International Journal of Engineering Sciences 2020 13(1) 21-28

INTERNATIONAL JOURNAL
OF
ENGINEERING SCIENCES

Mixture Surrogate Models for Multi- Objective Optimization

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(Received 2 January 2020, accepted 5 April 2020)

Doi: https://doi.org/10.36224/ijes.130104

Abstract

Multi-objective optimization problems (MOOP) involve minimization of more than one objective functions and all of them are to be simultaneously minimized. The solution of these problems involves a large number of iterations. The multi- objective optimization problems related structural optimization of complex engineering structures is usually solved with finite element analysis (FEA). The solution time required to solve these FEA based solutions are very high. So surrogate models or meta- models are used to approximate the finite element solution during the optimization process. These surrogate assisted multi- objective optimization techniques are very commonly used in the current literature. These optimization techniques use evolutionary algorithm and it is very difficult to guarantee the convergence of the final solution, especially in the cases where the budget of costly function evaluations is low. In such cases, it is required to increase the efficiency of surrogate models in terms of accuracy and total efforts required to find the final solutions.In this paper, an advanced surrogate assisted multi- objective optimization algorithm (ASMO) is developed. This algorithm can handle linear, equality and non- linear constraints and can be applied to both benchmark and engineering application problems. This algorithm does not require any prior knowledge for the selection of surrogate models. During the optimization process, best single and mixture surrogate models are automatically selected. The advanced surrogate models are created by MATSuMoTo, the MATLAB based tool box. These mixture models are built by Dempster- Shafer theory (DST). This theory has a capacity to handle multiple model characteristics for the selection of best models. By adopting this strategy, it is ensured that most accurate surrogate models are selected. There can be different kind of surrogate models for objective and constraint functions. Multi-objective optimization of machine tool spindle is studied as the test problem for this algorithm and it is observed that the proposed strategy is able to find the non- dominated solutions with minimum number of costly function evaluations. The developed method can be applied to other benchmark and engineering applications.

Keywords: Multi Objective Design Optimization, FEA, DST, Surrogate Models, FEA, RBF, NHV

1. Introduction

The real engineering problems have a large number of design variables and constraints. In such cases the number of objective functions is more than one and sometimes is conflicting nature. This class of optimization is termed as multi- objective optimization problem (MOOP). It is not possible to minimize all the objective functions simultaneously [3], and after performing some optimization cycles, there comes a stage when it is not possible to reduce objective function without increasing the other. This set of results is identified as the non- dominated, Pareto-optimal or Pareto-Front solution and the main objective of any MOOP solving algorithm is to determine the Pareto-front. In this paper, an advanced surrogate assisted multi- objective optimization (ASMO) algorithm is developed. This algorithm can handle linear, equality and non- linear constraints and can be applied to both benchmark and engineering applications.

This paper is organized in the following six sections: in Section II, the literature review and surrogate assisted optimization methods are presented along with the details of preset method

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ISSN 0976 – 6693.

used in this study. Section III explains the methodology developed for the creation of mixture surrogate model. In Section IV, details of developed algorithm ASAMO are provided for solving MOOP. In Sections V, the introduced techniques are applied on an engineering application of multi- objective optimization of machine tool spindle design. Section VI provides the details of key results and their discussion. In Section VII, overall conclusions of the studies are provided.

2. Literature review

MOOP solving is roughly divided into categories based on the solution techniques. These are of evolutionary and non- evolutionary types. NSGAII is an evolutionary type of MOOP solving algorithm (EMO) and was developed by Deb [4]. Nain et al. [15] have used the Artificial Neural network as a surrogate model and used it in combination with NSGA-II. Datta et al. [2] have developed a surrogate model-based evolutionary algorithm (SMES-RBF) which can handle constrained MOOP. Kunakote et al. [11] used different types of surrogate models with SPEA-II to study their effect on Pareto- optimal solutions. Knowles, J. [9], has developed a surrogate assisted algorithm, also known as ParEGO (Pareto- efficient global optimization), for solving. This algorithm utilizes Kriging as a surrogate model. Bhattacharjee et al. [1] have developed a surrogate assisted evolutionary algorithm (SAMO) to solve the constrained MOOP. In the related studies by authors ([6], [7] and [8]), the findings of surrogate assisted optimization are discussed. In this work, we used Dempster-Shafer Theory (DST) [13] for the development of advanced surrogate model for objective functions and constraints which takes into consideration several model characteristics for best model selection. Pradip Peter Dey et al. [17] presented a procedure for Dynamic Modeling. Srinivas Soumitri Miriyala and Kishalay Mitra [18] discussed the problems in using computationally expensive models for optimization. Byounghee Kim et al. [19] presented a neural network architecture for data modeling.

