SURROGATE MODELS FOR MULTI-OBJECTIVE EVOLUTIONARY ALGORITHMS, A SURVEY AND CURRENT RESEARCH TRENDS

Nguyen Duc Dinh[1], Nguyen Long[2*], Nguyen Hong Nghi[3], Nguyen Xuan Hoai[4]

Abstract: *Multi-objective problems (MOPs), a class of optimization problems in the real-word, which has multiple conflicting objectives. Multi-objective evolutionary algorithms (MOEAs) are known as great potential algorithms to solve difficult MOPs. With MOEAs, based on principle of population, we have a set of optimal solutions (feasible solution set) after the search. We often use concept of dominance relationship in population, it is not difficult to find out set of Pareto optimal solutions during generations. However, with expensive optimization problems in the real world, it has to use a lot of fitness function evaluations during the search. To avoid the expensive physical experiments, we can use computer simulations methods to solve the difficult MOPs. In fact, this way often costs expensive in computation and times for the simulation. In these cases, researchers discussed on the usage of surrogate models for evolutionary algorithms, especially for MOEAs to minimize the number of fitness callings. This paper we will take a short overview about surrogate models for MOEAs, state of the art and current research trends.*

Keywords: Surrogate models; Approximation models; Meta-models; MOEAs.

1. COMMON CONCEPTS

1.1. Expensive multi-objective problems

A multi-objective optimization problem involves at least two conflicting objectives and it has a set of Pareto optimal solutions. MOEAs use a population of solutions to approximate the Pareto optimal set in a single run. MOEAs have attracted a lot of research attention during the past decade. They are still one of the hottest research areas in the field of Computational Intelligence, especially to solve difficult MOPs in the real world.

A multi-objective problem is formed as follows [16]:

$$\text{minimize } \{f_1(x), f_2(x), \dots, f_k(x)\} \qquad (1)$$
$$\text{subject to } x \in S,$$

where k (≥ 2) is the number of objectives, f_i: $R^n \rightarrow R$ *are objective functions*. The vector of objective functions are denoted by $f(x) = (f_1(x), f_2(x),..., f_k(x))^T$. The *decision (variable) vector* $x = (x_1, x_2,..., x_n)^T$ belongs to the *feasible region (set)* S, which is a subset of *decision variable space* R^n. The term *"minimize"* means all objective functions are minimized simultaneously.

If there is no conflict between objective functions, then a solution can be found where every objective function attains its optimum. In this case, no special methods are needed. To avoid such trivial cases we assume that there does not exist a single solution that is optimal with respect to every objective function. This means that the objective functions are at least partly conflicting.

In multi-objective optimization, a problem is defined as a expensive problem when it has fitness functions which require time-consuming experiments or computer simulations.

1.2. Surrogate models

Surrogate models are used to approximate in simulation way to reduce the computational cost for expensive problems. The models are described as below:

If we call $f(\overrightarrow{x})$ is an origin fitness function of a MOP, then, we have $f'(\overrightarrow{x})$ is a meta function, which is indicated as below:

$$f'(\overrightarrow{x}) = f(\overrightarrow{x}) + e(\overrightarrow{x}) \tag{2}$$

function $e(\overrightarrow{x})$ is the approximated error. In this case, the fitness function $f(\overrightarrow{x})$ is not to be known, the values (input or output) are cared. Based on the responses of the simulator from a chosen dataset, a surrogate is constructed, then the model generates easy representations that describe the relations between preference information of input and output variables. There are some approaches for the surrogate models, which are divided into some kinds as below:

1.2.1. The radial basis function (RBF)

In the proposal [8], the authors suggest an approach to develop equations of topography and other irregular surfaces. To describe the method, the term *"multi quadric analysis"* is used. The radial basis function (RBF) is a real value function which is depended on the distance from a center point of the neuron to the input point. A specified point in the neuron may used as the center point. The radial function is formed as below:

$$\phi\left(\left\|\vec{x}\right\|\right) = \phi(\vec{x}) \tag{3}$$

The RBF often includes of three different layers, such as:

- Input layer: works on an identify function.
- Hidden layer: works on non-linear RBF activation function.
- Output layer: works on $\phi : R^n \to R\phi(\vec{x}) = \sum_{i=1}^{N} w_i \phi\left(\left\|\vec{x} - \vec{c_i}\right\|\right)$

In this approach, some parameters are used: the central vector $\overrightarrow{c_i}$, the weights w_i and the RBF widths β_i. The optimization process is the task of tuning these parameters. Based on the model, there are some proposals recently [11, 26, 5, 17], for details:

In [11], the authors proposed an algorithm which performs actual analysis for the initial population and periodically every few generations. An external archive of the unique solutions evaluated using the actual analysis is maintained to train the surrogate models. The data points in the archive are split into multiple partitions using k-Means clustering. A RBF network surrogate model is built for each partition using a fraction of the points in that partition. The rest of the points in the partition are used as a validation data to decide the prediction accuracy of the surrogate model. Prediction of a new candidate solution is done by the surrogate model with the least prediction error in the neighborhood of that point.

