	E-RBF NRMSE
1	2	**0.0000**	**0.00**	4.2500	10.39	**0.0000**	**0.00**
2	2	**2.9094**	**1.70**	17.6243	10.31	3.9705	2.32
3	2	3.3894	91.84	**0.2816**	**7.63**	**0.2816**	**7.63**
4	2	16.3495	12.67	1.3702	1.06	**1.2345**	**0.96**
5	5	0.3073	27.66	0.2131	19.18	***0.0180***	***1.62***
6	10	0.4849	25.06	0.2628	13.58	***0.0325***	***1.68***
7	10	**0.5626**	**0.051**	18.2715	1.65	0.6991	0.063



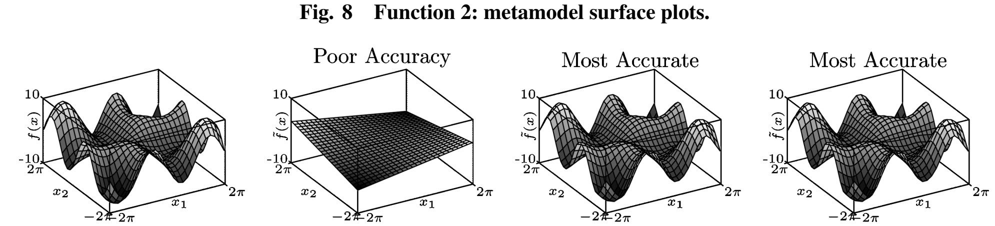
a) Actual function **b) RSM** **c) RBF** **d) E-RBF**

Fig. 7 Function 1: metamodel surface plots.



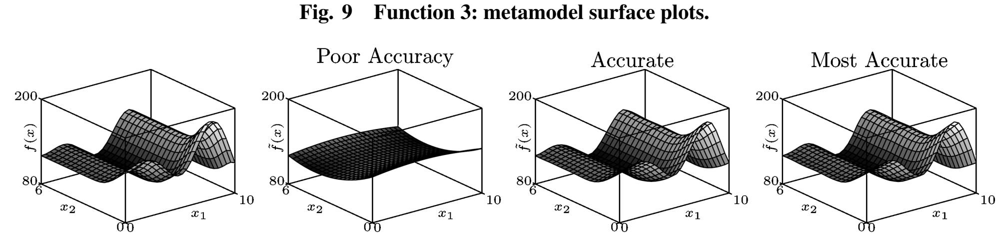
a) Actual function **b) RSM** **c) RBF** **d) E-RBF**

Fig. 8 Function 2: metamodel surface plots.



a) Actual function **b) RSM** **c) RBF** **d) E-RBF**

Fig. 9 Function 3: metamodel surface plots.



a) Actual function **b) RSM** **c) RBF** **d) E-RBF**

Fig. 10 Function 4: metamodel surface plots.

minima. Note that the RBF approach does not provide a systematic way to promote unimodality or convexity; it is likely to produce metamodels with irregular surfaces and possibly spurious local minima. As a consequence, the metamodel error using the typical RBFs is significantly higher than that using the E-RBF approach (Table 4).

The response surface methodology expectedly yields a perfect fit because it uses a quadratic polynomial. Similar results are obtained for function 2, which is a cubic polynomial. Figure 8 shows that the typical RBF approach again fails to accurately model the function. The E-RBFs again, by contrast, result in a highly accurate and convex metamodel.

2. Functions 3 and 4

Figures 9 and 10 show the surface plots for functions 3 and 4, respectively. These functions are highly nonlinear in nature. From the error values given in Table 4, we can see that the RSM is inadequate in handling such functions, whereas both the RBF and E-RBF approaches provide accurate metamodels. Note that we have used the pseudo-inverse approach [Eq. (27)] in the case of the E-RBF approach.