2.1. Surrogate models

Surrogate Model (also known as metamodels) is a model of a model. The computationally expensive simulation models are used to describe complex physical behaviour. The surrogate models are used to replace the computationally expensive function evaluations [13]:

$$f(x) = s(x) + e(x) \tag{1}$$

Here $f(x)$ shows the output of computationally expensive simulation model, $s(x)$ denotes the prediction of the surrogate model at point x, and $e(x)$ is the error function.

During the iterative optimization procedure, the surrogate model $s(x)$ is used instead of the true objective function $f(x)$ as much as possible because $s(x)$ is computationally cheap to evaluate. With this approach, computational times can be drastically reduced. The surrogate model $s(x)$ is built in the design space with minimum error $e(x)$. This robust surrogate model is used to predict the objective and constraint function values of points in the variable domain, and this information is then utilized for determining promising points (infill points) for doing the expensive function evaluations.

3. Mixture Surrogate Models

For solving single objective function problems, an algorithm has been developed by authors on the basis of dynamic partitioning based surrogate assisted optimization (DPSO) [5], which utilizes the advanced surrogate model-techniques as discussed above. DPSO is a surrogate model based optimization algorithm, which can locate all the local and global minima accurately for the benchmark and real application problems, with minimum function evaluations. The framework developed in the DPSO for the development of advanced surrogate models is extended for this algorithm also by following the below steps:

Step 1: Data points selection for a partition.

Step 2: Build the library of the M surrogate model from these data points. The mixture surrogate models are prepared by following expression.

$$f(x) = \sum_{i=1}^{M} w_i f_i(\mathrm{x}) \qquad (2)$$

Step 3: Metamodel characteristics (error metrics) are calculated by performing the actual simulations and predicted function values at each data point.

Step 4: There can be more than one surrogate model characteristics which can be conflicting in nature.

Step 5: Use DST to develop best single and mixture surrogate models by MATsuMoTo Toolbox [14].

4. Advanced Surrogate Assisted Multi-objective Optimization Algorithm (ASAMO)

In the current research, the concepts of SAMO- surrogate assisted multi-objective optimization (by Bhattacharjee et al. [1]) are developed further by improving the convergence properties of the final Pareto- optimal solution. This work utilizes the NSAGA-II [4] as basic EA.

