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Radial Basis Surrogate Model Integrated to Evolutionary Algorithm for Solving Computation Intensive Black-Box Problems

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Abstract**—**For design optimization with high-dimensional expensive problems, an effective and efficient optimization methodology is desired. This work proposes a series of modification to the Differential Evolution (DE) algorithm for solving computation Intensive Black-Box Problems. The proposed methodology is called Radial Basis Meta-Model Algorithm Assisted Differential Evolutionary (RBF-DE), which is a global optimization algorithm based on the meta-modeling techniques. A meta-modeling assisted DE is proposed to solve computationally expensive optimization problems. The Radial Basis Function (RBF) model is used as a surrogate model to approximate the expensive objective function, while DE employs a mechanism to dynamically select the best performing combination of parameters such as differential rate, cross over probability, and population size. The proposed algorithm is tested on benchmark functions and real life practical applications and problems. The test results demonstrate that the proposed algorithm is promising and performs well compared to other optimization algorithms. The proposed algorithm is capable of converging to acceptable and good solutions in terms of accuracy, number of evaluations, and time needed to converge.

Keywords**—**Differential evolution, engineering design, expensive computations, meta-modeling, radial basis function, optimization.

I. Introduction

IN today's world, there exist many computationally intensive and expensive mathematical or physical models and engineering problems. To solve these computationally expensive problems, an enormous number of fitness function evaluations are required during the evolution process when evolutionary algorithms (EAs) are used. To be able to solve these problems, it is very crucial to wisely explore and search the design space. Recently, EAs based surrogate models have attracted much attention [1]. In such algorithms, a meta-model also known as surrogate model is used to evaluate the objective function by constructing an approximate model [2]. Over the last few decades, many surrogate models have been proposed such as Kriging [3], polynomials [4], and RBF [5].

Global optimization using approximated or surrogate model based on search methods has attracted considerable interests lately due to their high efficiency, robustness, and ease of implementation. Giunta and Watson [6] and Forrester and Keane [7] have used analytical test problems with different design variables to compare response surface approximations, and Kriging [8] and Queipo [9] have reviewed different surrogate models used in various aerospace applications. Kaymaz and McMathon [10] introduced the ADAPRES method, in which a weighted regression scheme is applied instead of normal regression. Experimental points are selected from a region where the design point is most likely to exist. Schonlau et al. [11] presented a sequential algorithm to balance local and global searches using approximations for constrained optimization. Sasena et al. [12] used Kriging models for disconnected feasible regions. Osio and Amon in [13] developed a multistage Kriging strategy to sequentially update and improve the accuracy of surrogate approximations.

The use of surrogate models has largely contributed towards reducing the computations required to converge to the global solutions for the computationally intensive engineering design problems. These meta-models replace the expensive black-box functions with cheap, easy to construct, and visible functions that do not require powerful personal computers PCs and does not take much time to evaluate. The RBF or model, which is used in this work, has proven to be one of the most promising models for noisy, and highly non-linear functions.

DE, which is a heuristic and natural inspired optimization algorithm, has been used in many engineering and non-engineering fields because of its capabilities of yielding reasonable results that engineers can easily rely on in making their decisions. DE has also shown advantageous convergence properties and remarkable robustness. Cuevas et al. [14] introduced a circle detection method based on DE. Kettani et al. [15] proposed a quantum differential evolutionary algorithm for the independent set problem. Dattatray et al. [16] included an application of DE for the optimal operation of multipurpose reservoir. The objective of their study was to maximize the hydropower production.

The question that needs to be answered is how long it takes to search and converge to a global solution. For that reason, using meta-models to assist DE is considered as a promising approach. Combing and utilizing the EA and RBF met-model advantages will increase the convergence speed. Hence, reducing the number of expensive function and constraints evaluations. DE is introduced in the next section to give an idea how such algorithm functions.

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II. Differential Evolution

DE is arguably one of the most powerful stochastic optimization algorithms in recent time. DE operates through the same computational steps as EA. However, unlike traditional EAs, the DE-variants perturb the current generation population members with the scaled differences of randomly selected and distinct population members. Therefore, no separate probability distribution has to be used for generating the offspring. Since it was introduced in 1995, DE has been continuously developed by many researchers resulting in a lot of variants of the originally introduced algorithm with improved performance.