3. Functions 5–7

Functions 5 to 7 are larger problems with 5 and 10 variables. The error measures, RMSE and NRMSE, are provided in Table 4. The performance of the E-RBFs for functions 5 and 6 is particularly noteworthy, as is evident from the results. The error measures for functions 5 and 6 are shown in italicized boldface in the case of the E-RBFs to show their marked improvements in comparison to the error measures obtained using the RBF approach and the RSM. Indeed, the RMSE values obtained using the E-RBFs for these two functions are almost 1/10 of those obtained using the RBFs. The RMSE values for the E-RBF approach are also significantly lower than those obtained for the RSM, reported in Giunta and Watson[12] under similar conditions. The poor performance of the RSM for functions 5 and 6 can be attributed to the presence of sinusoidal terms in these functions (Table 3), which a quadratic polynomial cannot effectively capture over a large domain.

Function 7 is a 10-variable example, but the nonlinearity level is low. As such, the RSM performs satisfactorily (RMSE = 0.5626), whereas the RBFs yet again fail to provide a good fit. The E-RBF approach, on the other hand, performs almost as well as the RSM with an RMSE of 0.6991.

F. Additional Computational Expense Using E-RBF

In general, the linear optimization problem under the E-RBF approach requires more computational effort compared with that required to solve a system of linear equations (RBF or RSM). The linear-programming approach is used for functions 1 and 2, but both of these examples are small-scale examples with two variables and 10 data points. In such cases, the computational expense for all three metamodeling techniques is approximately the same (less than 1 s on a single 1.5-GHz processor). For large-scale problems, the linear program will require more computational effort than the square system of equations (RBF) or the least-squares fit (RSM), and a detailed investigation is warranted for such cases.

In the present paper, we have used the pseudo-inverse approach for nonconvex problems (functions 3–7). Under the E-RBF approach, we need to handle a matrix with $3mn_p$ more columns than that using the typical RBF approach. For functions 3–7, on average, the RSM and the RBF approach required 0.02 s for model fitting using MATLAB on a 1.5-GHz processor, whereas the E-RBF approach, on average, required 0.843 s. This additional expense, though, will generally be negligible in the context of the potential applications [finite element analysis (FEA), computational fluid dynamics (CFD)] that are being considered. The computational effort required for a single FEA or CFD simulation could be on the order of several hours to even several days. Thus, the preceding increased computational effort required for E-RBF can be considered insignificant. Also, more efficient solvers can be used to solve the underdetermined system of equations [Eq. (27)], which take into account special properties of the system of equations (such as symmetry), further reducing the computational expense.

A common theme emerging from the preceding results is that the E-RBFs perform consistently well under widely varying conditions, such as simple polynomial functions and highly nonlinear large-scale problems. On the contrary, the RSM tends to perform well for problems with low nonlinearity, and the RBF approach performs satisfactorily for highly nonlinear problems, although it did not perform adequately for the functions 5 and 6 considered in this study. Following these promising results in favor of the E-RBF approach, its applicability for large-scale problems ($m > 100$) can be investigated in the future.

Under the E-RBF approach, as we saw in the case of functions 1 and 2, we were able to impose convexity constraints to obtain metamodels that are guaranteed to be convex under some given conditions. A logical next step is to consider incorporating different constraints within the E-RBF formulation to handle other critical issues in addition to convexity.

VI. Conclusions

In this paper, the extended radial basis function (E-RBF) approach to metamodeling is presented, where the novel idea of more than one basis function for every data point is proposed and successfully implemented. A new class of basis functions—nonradial basis functions—which offer more flexibility than the typical multiquadric RBFs, is developed. In contrast to the typical RBF approach, which yields a square system of linear equations, the E-RBF approach results in an underdetermined system of linear equations, which leads to a family of interpolative solutions. The additional degrees of freedom in such a linear system provide a more flexible metamodeling environment, where the designer can express important requirements in the form of constraints in a linear-programming problem. A series of mathematical examples demonstrate the effectiveness of the E-RBF approach under widely varying conditions, such as simple polynomial functions and highly nonlinear large-scale functions.

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