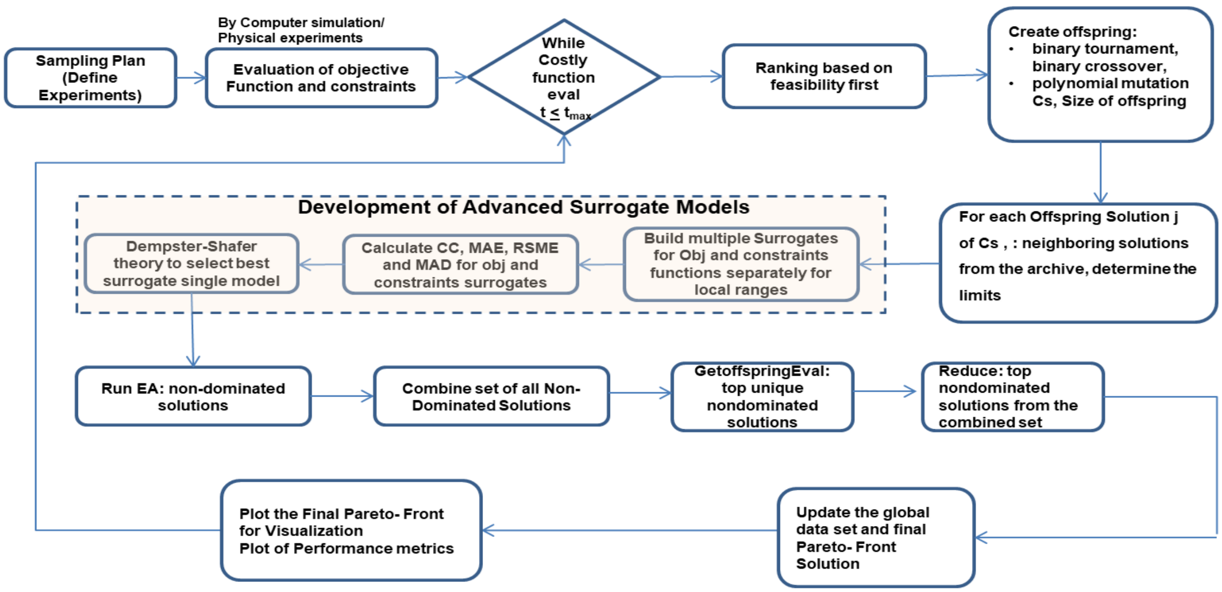

Figure 1: Advanced Surrogate Assisted Multi-objective Optimization Algorithm (ASAMO)

In this research, the concepts of original SAMO [1] are used as a framework for our purpose. The original SAMO is base lined with the following improvements:

- For the choice of the finest metamodel, Matlab [12] based MATSuMoTo [14] is used, which utilizes DS theory to combine the effect of four surrogate model characteristics. This improved the performance of the original algorithm.
- MATSuMoTo toolbox can utilize parallel pool computations which allows parallel computations for the simultaneous generation of multiple surrogates

This is achieved by improvements with reference to the development of advanced metamodels. For further details, the reference [1] can be referred. The shaded boxes in the dotted lines show the areas of improvements in SAMO.

5. Numerical analysis

In the surrogate-based multi-objective problem solution approach, non- dominated (Pareto- front) solutions are obtained by approximation of these functions by equivalent surrogate models (s_i *and* $\hat{g}_j$) .The problem is formulated as follows [1] :

$$min\ [s_1(x),\ s_2(x),\ ,\dots, s_m(x)]^T \tag{3}$$

subjected to $\hat{g}_j(x) \leq 0$, j = 1, 2,….,k

$$x_j^l \leq x_j \leq x_j^u, \qquad j = 1, 2, \dots., d$$

The concepts developed in the above sections are applied to the real engineering applications related to optimization of machine tool spindle design. The real engineering application is chosen instead of mathematical benchmark test functions due to challenges involved due to multiple objectives and constrains [1]. The quality of Pareto-front for these problems is usually disconnected in nature. The details of these parameters are given in the reference [10]. The current machine tool spindle design study is a MOOP with the following two objectives to be minimized Spindle Volume (f_1) and Spindle deflection (f_2) [10].
The schematic diagram of MTS is shown in Figure 2.

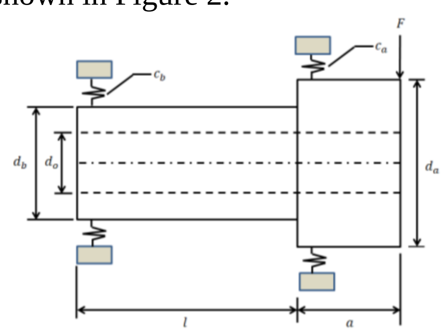

Figure 2: Details of machine tool spindle

After performing the design sensitivity analysis, four design parameters [10] are selected as design variables $x = \{l, d_o, d_a, d_b\}$. The problem is formulated in Equations (4) to (8).