The authors in [26] introduced a modified version of MOEA/D which is assisted by cooperative RBF networks, with the aim of improving the prediction of the function value. The RBF networks employed here, use different kernels in order to have different shapes of the fitness landscape. With that, each RBF network provides information which is used to improve the value of the objective function. In [14] the authors presented a meta-model assisted memetic algorithm, using online trained local meta-models supporting both the inexact pre-evaluation of evolving populations and the local search. The use of RBF networks to screen out non-promising individuals in each generation, so as to avoid evaluating them with the exact and costly evaluation tool, is currently a well established technique; it considerably reduces the CPU cost of evolutionary computations and makes them competitive for engineering applications with computationally expensive evaluation tools.

In [17], the authors proposed a new MOEA called MODE-LD+SS, which combines differential evolution with local dominance and scalar selection mechanisms. Local dominance aims to improve the convergence rate and the scalar selection mechanism intends to improve the distribution of solutions along the Pareto front.

1.2.2. The polynomial response surface (PRS)

The authors in [21] suggested using concept of statics to regress and analyst the variances to find out the minimum responsive variance. This methodology called The response surface methodology (RSM). Based on the RSM and polynomials, and popular approach is proposed, which called polynomial response surfaces (PRS). In PRS, a function is a linear aggregate (or combination) of powers and products of the training set. The model is formed as below:

$$\hat{y}^{(p)} = \beta^T \vec{x}^p \tag{4}$$

Here, dataset sized n is presented as $\vec{x_1}, \vec{x_2}, ..., \vec{x_n}$, β is the vector of coefficients to be estimated, $\vec{x}^p$ is the vector corresponding to the form of a pair of $x_1^{(p)}$ and $x_2^{(p)}$.

In the proposal, there are two common methods are used to estimate unspecified coefficients: gradient and least squares methods. In this case, the number of coefficients is the number of samples which we need.

In [3], the authors used stepwise regression to build up PRS as below:

- Determine an initial model.
- In a loop, the model is altered with one of two actions (add or remove a predictor variable in accordance with a special criterion.
- Stop the search when the loop size is reached.

Based on the approach, there are some proposals in [6, 13, 4, 20,18], for details:

Based on NSGA-II, the authors on [6] introduced a proposal which applied to study trade-offs among objectives of a rocket injector design problem where performance and life objectives compete. The Pareto Optimal Front (POF) is approximated using a quintic polynomial. The compromise region quantifies trade-offs among objectives.

In [13], to solve the problem on crash safety design of vehicles, the authors suggest to use stepwise regression model for NSGA-II. The authors present a multi-objective optimization procedure for the vehicle design, where the weight, acceleration characteristics and toe-board intrusion are considered as the design objectives. The response surface method with linear and quadratic basis functions is employed to formulate these objectives, in which optimal Latin hypercube sampling and stepwise regression techniques are implemented.

The authors in [4] presented and analyzed in detail an efficient search method based on evolutionary algorithms (EA) assisted by local Gaussian random field meta-models (GRFM). It is created for the use in optimization problems with one (or many) computationally expensive evaluation function(s). The role of GRFM is to predict objective function values for new candidate solutions by exploiting information recorded during previous evaluations. Moreover, GRFM are able to provide estimates of the confidence of their predictions. Predictions and their confidence intervals predicted by GRFM are used by the meta-model assisted EA. It selects the promising members in each generation and carries out exact, costly evaluations only for them. The extensive use of the uncertainty information of predictions for screening the candidate solutions makes it possible to significantly reduce the computational cost of single and multi-objective EA.

In [18], the authors used a special memetic operator, which performs local search on some of the newly generated individuals. This operator used the meta-model constructed based on previously evaluated points in the decision space. The meta-model is trained to predict the distance to the currently known Pareto front. In the proposal, the known points do not have the same weight, as those that are closer to the locally optimized one are considered more important. The author's idea is that points closer to the Pareto front are more interesting during the run of the algorithm, and the memetic operator moves the individuals towards the front. The meta-model provides a general direction in which the search should proceed. To obtain a training set for the meta-models we also added an external archive of individuals with known objective values.

