An Adaptive Sampling Algorithm and Approximate-Model-Based Optimization Method

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Abstract: The approximate model based optimization algorithm can improve the speed of optimization convergence and save the time of calculation, which is very consistent with the development requirements of modern industrial rapid design. In this work, an adaptive and approximate model based optimization method is introduced, which is improved on the basis on HAM. This method uses three different types of approximate models at the same time to the full advantage of the three models’ characteristics. Besides, an adaptive sampling algorithm is applied to achieve the self-setting mechanism for new sampling points in the search process. By testing on several standard test functions, the method performed better than GA, PSO and HAM in computational efficiency and accuracy. The method is also applied in the optimization design of rocket engine design to get the maximum thrust. Only after fifty-seven times of simulation calculation, optimal is obtained and the thrust is improved by 2.56%. the method is particularly suitable for design problems involving computation intensive analyses and simulations.

1. Introduction

Today, with the great improvement in the accuracy of computer analyses and simulations, the physical characteristics of the modelled systems can be well predicted and expensive physical experiments for a given design are replaced by computer simulations widely. Besides, these computer simulation softwares are also used for optimization design. Then appropriate search algorithms for design optimization are essential. In recent years, many efficient, capable, and robust optimization methods has been developed. Optimization methods based on approximate model are widely applied to solve time-consuming design optimization problems.

Many approximate models with high efficiency and accuracy are proposed and applied widely, for instance, response surface method (RSM), radial basis function (RBF), multivariate adaptive regression spline (MARS) and Kriging methods [1]. These approximate models have different characteristics and suitable for different kinds of design problems [2]. Then a strategy to choose the most suitable approximate model from several models for an optimization design problem becomes invaluable.

Many strategies proposed to solve the problems are using several approximate models to predict at the same time. Zerpa proposed the concept of combination of approximate models [3]. Combination of approximate models superimposes several approximate models together in the form of weights and the...
weight coefficient is generally determined by a certain error index. The robustness and accuracy of the combined approximate model are higher than that of a single approximate model. This strategies has been applied on the optimization of helicopter propeller blade noise reduction [4]. Gu introduced a hybrid and adaptive meta-model-based global optimization methods (HAM) and applied in vehicle design [5]. This method incorporates three different approximate models into the search process.

In this work, an approximate model based optimization method is introduced to meet the need of optimization design problems which are characteristics unknown, computation intensive, time-consuming and computer simulation based. Developed on the basis of HAM, the method incorporates three different approximate models and sets new sampling points adaptively in each iteration. The adaptive sampling mechanism increases the accuracy of the approximate models and the efficiency of optimization process. Performance tests on several standard test functions showed considerable improvements over other global optimization methods that are single approximate model based and conventional. A real industrial design problem in rocket engine nozzle is used to demonstrate the feasibility and advantages of the method.

2. Introduced method
In this article, a method for global optimization is introduced that three different approximate models are used for modelling and new sampling points are set adaptively in the search process. In this strategy, three approximate models are constructed on initial sample points. Then, three set of points are calculated using the three constructed approximate models. Finally, several new sample points are choose from the three set of points, and the models are reconstructed.

The use of three approximate models presents a good balance in complexity and performance. Because the three approximate models have different characteristics for different types of optimization design problems, when one of the three models is not suitable for the optimization design problem, the other two approximate models are likely to be suitable for the problem. Response surface method (RSM), radial basis function (RBF) and Kriging methods are chosen in this work, because each of them have different performance characteristics and present a unique capability to cover a specific type of objective functions. Kriging method is better for high order problems; RSM is suitable for lower order problems; and RBF has the advantage of local approximation.

Given a simulation function, $f(x)$, the proposed optimization method contains the following parts:

2.1. Get the initial sampling points
The simple Latin hypercube sampling (LHS) technique is used to obtain design data samples that best represent the objective function. A few points sampled by LHS and several boundary points are used as initial sampling points. The purpose of adding boundary points as initial sampling points is Improve the efficiency of calculation under these circumstances where the optimum points are on the boundary.

2.2. Adaptive sampling algorithm (ASA)
(1) Construct the initial approximate models, $f'(x)$, $g'(x)$ and $h'(x)$, using the three different approximate models with the initial points from $f(x)$.
(2) In design space, $S$, Generate $N$ points using LHS method and put these points into group $P$.
(3) Use the three constructed approximate models to calculate the values of the $N$ points in $P$, and sort these points in the descending order of the values calculated by the models independently. The obtained three group of points have the same elements, but in different order.
(4) Select a small portion ($n=0.01N$) of the three group of points independently with the low values associated with each of the three approximate models. Then three group of points are obtained: $F$ for $f'(x)$, $G$ for $g'(x)$ and $H$ for $h'(x)$.
(5) The points in the three groups, $F$, $G$ and $H$, are divided into seven new groups again:
$S_1 = F \cap G \cap H$, covers $t_1$ points that are selected by all three approximate models: $f'(x)$, $g'(x)$ and $h'(x)$.
$S_2 = F \cap G - S_1$, covers $t_2$ points that are selected by two approximate models: $f'(x)$ and $g'(x)$.
2.3. Weight calculation
The weight of each group is calculated based upon the number of points in the group, as in equation (2):

\[ w_i = \frac{t_i \times t_i}{\sum t_i \times t_i} \quad (i = 1, ..., 7) \]  

(2)

Where \( t_i \) is the number of the points in the \( i \)th group, \( w_i \) is the weight of the group, and \( k_i \) is the integer value after rounding.