DE is an evolutionary stationary optimization method that is fairly fast and reasonably robust. DE, which is originally due to Storn and Price [17], [18], is a method that optimizes a problem by iteratively trying to improve a candidate solution with regard to a given measure of quality. Such methods are commonly known as metaheuristics as they make few or no assumptions about the problem being optimized and can search very large spaces of candidate solutions. However, metaheuristics such as DE do not guarantee converging to an optimal solution, yet it efficiently explores and searches the design space. DE is used for multidimensional real-valued functions but does not use the gradient of the problem being optimized, which means that DE does not require for the optimization problem to be differentiable as it is required by classic optimization methods such as gradient descent and quasi-newton methods. DE can therefore also be used on optimization problems that are not even continuous, are noisy, change over time, etc. [19] What makes DE a powerful algorithm is its capability of handling non-differentiable, nonlinear, and multimodal objective functions. It has been used to train neural networks having real and constrained integer weights [20], [21].

In a population of potential solutions within an n-dimensional search space, a fixed number of vectors are randomly initialized, then evolved over time to explore the search space and to locate the minima of the objective function. At each iteration, called a generation, new vectors are generated by the combination of vectors randomly chosen from the current population (mutation). The outcoming vectors are then mixed with a predetermined target vector. This operation is called recombination and produces the trial vector. Finally, the trial vector is accepted for the next generation if and only if it yields a reduction in the value of the objective function. This last operator is referred to as a selection. In the other words, DE optimizes a problem by maintaining a population of candidate solutions and creating new candidate solutions by combining existing ones according to its simple formulae, and then keeping whichever candidate solution has the best score or fitness on the optimization problem at hand. In this way, the optimization problem is treated as a black box that merely provides a measure of quality given a candidate solution and the gradient is therefore not needed. In DE, the choice of DE parameters, differential weight [0 2], crossover probability [0 1], and population size [≥4] can have a large impact on optimization performance. Selecting the DE parameters that yield good performance has therefore been the subject of much research.

III. Meta-Modeling

Approximation models or meta-models (surrogate models) play a major role in the meta-models based global design optimization. The meta-model in simple and easy-to-calculate form is used to replace the original, black-box computer analysis and simulation model. The introduced meta-model also provides an insight to the optimization problem by visualizing the interactions among design variables, objective functions, and constraints. The overall objective is to reduce the computation cost of computationally intensive design simulations and analyses, using inexpensive surrogates of these analyses and simulations [22].

The main benefits of meta-models can be summarized as follows:

- It is much cheaper to evaluate a meta-model than to perform a complex computer simulation. This yields a reduction in computational effort where many function evaluations are necessary (e.g. in optimization or stochastic analyses).
- By the use of meta-models, the designer can easily explore the entire design space to get a more profound understanding of the system under investigation.
- Meta-models can be used to combine information gathered from different sources, for instance analysis codes for different disciplines (e.g. fluids, structures, or thermodynamic problems), or physical experiments and computer simulations.
- Parallel computing is simple since in general the individual sampling points are appointed simultaneously. Hence, the necessary computer experiments can be performed independently and in parallel.
- Meta-models can be used to the smooth response values if noise is present in the observations.
- In the next section, RBF model, which is used in this paper, is introduced.

IV. Radial Basis Function

Originally introduced by Hardy [23] and further improved by Dyn et al. [24], RBF is an effective algorithm for smoothing and interpolating the experimental data. The form of the approximate model is a basis function of the Euclidean distance between the sampled data point and the point to be predicted. Developed as an analytical method for representing irregular surfaces, RBF uses linear combinations of radial symmetric functions of the Euclidean distance to build approximation models.

Mathematically, the model can be expressed as shown in (1).

$$\hat{y}(x) = \sum_{i=1}^{N} w_i\, \varphi(\|x - c_i\|) \qquad (1)$$

where the approximated function $\hat{y}(x)$ is represented as a sum of N RBF φ, each associated with a difference center c_i and weighted by an appropriate coefficient, w_i RBF approximation is capable of producing good fits to arbitrary contours of both deterministic and stochastic response functions [25]. The radial function $\varphi(r)$ can take many forms as shown in Table I.