A meta-model based approach is introduced in [20] to the reduction in the needed number of function evaluations is presented. Local aggregate meta-models are used in a memetic operator. The algorithm is first discussed from a theoretical point of view and then it is shown that the meta-models greatly reduce the number of function evaluations.

1.2.3. The support vector machine (SVM)

In [24], based on the theory of statistical learning, the authors introduced to use support vector machines (SVMs) which is a set of related supervised learning methods. Here, the data is analyzed to recognize patterns. In this approach, to classify, regress, analyst one or set of hyper-planes in corresponding multi-dimensional space is suggested to use. The set of inputs are map to a larger space, then, it calculates the cross product in terms of the variables in original space which makes the computational load reasonable. The concept of *"kernel function"* (as K(x, y)) is defined as the cross products in larger space. The kernel function can be chosen as a solver for the regression problem. One of other function is introduced is *"loss function"* with a measure of distance. The problem of approximating the set of data is formed as:

$$f(x) = g(w,x) + b \tag{5}$$

Then, the minimum of the function:

$$\phi(w,\xi)=\frac{1}{2}\|w\|^2+C\sum_{i=1}^{n}\left(\xi_i^-+\xi_i^+\right) \quad (6)$$

is known as the optimal regression function. Here, C is specified value, ξ^- and ξ^+ are slack variables which present the lower and upper constraints on the results.

Based on the SVM, there are some proposals in [14, 19, 20], for details:

In [14] the authors proposed a meta-model based approach to the reduction in the needed number of function evaluations is presented. Local aggregate meta-models are used in a memetic operator. The algorithm is first discussed from a theoretical point of view and then it is shown that the meta-models greatly reduce the number of function evaluations.

In [19], the authors proposed a surrogate-based evolutionary strategy for multi-objective optimization. The evolutionary strategy uses distance based aggregate surrogate models in two ways: as a part of memetic search and as way to pre-select individuals in order to avoid evaluation of bad individuals. The model predicts the distance of individuals to the currently known Pareto set.

In [20], the authors presented a memetic evolutionary algorithm for multi-objective optimization with local meta-models. The proposal shows that the local models give better results than a single global model, usually reducing the number of needed function evaluations by 10%, with occasional reductions as high as 48%. Although this difference may seem rather small, it may better reduce the associated costs in practical tasks.

1.2.4. The kriging (KRG)

In [15], the authors proposed a method named *"Kriging"*, which is a response surface method bases on spatial prediction techniques. This method minimizes the mean squared error to build the spatial and temporal correlation among the values of an attribute. In [22], the authors developed a parametric regression model which design and analysis of computer experiments, called DACE. The model is an extension of Kriging approach for at least three dimensions problems. The model is a combination of a known function *f(x)* and a Gaussian random process *f'(x)* that is assume to have mean zero and covariance, like as:

$$E(f'(\vec{x}^{(i)}),f'(\vec{x}^{(j)}))=Cov(f'(\vec{x}^{(i)}),f'(\vec{x}^{(j)}))=\sigma^2R(\vec{\theta},\vec{x}^{(i)},\vec{x}^{(j)}) \quad (7)$$

here, $\vec{x}^{(j)}$ is the correlation function with parameters θ, σ is the process variance of the response and $R(\vec{\theta},\vec{x}^{(i)},\vec{x}^{(j)})$.

With KRG model and popular MOEAs, there are some works, recently [2, 7, 10, 25, 4, 1], for details:

In [2] the authors built a procedure which uses Kriging approximations and NSGA-II algorithm to optimize the aircraft design. The Kriging based genetic algorithm procedure gives shapes which are optimized for both the initial peak and perceived noised level of the signature along with minimum drag. The design problem concerns three objectives: the aircraft drag coefficient and the strength of the ground boom signature (using both the initial pressure rise and the perceived noise level) for each design point. In the study, Kriging approximation models are constructed from a large number of members of an initial population using the results from repeated analyses carried out with BOOM-UA (a specified analysis tool). The approximation model is combined with the NSGA-II algorithm to minimize ground boom intensity while maintaining acceptable levels of aerodynamic cruise performance.

In [7], by providing a Design of Experiments (DOE) capability into the framework, the authors hybridized the desirable characteristics of EAs and surrogate models such as RSM to obtain an efficient optimization system. Within this context, the DOE samples a number of design candidates at which the analysis code, the surrogate model is then constructed for the computationally expensive problem. Different sampling and DOE strategies can be used; Latin hypercube, Response Surface Methods or DACE/Kriging.