If \( t_1 > 0 \) and \( k_1 = 0, k_1 \) is reset to 1. This can avoid the situation that the points in \( S_1 \) is ignored after weighted calculation because the number of points in \( S_1 \) is too small.

2.4. Termination criteria
The mean of the ten lowest function values, \( \bar{m}n \), are set as the terminating parameters of the search process. When the improvement on \( \bar{m}n \) becomes negligible, the search process terminates. As in equation (3):

\[ \left| \bar{m}n_{i+1} - \bar{m}n_i \right| \leq \varepsilon \quad (3) \]

\[ \bar{m}n = \frac{\sum_{j=1}^{10} f_j}{10} \quad (4) \]

Where \( \varepsilon \) is a small value given by designer, and \( f_j \) is the \( j \)th smallest function value.

3. Test of the new ASA method on standard test functions
The proposed ASA method has been tested on several well-known test functions, and compared with several widely used global optimization methods, including particle swarm optimization (PSO) and genetic algorithm (GA). Besides, GU’s HAM method is also used as comparison, since ASA is improved on the basis of HAM.

The standard test functions are:
(1) Generalized polynomial function (GF)
\[ f(x_1, x_2) = \left( 2.625 - x_1(1 - x_2^2) \right)^2 + \left( 2.25 - x_1(1 - x_2^2) \right)^2 + (1.5 - x_1(1 - x_2))^2, \]
\[ x_1, x_2 \in [-2, 2] \]

Its known minimum is 0.5233.

(2) Goldstein and Price function (GP)
\[ f(x_1, x_2) = (1 + (x_1 + x_2 + 1)^2(19 - 14x_1 + 3x_1^2 - 14x_2 + 6x_1x_2 + 3x_2^2)) \times (30 + 2x_1 - \]
\[ 3x_2)^2(18 - 32x_1 + 12x_2^2 + 48x_2 - 36x_1x_2 + 27x_2^2)) \]
\[ x_1, x_2 \in [-2, 2] \]

Its known minimum is 3.

(3) Griewank functions (GN)

\[ f(x_1, x_2) = \]
\[ \frac{1}{4000} \sum_{i=1}^{d} x_i^2 - \cos(\frac{\pi}{2} \sum_{i=1}^{d} x_i^2) \]
\[ x_1, x_2 \in [-600, 600] \]
\[ f(x) = 1 + \frac{(x_1^2 + x_2^2)}{200} - \cos(x_1) \cos\left(\frac{x_2}{\sqrt{2}}\right), \quad x_1, x_2 \in [-100, 100] \]  

(7) Its known minimum is 0.

(4) Six-hump Camel-Back function (SC)

\[ f(x_1, x_2) = 4x_1^2 - 2.1x_1^4 + \frac{1}{3} x_1^6 + x_1 x_2 - 4x_2^2 + 2.9484x_1^4 + x_1^2, x_1, x_2 \in [-2, 2] \]  

(8) Its known minimum is -1.0316.

(5) Leon function

\[ f(x_1, x_2) = 100(x_2 - x_1^3)^2 + (x_1 - 1)^2, x_1, x_2 \in [-10, 10] \]  

(9) Its known minimum is 0.

In the test, seven points sampled by LHS and four boundary points are used as initial sampling points. And \( N \) is set as 10000, then \( n \) is 100. For each standard test function, the search process runs 10 times to avoid unrepresentative numerical results. The number of iterations (NIT) and the number of sample points (NSP) are used to measure computation efficiency. The average of all values are illustrated in table 1. The calculated minimum is also shown to illustrate the accuracy of the search.