TABLE I
RBF FORMS

Function Type	Radial Basis Form
Linear Function	$\varphi(r) = r$
Cubic Function	$\varphi(r) = r^3$
Thin Plate Function	$\varphi(r) = r^2 \log r$
Multi-quadratic Function	$\varphi(r) = \begin{cases} \sqrt{r^2 + a^2}, & r > 0 \\ 0, & r > 0 \end{cases}$
Gaussian Function	$\varphi(r) = e^{-ar^2}$

V. DE BASED RBF MODEL (RBF-DE)

There has been much attention to hybrid optimization algorithms in the past few decades; recently, more attention is given to the optimization algorithm based meta-modeling techniques. Recently, researchers are interested in combining meta-models (either Kriging, polynomial, RBF, etc.) and evolutionary algorithms (EA) [26], which is one of the categories of nature-inspired global optimization approaches that have been around for many years in dealing with the different types of optimization problems. Over the years, considerable progress has been achieved in developing more flexible, capable, and efficient nature-based global optimization methods. Nature-based algorithms are based on random observations that give different final solutions each run, starting from an identical initial point. Specifically, EA population based approaches deal with a set of candidate solutions that can be improved via a number of iterations. Evolutionary algorithms are the optimization algorithms based on the Darwin's principle [27] which uses the four general steps: reproduction, crossover, mutation, and selection. Finally, the fitness function is used to reach the optimal solution. DE belongs to EA family. In this paper, RBF model is utilized to assess DE in the search for the global solution of black-box functions. The integration of DE and RBF is unique in terms of the search capability and the speed of convergence. In this paper, many benchmark test problems were tested, and the promising results were reported.

VI. DESCRIPTION OF THE ALGORITHM

Fig. 1 explains how the proposed algorithm searches and converges to global solution.

VII. VALIDATION

The goal of any global optimization method is to find the best possible solutions among many other local solutions. The Benchmark test functions shown in Table II were used to evaluate the proposed algorithm' robustness, capability and efficiency over Convex and Non-Convex functions shown in Fig. 2.

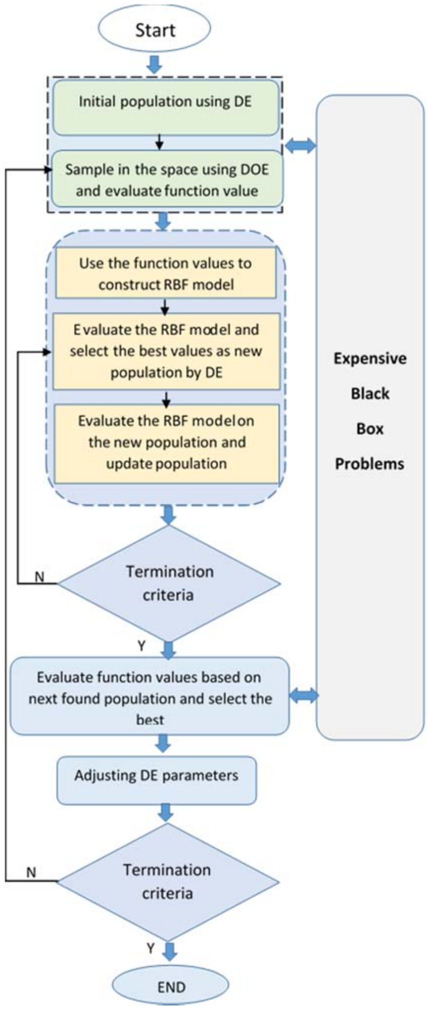

Fig. 1 RBF-DE proposed method flowchart

TABLE II
BENCHMARK FUNCTIONS

Symbol	Search space	
Alpine	[-10 10]	$f(x) = \sum_{i=1}^{n} \lvert x_i \sin(x_i) + 0.1x_i \rvert$
Zakharo	[-5 10]	$f(x) = \sum_{i=1}^{n} x_i^2 + \left(\frac{1}{2}\sum_{i=1}^{n} ix_i\right)^2 + \left(\frac{1}{2}\sum^{ni=1} ix_i\right)^4$
ACKELY	[-5.12 5.12]	$f(x) = -20e^{-0.2\sqrt{\frac{1}{n}\sum_{i=1}^{n} x_i^2}} - e^{\frac{1}{n}\sum_{i=1}^{n}\cos(2\pi x_i)} + 20 + e$
SARGAN	[-10 10]	$f(x) = \sum_{i=1}^{n} n\left(x_i^2 + 0.4\sum_{i \neq j}^{n} x_i x_j\right)$

VIII. PERFORMANCE TEST RESULTS

The principal objective of this paper is to increase the performance of the DE algorithm for expensive black-box problems. A series of modifications has been proposed, and RBF-DE can find the optimum with remarkably fewer NFE. In order to prove this assertion, the performance of DE algorithm has been compared to the modified version on four standard with different dimensional test problems. Table III shows a summary of these results. It is notable that, for a fair comparison, the same stopping criteria have been used for the original DE algorithm.