In [10], in the problems with two objective functions, thermal resistance and pumping power have been selected to assess the performance of the micro channel heat sink. The design variables related to the width of the micro channel at the top and bottom, depth of the micro channel, and width of fin, which contribute to objective functions, have been identified and a three-level full factorial design was selected to exploit the design space. The numerical solutions obtained at these design points were utilized to construct surrogate models Kriging and Radial Basis Neural Network. A hybrid multi-objective evolutionary algorithm coupled with surrogate models is applied to find out global Pareto-optimal solutions.

In [25], the authors deeply discussed on surrogated MOEAs and indicated that: Kriging appears to perform well in most situations, however it is much more computationally expensive than the rest. It is obvious that a careful consideration of RSM could lead to a situation where all objectives in multi-objective problems are modeled using different methods, in order to maintain high quality and reduce optimization costs.

In [4] the KRG is used, the term Kriging points directly to the origin of these prediction methods dating back to the sixties, when the mining engineer Krige used Gaussian Random Field Models (GRFMs) to predict the concentration of ore in gold and uranium mines.

In [27], the authors proposed such a method, MOEA/D-EGO, for dealing with expensive MOPs. The algorithm decomposes an MOP into a number of single-objective optimization sub-problems. At each iteration, a predictive distribution model is built for each individual objective in the MOP by using Fuzzy clustering and Gaussian stochastic process modeling. Then, a predictive model for the objective of each sub-problem can be induced. MOEA/D is used for maximizing the expected improvement metrics of all the sub-problems and several test points are then selected for evaluation.

2. ADVANTAGES AND DISADVANTAGES

2.1. Advantages

- RBF: The RBF networks have advantages of easy design, good generalization, strong tolerance to input noise, and online learning ability. The properties of RBF networks make it very suitable for design problems in the real-world. The RBF is training faster than multi-layer perceptron (MLP). In RBF, the hidden layer is easier to interpret than the hidden layer in an MLP.

- PRS: The integration of multiple disciplinary codes with an optimization code becomes more manageable. The statistical methods can be used to detect and repair bad data and to estimate the average error in the data [9]. The model is suited to simple design landscapes with low dimensionality where data is cheap to obtain [23].

- SVM: With the concept of kernel, SVMs gain flexibility in the choice of the form of the threshold separating solvent from insolvent companies, which needs not be linear and even needs not have the same functional form for all data, since its function is non-parametric and operates locally. In the model, by choosing an appropriate generalization grade, SVMs can be robust, even when the training sample has some bias. By choosing different r values for different input values, it is possible to rescale outliers. SVMs deliver a unique solution, since the optimality problem is convex. With appropriate kernel, such as the Gaussian kernel, one can put more stress on the similarity between companies, because the more similar the financial structure of two companies is, the higher is the value of the kernel.

- Kriging: Kriging treats clusters as like as the point's help to carry estimate the effects of data clustering. With the model the known value of estimation errors (kriging variance) along with the z variable and it gives estimation of errors for stochastic simulation of possible realizations of *Z(u)* [12].

2.2. Disadvantages

The models for surrogate assisted MOEAs show a lot of advantages in optimization area, but they also give some disadvantages:

- RBF: Although the RBF is quick to train, when training is finished and it is being used it is slower than a MLP, so where speed is a factor a MLP may be more appropriate.

- PRS: Care is needed with the selection of the polynomial order. For problems with a high number of dimensions, it is difficult to gain sufficient data. Care is needed with order selections.

- SVM: the biggest limitation of the SVM model which lies in choice of the kernel, speed and size, both in training and testing, high algorithmic complexity and extensive memory requirements of the required quadratic programming in large-scale tasks.

- Kriging: This model is expensive to train for higher dimensional problems.

3. CURRENT RESEARCH TRENDS

Through a short review and analysis about the common models for surrogate multi-objective evolutionary algorithm, recently proposals, research issues and discussions, there are some promised trends for academic researchers in this area:

1. Surrogates in interactive evolutionary multi-objective (EMO) algorithms: in an interactive EMO algorithm, humans calculate the fitness value for all individuals. This is necessary in case of no fitness functions are available. It is difficult for the algorithm when humans feel tired, have no choices, no actions. To

solve the problem, the usage of surrogate models can be used to replace the evaluations by the human. This case, machine learning model is used to predict the fitness value the human may assign to a design based on history data.

2. Surrogated-assisted evolution for solving dynamic multi-objective optimization algorithms: Recently, researchers discussed a lot about evolutionary algorithms for dynamic MOPs. The research idea is to design an evolutionary search strategy to drive solutions belong POF. In this, the maintaining of diversity of population is an important part of the evolutionary algorithm. Then, memory mechanisms which include sub-populations, archives, external population need to construct as research directions. To implement the strategy to maintain the diversity of the population anticipation and prediction of the change in the fitness function can be helpful in solving dynamic problems more efficiently. In such strategies, a surrogate can be helpful in learning the changing fitness function.