**Table 1.** the test data of GA, PSO, HAM and ASA on five standard test functions.

(a) calculated minimum(MIN).

|        | GA     | PSO    | HAM    | ASA    |
|--------|--------|--------|--------|--------|
| GF     | 0.5234 | 0.5233 | 0.5467 | 0.5461 |
| GP     | 11.2539| 3.0036 | 3.0006 | 3.0039 |
| GN     | 0      | 0      | 0.0537 | 0.0306 |
| SC     | -1.0316| -1.0316| -1.0310| -1.0311|
| Leon   | 0.0379 | 0.0059 | 0.0053 | 0.0055 |

(b) number of iterations(NIT).

|        | GA     | PSO    | HAM    | ASA    |
|--------|--------|--------|--------|--------|
| GF     | 51.5   | 276.2  | 12.8   | 11.8   |
| GP     | 103.1  | 335.7  | 23.4   | 19.3   |
| GN     | 51     | 382.7  | 13.1   | 8      |
| SC     | 51     | 412.8  | 6.7    | 6.3    |
| Leon   | 84.4   | 406.6  | 21.9   | 19.1   |

(c) number of sample points(NSP).

|        | GA     | PSO    | HAM    | ASA    |
|--------|--------|--------|--------|--------|
| GF     | 1030   | 5524   | 88.4   | 87.7   |
| GP     | 2062   | 6714   | 165.1  | 138.9  |
| GN     | 1020   | 7654   | 72.8   | 65.1   |
| SC     | 1020   | 1729   | 49.6   | 51.8   |
| Leon   | 1688   | 8132   | 160.6  | 132.6  |

As the results shown in Table 1 (a), the ASA method preserves the accuracy of HAM, which is equivalent to the genetic algorithm. Only on test function GN, ASA perform poor in accuracy, and the reason is that the GN function has hundreds of Local optimum points in the design space.
As the results shown in Table 1 (b) and (c), the ASA method performed well on all functions, with both NEF and NIT lower than GA and PSO. GA and PSO require too many sample points and cost function evaluations. ASA method performed well than HAM on all test functions except SC, because ASA has more initial sample points than HAM which lead to larger NIT.

In summary, the proposed ASA method has improved the calculation efficiency on the premise of keeping the accuracy of the HAM.

4. Application on the nozzle profile optimization

As an important part of the rocket engine, the design of the nozzle has an important influence on the thrust of the rocket engine. The change in the nozzle profile of the rocket engine will affect the thrust, when all the other conditions remain unchanged. In order to obtain larger engine thrust, the ASA method is used to optimize the design of the nozzle of a small thrust rocket engine.

4.1. Simulation model

The physical model used in numerical calculation is a curved nozzle. Considering the symmetry of the physical model, the model in the numerical analysis and calculation is simplified, that is, only half of the model is established, so that the computation cost of the whole simulation can be largely reduced. The FLUENT software based on the finite volume method is used to simulate the flow field of the nozzle. The surface mesh of the rocket engine nozzle is shown in Figure 1.

![Figure 1. The rocket engine nozzle](image)

In the process of numerical calculation, Nitrogen is set to a gas flow medium inside the nozzle, the inlet and outlet boundary condition are set to the pressure inlet boundary, wall boundary condition is set to non-slip adiabatic wall boundary.

4.2. Optimization process

Three key design variables are considered, which are nozzle diffuser angle $\beta_e$, ratio of the radius of the contraction section surface to the nozzle throat radius, $k = R_e/R_t$, and ratio of the radius of the throat section surface to the nozzle throat radius, $\rho = R_3/R_t$. Other parameters, such as the nozzle throat radius, inlet radius and outlet radius, remain unchanged. The design objective is to maximize the thrust:

$$\begin{align*}
\text{Min} & \quad (-F) \\
\text{s.t.} & \quad 1.3 \ll k \ll 2 \\
& \quad 2 \ll \rho \ll 4 \\
& \quad 5 \ll \beta_e \ll 10
\end{align*}$$

Optimization results using the ASA optimization program are obtained as shown in table 2. The optimization process has only seven iterations and fifty-seven times of simulation calculation, taking
550 minutes in total. Compared with the initial design, the optimal design increases 2.56% of the thrust.

|        | k   | ρ   | β_e | F/N |
|--------|-----|-----|-----|-----|
| Initial design | 1.5 | 3   | 7.5 | 44.252 |
| Optimal design   | 2.001 | 2.046 | 5.194 | 45.386 |

5. Conclusions
In this work, an adaptive and approximate model based optimization method is introduced, which is improved on the basis on HAM. The objective of this work is to further improve the efficiency and accuracy of the approximate model based optimization technique and make it applicable to a broad spectrum of design optimization applications.

This method uses three different types of approximate models at the same time, so that it can takes the full advantage of the three models’ characteristics and be suitable for different kinds of optimization design problems. Besides, the method applied an adaptive sampling algorithm (ASA) to achieve the self-setting mechanism for new sampling points in the search process.

By testing on several standard test functions, the method preserves the accuracy of HAM, which is equivalent to the genetic algorithm. The method also performed well than GA, PSO and HAM in computational efficiency.

The method has been applied in the optimization design of rocket engine design to get the maximum thrust. Only after seven iterations and fifty-seven times of simulation calculation, optimal is obtained and the thrust is improved by 2.56%, then the feasibility and efficiency of this method have been proved.

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Conflict
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