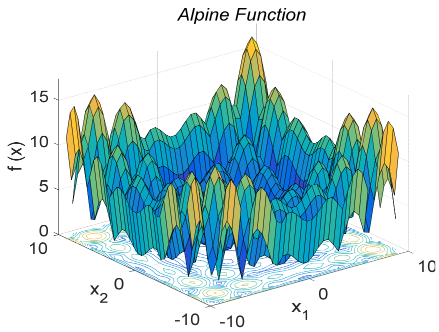

Fig. 2 Alpine function

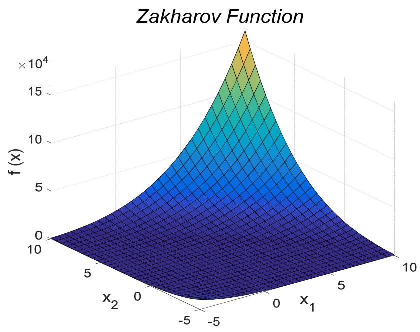

Fig. 3 Zakharov function

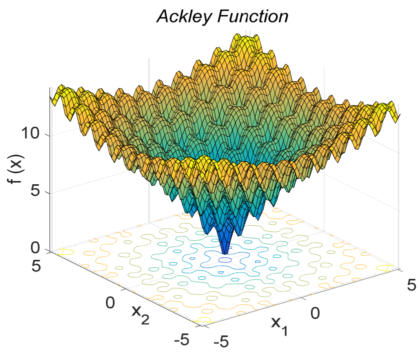

Fig. 4 Ackely function

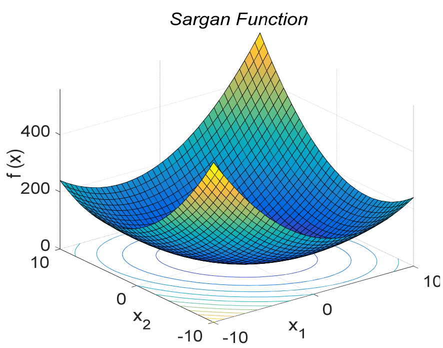

Fig. 5 Sargan function

The history of convergence in both methods can clarify the effect of the proposed modification. Figs. 6 (a)-(d) show the convergence rate of 2-variable, 3-variable, 6-variable and 10-variable test problems. One can see that in order to reach the same accuracy, the NFE required by the RBF-DE is significantly smaller than that for the original DE algorithm.

TABLE III
COMPARISON RESULTS

f	D	DE			RBF-DE		
		*f**	N.F.E	K	*f**	N.F.E	K
Alpine	2	2.9991E-5	2500	90	3.8275E-5	452	28
Zakharov	3	8.9691E-6	2500	98	2.1773E-5	659	34
Ackley	6	4.2960E-4	5000	200	4.5061E-4	973	80
Sargan	10	7.3774E-4	6250	260	2.8522E-5	1061	76