3. Surrogates for robust multi-objective optimization: In the real-world applications, we need to concern the performance of MOEAs to obtain optimal solution and also the sensitivity of the performance to small. If an optimal solution is insensitive to such changes, the solution is known as robust optimization. This case, an implicit averaging or explicit averaging can be used in MOEAs to obtain robust optimal solutions. Wherein an assumption on the probability distribution of the noise is often made. By contrast, one can predefine the allowed performance decrease and then search for an optimum that has the maximum tolerance of changes in the design variables or in the environment, which is termed inverse robust optimization. In both cases, explicit averaging based or inverse robust optimization additional fitness evaluations are needed. Then, a surrogate is promised direction to improve the efficiency and extra fitness evaluations.

4. Surrogate-assisted combinatorial multi-objective optimization: In the real-world applications, there are also many computationally intensive combinatorial optimization problems. In these cases, we can use discrete modeling techniques such as binary neural network, which is used to assist a mixed integer evolution strategy for medical images analysis. Then, the Kriging model is suitable to be used for telecom network optimization problems.

5. Surrogates for constrained optimization: In the real-world, MOPs often have one or more constraints. To determine if a given solution is feasible, we need to evaluate the constraint functions. In case of the evaluations of constraint functions are time consuming, it is desirable to replace the constraint functions with others by using approximate models. Then, surrogates are applied to manipulate the shape and size of the feasible region to ease the solution of highly constrained MOPs. The usage of surrogate models to deliberately enlarge the feasible region by building up a very simple surrogate for each constraint function. As the optimal proceeds, the complexity of the surrogates increases gradually so that the approximated feasible region can converge to the real feasible region.

4. CONCLUSION

The usage of surrogate models for multi-objective evolutionary algorithms are motivated from real-world applications. As multi-objective optimizations are increasingly applied to solving complex problems, expensive problems research trends in using surrogate models for MOEAs have considerably increased in recent years. This paper provides a brief overview of recent advances in this research area and raised some research trends that remain to be resolved in the future. Based on research trends, researchers need to apply new techniques to incorporate with the surrogate models for MOEAs such as Artificial Intelligence (AI), Deep Learning, Cloud Computing,... with which more computing resources will be made available to common users via computer networks.

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TÓM TẮT

MÔ HÌNH ĐẠI DIỆN CHO GIẢI THUẬT TIẾN HÓA ĐA MỤC TIÊU. KHẢO SÁT VÀ VẤN ĐỀ NGHIÊN CỨU

Bài toán tối ưu đa mục tiêu là một lớp bài toán tối ưu trong thực tế, có nhiều mục tiêu xung đột với nhau. Giải thuật tiến hóa tối ưu đa mục tiêu thường khá hiệu quả để giải các bài toán tối ưu đa mục tiêu khó. Với giải thuật tiến hóa đa mục tiêu, dựa trên nguyên lý quần thể, chúng ta đạt được một tập giải pháp tối ưu (tập giải pháp khả dụng) sau quá trình tìm kiếm. Chúng ta thường sử dụng quan hệ trội trong quần thể và không khó khăn để xác định được các giải pháp Pareto qua mỗi thế hệ. Tuy nhiên, với các bài toán tối ưu khó trong thực tế, cần phải có nhiều đánh giá của hàm thích nghi trong quá trình tìm kiếm. Để tránh các thí nghiệm tốn kém, chúng ta có thể dùng phương pháp mô phỏng trên máy tính để giải quyết các bài toán khó này. Thực tế, phương pháp này đòi hỏi chi phí tính toán và thời gian lớn cho quá trình mô phỏng. Vì thế, có nhiều nghiên cứu thảo luận về việc sử dụng mô hình đại diện cho giải thuật tiến hóa, đặc biệt là tiến hóa đa mục tiêu để giảm số lượng tính toán thích nghi. Bài báo này đưa ra một khảo sát ngắn về mô hình đại diện cho giải thuật tiến hóa tối ưu đa mục tiêu, những kết quả hiện tại và vấn đề nghiên cứu đặt ra.

Từ khóa: Mô hình đại diện; Mô hình xấp xỉ; Mô hình meta; Giải thuật tiến hóa đa mục tiêu.

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Address: [1]MITI, Military Academy of Science and Technology;
[2]National Defense Academy;
[3]VNPT Information Technology;
[4]AI Academy.
[*]Email: nddinh76@gmail.com.