ANovelAlternate Point-taking Strategy for Surrogate-AssistedEvolutionary Algorithm

ABSTRACT

The essence of surrogate model is a low-cost alternative, which mainly replaces the computationally heavy simulation process to reduce the time cost consumed. In the past two decades, this approximation based optimization method has made remarkable progress, and surrogate models are widely used in computationally expensive simulation model analysis and optimization. In addition, with the development of technology, the surrogate model is no longer a simple substitute, but can drive new sample points to join the training process based on historical data, so as to gradually approach the global optimal solution of the problem.For optimization problems, there are many surrogates-assisted optimization algorithm methods. However, the selection of sample points has great influence on the accuracy of the surrogate model.In order to obtain a more accurate surrogate model, the newly added sample points should meet the sample diversity criterion of the specified distance, and at the same time, corresponding strategies should be adopted to fully explore sparse regions, so as to avoid falling into the local optimal phenomenon in the optimization process.Therefore, an ensemble of surrogates based on alternate point-taking strategy(APTS) is proposed, and a hierarchical search framework is designed, using different algorithms at each stage. The effectiveness of APTS is verified on three benchmark examples with different dimensions and compared with several advanced methods. The results show that this method has better accuracy and robustness than other methods on most test problems.

Keywords: Surrogate model, Optimization algorithm, Hierarchical search, Ensemble, Point-taking strategy

1. INTRODUCTION

In many engineering problems, highly complex and costly computer simulations or physical experiments are usually required to quantify the economic and engineering performance of complex systems[1]. However, the high computational cost associated with the high fidelity model involved in this process poses a serious obstacle to practical application. As the dimension increases, so does the cost of computer simulation, even beyond the range of affordable projections. As an approximate model, surrogate model can significantly reduce the calculation cost. Commonly used surrogate models include radial basis function (RBF)[2], Gaussian process (GP) or Kriging model[3], support vector regression

(SVR)[4]and polynomial response surface (PRS)[5], etc. After in-depth study and comparison of the performance of these surrogate models, it is found that RBF performs well in terms of robustness and accuracy, while KRG is more suitable for low-dimensional problems, and its performance deteriorates as the problem dimension increases.

In order to effectively apply the surrogate model tosurrogate-assisted evolutionary algorithms (SAEAs), various fill sampling criteria (also known as pre-screening criteria, model management, or evolutionary control) have been developed to select promising individuals for precise FEs and alternative reconstruction[6,7]. Based on the criteria of optimization accuracy, individuals with the best predictive value of the surrogate model are selected for accurate evaluation, so as to promote the development of the current potential areas[8, 9]. Indetermination based criteria select individuals with maximum uncertainty for accurate FEs evaluation, so as to conduct exploration in sparse areas and avoid missing the true global optimal solution[10, 11]. However, studies[12] have shown that filling criteria that only consider individuals with the best predicted value may lead to premature convergence of the algorithm or make the search fall into local optimal phenomenon, while those criteria that only focus on approximate uncertainty may lead to slow convergence.Therefore, standards based on optimization accuracy and uncertainty are adopted in this paper to facilitate the exploration and in-depth mining of the algorithm.

EAs[13-16] assisted by global surrogate model constructs a global surrogate model on the entire decision space to assist global search in the optimization process. Local surrogate model-assisted EAs[17, 18] constructs local surrogate models by capturing local scope details in the decision space, thereby improving model accuracy and speeding up the search for promising subspaces.A large number of SAEAs have been developed. For example, Li et al. [19] developed a PSO assisted by a global RBF surrogate model (FSAPSO) to optimize medium-dimension problems; Pan et al. [20] developed a surrogate-assisted hybrid algorithm (SAHO) for expensive optimization problems from low to high dimensions. Wang et al. [21] proposed a PSO assisted by a committee active learning surrogate model (CAL-SAPSO) for medium-dimension problems, in which both global search and local search were assisted by a composite surrogate model. However, these methods only use one search method or fill sampling criterion in each iteration, and it is easy to fall into local optimal. Therefore, this paper proposes a new alternate point-taking strategy (APTS) and designs a hierarchical search framework, which uses different algorithms at each stage to make the search results more accurate.