N.F.E= Number of Function evaluations, K= Number of Iterations

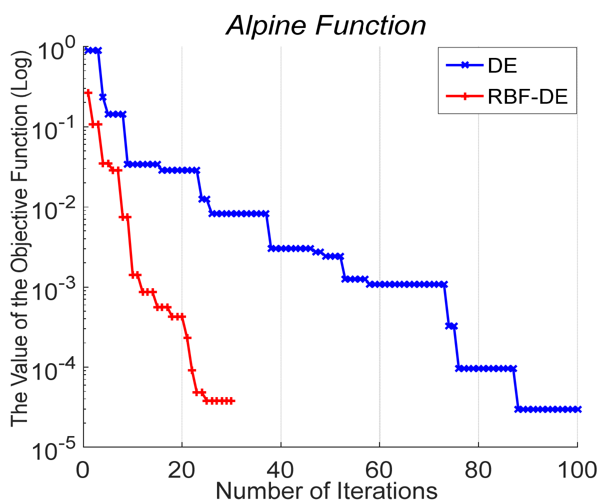

Fig. 6 (a) Convergence rate of Alpine function

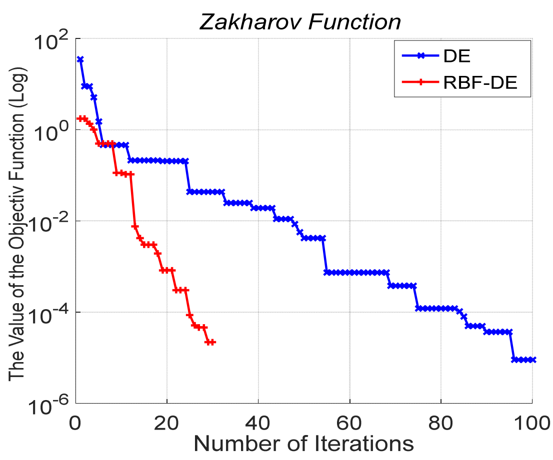

Fig. 6 (b) Convergence rate of Zakharov function

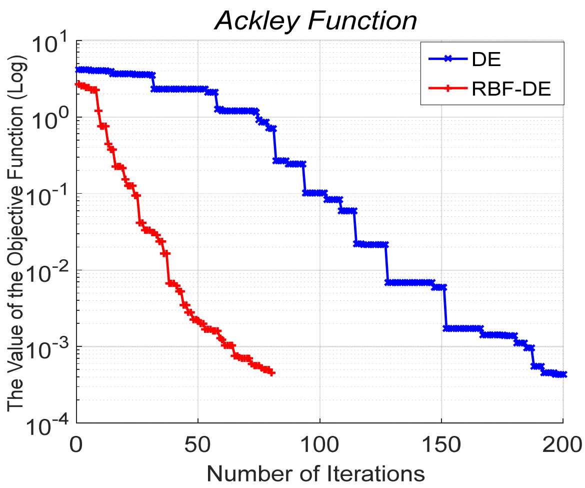

Fig. 6 (c) Convergence rate of Ackley function

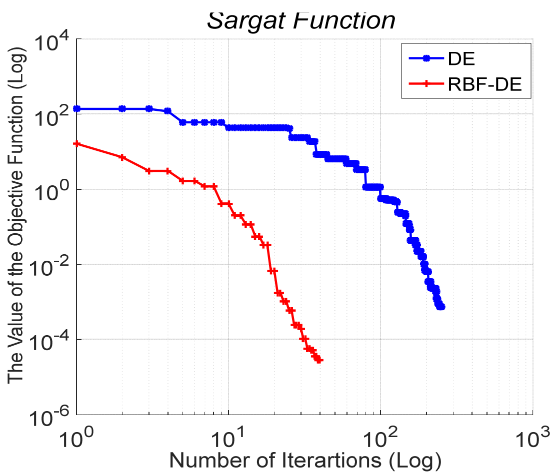

Fig. 6 (d) Convergence rate of Sargat function

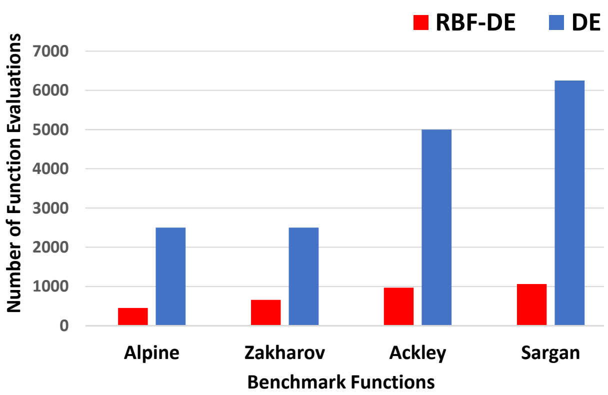

Fig. 7 Number of function evaluations in RBF-DE *versus* DE

Fig. 7 illustrates the required NFE in RBF-DE versus DE method for all test functions. In each case, the horizontal axis shows the function, while the vertical axis demonstrates its corresponding NFE. It is evident from these graphs that the proposed method not only decreases the required NFE, but also gives the user the opportunity to reach more accurate solutions at the cost of a much lower number of samples.

The main focus of this modification was to increase the performance of DE algorithm on expensive black-box problems. As we have expected, the performance of DE method has been increased for solving expensive functions is explicit.

IX. Conclusion

DE algorithm is found to be costly for expensive black-box problems with an exponentially increasing demand for function evaluations. In this work, modification of original DE was achieved by integrating RBF model with DE and progressive reduction on the search region is evident. The proposed RBF-DE has been benchmarked using four standard tests, and the performance increase has been illustrated and discussed. At the end, it is notable that the exponentially increasing demand of DE algorithm for function evaluations in expensive black-box problems has been replaced with the new strategy. This makes RBF-DE method a suitable choice for high cost functions, although further improvements are needed to make it more efficient for high expansive black-box (HEBB) problems.

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