Objective function 1 : Minimize volume, $f_1(x)$ -

$$f_1(x) = \frac{\pi}{4}[a(d_a^2 - d_0^2) + l(d_b^2 - d_o^2)] \tag{4}$$

Objective function 2 : spindle deflection constraint, $f_2(x)$

$$f_2(x) = \frac{Fa^3}{3EI_a}\left(1 + \frac{l\,I_a}{a\,I_b}\right) + \frac{F}{c_a}\left[\left(1 + \frac{a}{l}\right)^2 + \frac{c_a a^2}{c_b l^2}\right)\right] \quad (5)$$

Here, $I_a = 0.049(d_a^4 - d_o^4);\ I_b = 0.049(d_b^4 - d_o^4)$

Bearing stiffness, $c_a = 35400|\delta_{ra}|^{1/9} d_a^{10/9};\ c_b = 35400|\delta_{ba}|^{1/9} d_b^{10/9}$

Design proportionality constraint $g_2(x),\ g_3(x)$

$$g_2(x) = p_1 d_o - d_b \leq 0 \quad (6)$$

$$g_3(x) = p_2 d_b - d_a \leq 0 \quad (7)$$

Spindle nose radial runout, $g_4(x) = \left|\Delta_a + (\Delta_a - \Delta_b)\frac{a}{l}\right| - \Delta \leq 0$ (8)

Bound Constraints: $l_k \leq l \leq l_g;\ d_{a2} \leq d_a \leq d_{a1};$
$d_{b2} \leq d_b \leq d_{b1};\ d_{om} - d_o \leq 0$

ASAMO algorithm is applied and the key results are shown in the following Section 6.

6. Results and discussion

In this study ASAMO algorithm is tested with four types of surrogate models. The number of costly function evaluations is set at 500. These models are RBF linear, RBF Cube, Poly cube and Poly Quad surrogate models. Out of these models based on various model characteristics, best single and mixture surrogate models are developed.