2. TheProposedMethod

2.1 Flow Chart

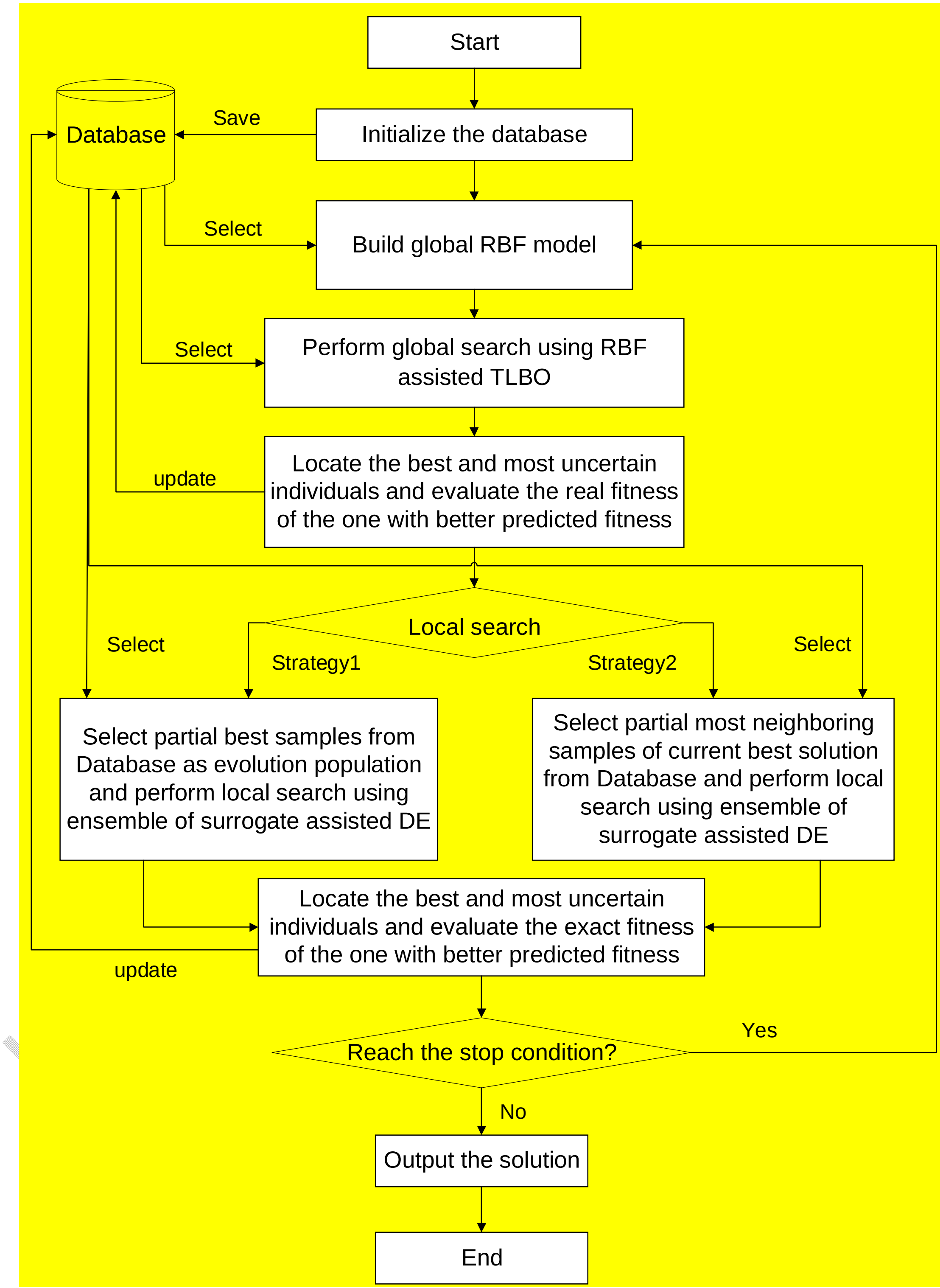


Figure 1: The flowchart of the proposed APTS

Figure 1 shows a general flow diagram for APTS. In this method, RBF model is used to assist TLBO algorithm for global search, and then an ensemble of surrogate is used to assist DE algorithm for local development search.

2.2 Online Data-driven

The ensemble of surrogates used in this paper is based on Unified Ensemble of Surrogates (UES). Zhang et al.[22] adopted the fixed integration of three models, PRS, KRG and RBF, and combined the global error criterion and local error criterion to evaluate the weight factor, which was defined as follows:

$$w_i = \frac{w_i^*}{\sum_{j=1}^{N} w_j^*}$$

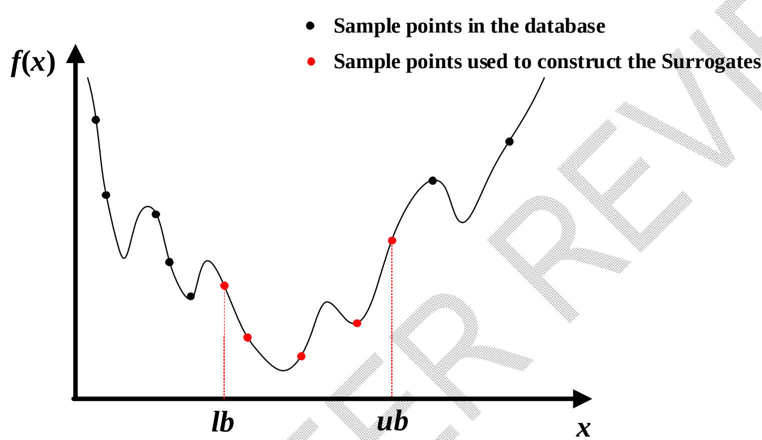
$$w_i^* = w_i^g(x)\lambda(x) + w_i^l(x)\big(1 - \lambda(x)\big)\#(1)$$

Where N represents the number of surrogate models participating in the combination. w_i^g and w_i^l represent the global weight factor of the i-th model and the local weight factor at the prediction point, respectively. $\lambda(x)$ is the control function used to determine the magnitude of the influence of the global error measure and the local error measure, its formula is $\lambda(\boldsymbol{x}) = sin\left\{\frac{\pi}{2}\left(\frac{d_1(x)}{d_2(x)}\right)\right\}$. In the formula, $d_1(\boldsymbol{x})$ and $d_2(\boldsymbol{x})$ respectively represent the distance between the prediction point $\boldsymbol{x}$ and the nearest sample point and the second nearest sample point.

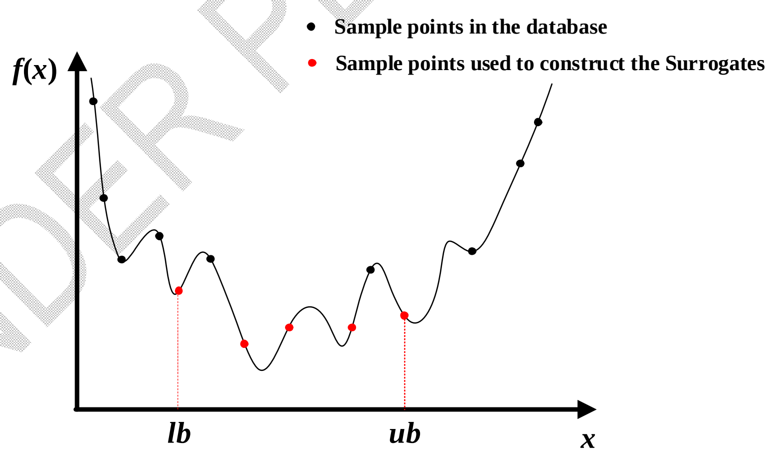
The UES is an off-line data-driven optimization, that is, an ensemble of surrogates is constructed with sample points, and then the model is used for optimization. The characteristic of off-line data drive is that the optimization process cannot generate new data actively, which requires that the initially constructed surrogate model must be high fidelity. However, in the absence of any optimization, it is difficult to guarantee the accuracy of the surrogate model around the true global optimal solution, even with Latin Hypercube sampling (LHS), which can efficiently sample from the distribution interval of variables. Therefore, in this paper, UES is changed to adaptive point method, that is, online data-driven optimization. An initial model is constructed, and then the surrogate model is constantly updated with the points found in the iterative process, so that its accuracy around the global optimal solution becomes higher and higher, and the algorithm is guided to search for optimization more accurately.

2.3 Alternate Point-taking Strategy

The accuracy of the surrogate model largely depends on the training sample points. In the existing literature, the training points for constructing the local model are usually the best part in the database. However, when the new sample points found are not significantly better than the results obtained in the last iteration, the constructed local model is easy to lead to optimization stagnation or local optimization. Therefore, an alternate point-taking strategy is proposed in this paper. One is to select the best part of sample points in the database according to the fitness value, and the other is to select the part of sample points closest to the current optimal solution. According to the comparison results between the optimal solution obtained in each iteration and the optimal solution of the previous iteration, the two strategies are carried out alternately to construct the combinatorial surrogate model in the local search stage, which effectively prevents the proposed method from falling into the local optimal phenomenon. The schematic diagram of the alternate point-taking strategy is shown in Figure 2.