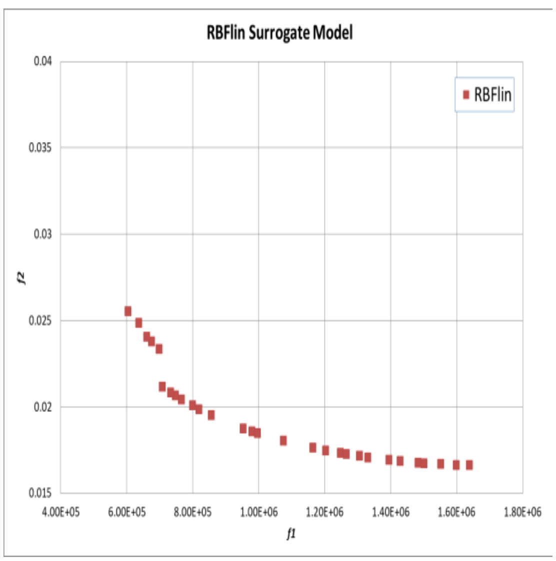

Figure 3: Non dominated front for ASAMO algorithm for RBF-linear surrogate model

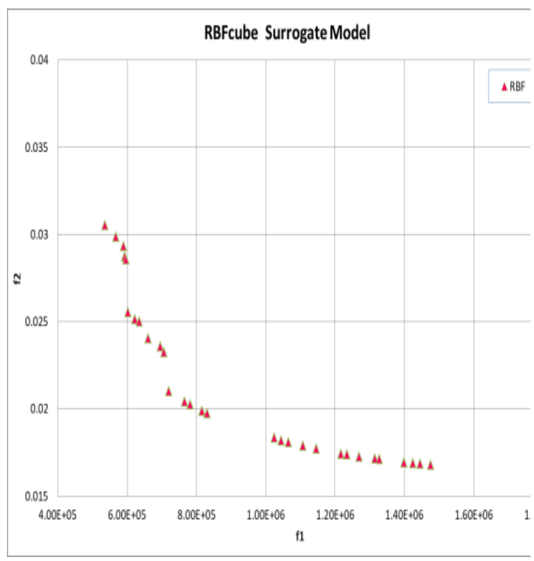

Figure 4: Non dominated front for ASAMO algorithm for RBF-cube surrogate model

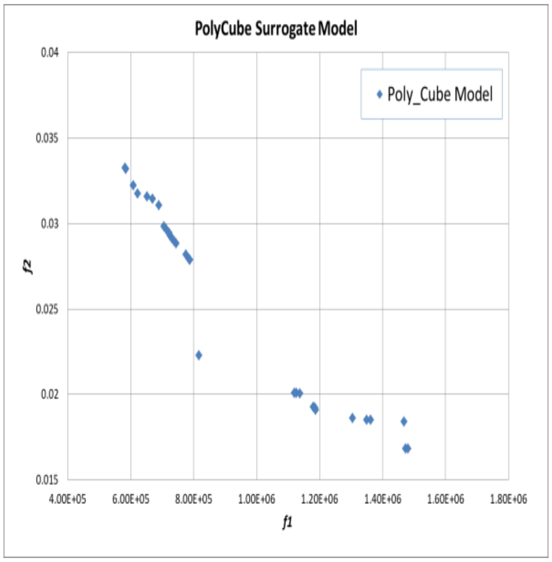

Figure 5: Non dominated front for ASAMO algorithm for Poly-cube surrogate model

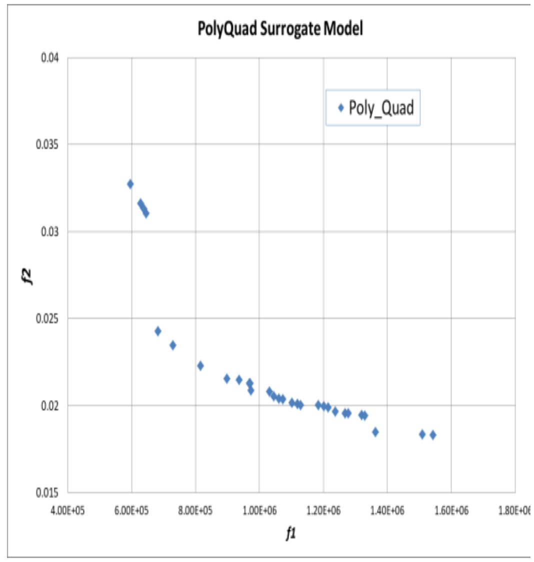

Figure 6: Non dominated front for ASAMO algorithm for Poly-quad surrogate model

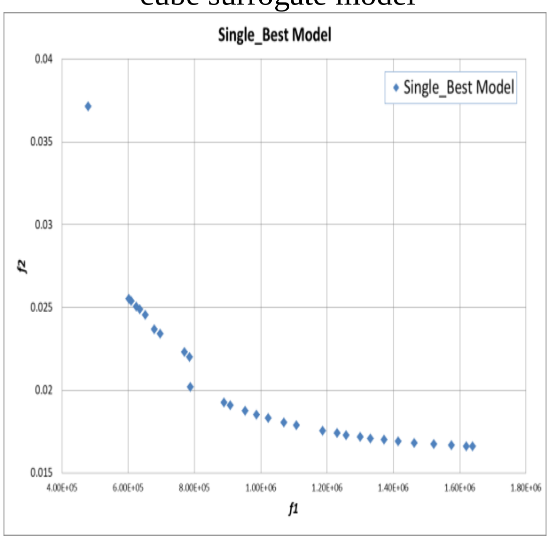

Figure 7: Non dominated front for ASAMO algorithm for single-best surrogate model

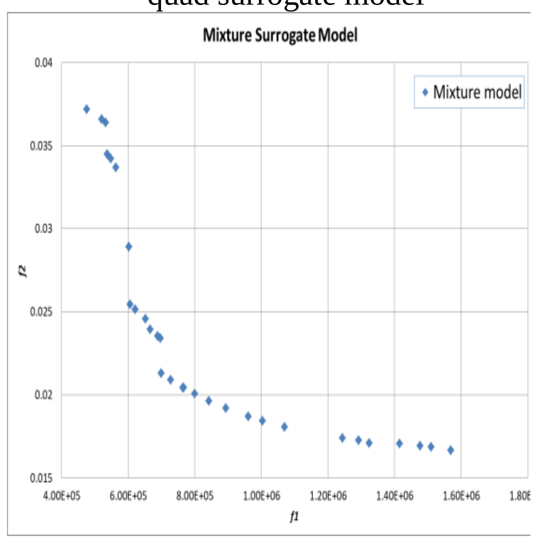

Figure 8: Non dominated front for ASAMO algorithm for mixture- surrogate model

Figures 3 to 8 display the Pareto- Front solution obtained by ASAMO for the various surrogate models as discussed above. These performances of these final Pareto- Front solutions are measured by the diversity and spread of the final solutions. From the study of these observations, it can be observed that the Pareto- Front solution obtained by mixture surrogate models are most diversified solutions and they are able to find all the 4 regions of Pareto- Front solutions. The next best performance was achieved for the single best models. For the individual surrogate models, the performance of RBF cube model is best for the divergence and spread of the solutions.