(a)



(b)

Figure 2: (a) Select the partial sample points closest to the current optimal solution

(b) Select the best partial sample points

2.4 Hierarchical Search Framework

Teaching Learning-Based Optimization (TLBO) has strong development ability in the global scope, but its convergence speed is slow. Differential evolution (DE) algorithm, though able to converge quickly, tends to fall into local optimal phenomenon, thus missing the real global optimal solution. Existing literature usually selects only one of these algorithms, or one of the two each time a new iteration is entered. This paper designs a hierarchical search framework, which mixes TLBO and DE to give full play to their respective advantages. In the global stage, the RBF model is constructed to assist TLBO to search the whole decision space and locate the most promising region. In the local stage, the ensemble of surrogates is used to assist DE to search the located region and find the global optimal solution. The innovation of this method is that it takes into account the characteristics of TLBO and DE, and gives full play to their respective advantages when doing search work.

3. Example Problems

In order to verify the effectiveness of the APTS, three test functions of different dimensions (Table 1 for details of the functions) were selected to evaluate the performance of the proposed method, and the APTS was compared with two SAEAs: FSAPSO[19] and CAL-SAPSO[23].

Table 1 Characteristics of three test problems

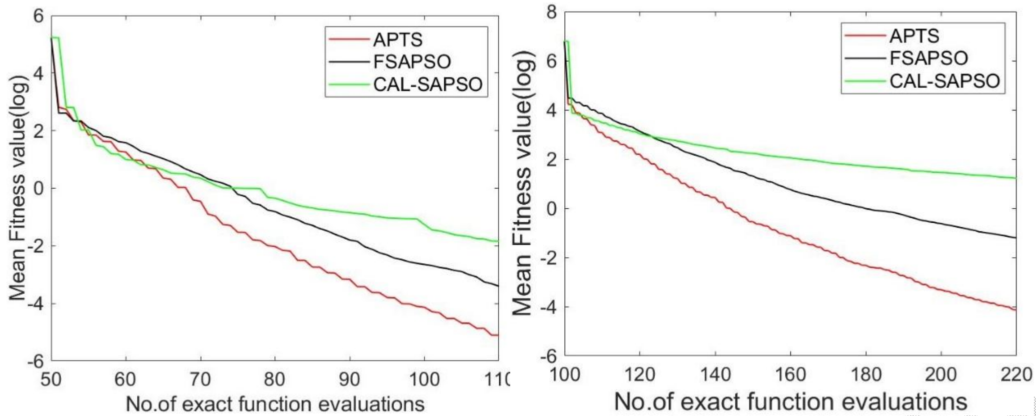
No.	Problem	Dimension(d)	Optimum	Characteristics
F1	Ellipsoid	10,20	0	Unimodal
F2	Ackley	10,20	0	Multimodal
F3	Griewank	10,20	0	Multimodal

Set the initial number of sample points $N_0 = 5 \times d$, The stop condition is set to reach the maximum number of exact values $NFE_{max} = 11 \times d$. All algorithms run independently 20 times.

Table 2 The results of several methods on three test problems in 10 and 20 dimensions

Methods		APTS	FSAPSO	CAL-SAPSO
No.	D	Mean	Mean	Mean
F1	10	**6.0728E-03**	3.2195E-02	1.5846E-01
	20	**1.6093E-02**	3.3654E+00	3.0142E-01
F2	10	**1.4257E+00**	6.5997E+00	1.9360E+01
	20	**1.9997E-02**	1.7874E+01	8.0361E+00
F3	10	**5.2306E-01**	9.1890E-01	1.3045E+00
	20	**2.3938E-01**	1.4236E+00	7.8814E-01