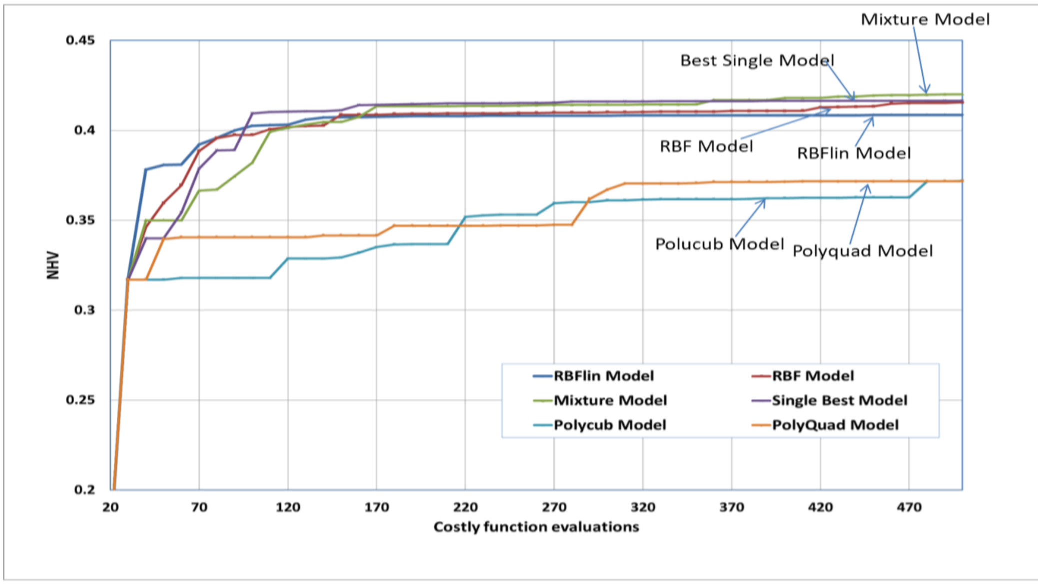

Figure 9: NHV for ASAMO algorithm for all surrogate models

Normalized Hyper Volume (NHV) is considered for evaluation of performance metric for this algorithm as this parameter evaluates the combined effect of two properties of the non-dominated solution. They are 1) convergence properties 2) diversity of the solution. The algorithm with a high value of NHV is considered as better (Zitzler et al. [16]). From the study of following table, it is observed that the mixture surrogate model performs best for ASAMO algorithm.

Table 1: NHV value at 500 at costly function evaluations

Type of surrogate model	NHV value
RBFlin Model	0.408439
RBF cub Model	0.415511
Polycub Model	0.371893
PolyQuad Model	0.371695
Single Best Model	0.416465
Mixture Model	0.420057

7. Conclusion

The present study shows efficiency of ASAMO algorithm with mixture surrogate model to solve complex multi- objective optimization problems with constraints. The performance of the ASAMO with the reference [1] clearly shows that the method is efficient in finding the well converged solutions with in 500 function evaluations as compared to 1000 function evaluation in the original study. The results clearly show that the performance of mixture surrogate models is better than all types of single surrogate models. This is observed on the basis of the quality of final Pareto-Front solutions obtained for mixture surrogate models. The non- dominated solutions obtained by mixture surrogate models have diversified solutions and are equally spaced in the objective space. The performance metric (NHV) shows highest value for the mixture surrogate models at 500 costly function evaluations. The developed algorithm can be easily extended for the benchmark problems and complex engineering applications which requires solutions of MOOPs.

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