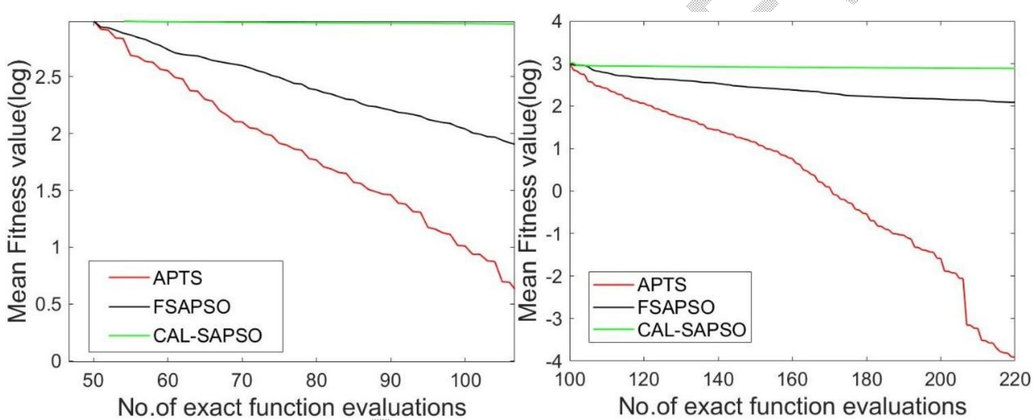
Table 2 shows the comparison results of APTS, FSAPSO and CAL-SAPSO in the 10 and 20 dimensional problems. Mean represents the average value of 20 independent runs of the algorithm. As can be seen from Table 2, APTS has the best average value on the six test functions.



(a) (b)

Figure 3: (a) Convergence graphs of several methods on 10-dimensional F1 functions

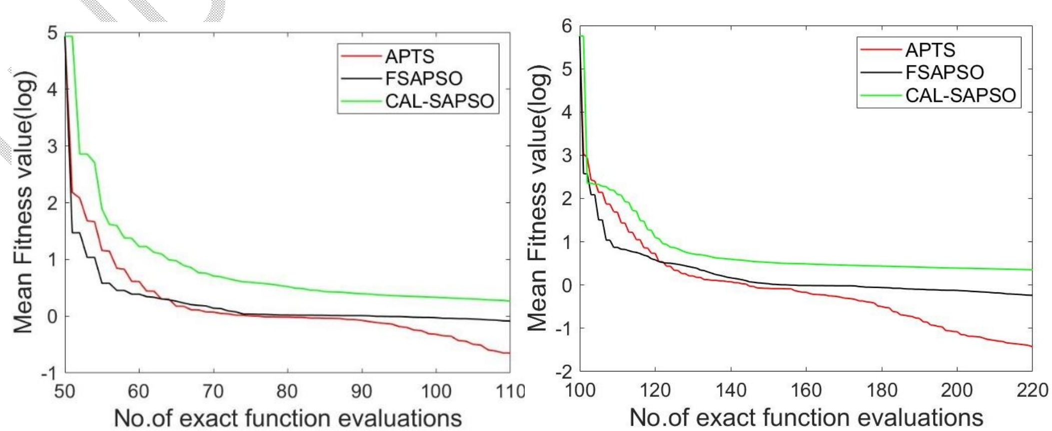
(b) Convergence graphs of several methods on 20-dimensional F1 functions



(a) (b)

Figure 4: (a) Convergence graphs of several methods on 10-dimensional F2 functions

(b) Convergence graphs of several methods on 20-dimensional F2 functions



(a) (b)

Figure 5: (a) Convergence graphs of several methods on 10-dimensional F3 functions

(b) Convergence graphs of several methods on 20-dimensional F3 functions

Figure3-5 shows the convergence diagram of APTS, FSAPSO and CAL-SAPSO in 10 and 20 dimensions respectively. The abscess is the number of exact FEs, and the ordinate is the average value of 20 operations in different algebraically corresponding fitness values. The faster the convergence rate, the better the result under the same number of iterations.As can be seen from the figure, the convergence rate of APTS is the fastest, indicating the superiority of this method.

4. CONCLUSIONS

In this paper, UES is changed to online data-driven optimization, and the surrogate model is constantly updated with newly discovered points in the iterative process, which gradually improves its accuracy and guides the algorithm to search for the optimal solution more accurately. In order to prevent the algorithm from falling into the local optimal phenomenon in the search process, two kinds of point-taking strategies (namely, selecting the best fixed number of sample points from the database and the fixed number of sample points closest to the current optimal solution) were proposed, which were used alternately to construct the local ensemble of surrogates. In addition, a layered framework with a hybrid optimization algorithm is designed to combine TLBO and DE in order to enhance the global exploration capability and local development capability. Firstly, a single RBF model is constructed using all the sample points in the database to assist TLBO algorithm in global search. Secondly, the ensemble of surrogates is used to assist DE algorithm in local search. The proposed APTS is compared with the other two methods on several test problems, and the experimental results show that the performance of APTS is the best, and the convergence rate is the fastest. In the future, we will focus on more point-taking strategies and build a more accurate surrogate models to make the optimization more accurate.

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