Using Empirical Knowledge for Adaptive Selection of Reduplicate Simulation Times in Simulation Optimization

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Summary
Simulation optimization studies the optimization problem of simulation-based objectives in the foundation of mature modern optimization theory system. In order to improve the disadvantages of current selection of reduplicate simulation times in simulation optimization, this paper presents an adaptive selection of reduplicate simulation times in simulation optimization by using empirical knowledge. The method is based on the empirical knowledge from simulation optimization practice. Empirical knowledge from simulation optimization studies is an important source for the creation of accurate simulation models. This paper focuses on the use of empirical knowledge for the development and calibration of simulation models. At first, the author summarizes some empirical knowledge from simulation optimization studies. At second, the author describes the method of this paper in detail. The method of this paper mainly consists of three steps: complexity estimation to the optimization problem, classified operation of trial point and adaptive selection of the reduplicate simulation times. At third, the author uses two numerical examples to testify the validity of this method. From the computing result of numerical examples, we can see that, through the adaptive selection of reduplicate simulation times to the different trial points, the computing time is decreasing and the global optimization solution is improving in the given computing precision. In conclusion, the method of this paper is feasible, correct and valid. Finally, the conclusions of this study are drawn with possible directions for subsequent studies.

Key words:
simulation optimization; orthogonal genetic algorithm; statistical test; computer simulation; optimization technology

1. Introduction

Simulation optimization studies the optimization problems of simulation-based objectives on the foundation of mature modern optimization theory system. Simulation optimization has been applied to the fields of system design, automation and simulation algorithm optimization widely [1-4]. In tutorials on simulation optimization, such as [5-7], four major classes of approach can be distinguished: gradient-based search methods, stochastic approximation methods, response surface methodology and heuristic methods. Those methods have been applied in various application fields and particularly in manufacturing systems [8] and economic systems [9]. Basically, the aim of each of these approaches is to propose a strategy to explore the solution space, with a limited number of simulation experiments [10].

In general, Simulation Optimization problems can be mathematically formulated as follows:

$$Min \quad F(X) = \underset{X \in D}{E}\left[y\left(X, f\left(X, w \right)\right)|_X \right] \tag{1}$$

Where X denotes the controllable factor (decision variables). To most practical engineering optimization problems, X is mixed decision variables, including the continuous variables and discrete variables. w denotes the uncontrollable factor, for example, all kinds of random perturbation. D denotes the solution space of the decision variables.

$f(X,w) = \left(f_1(X,w), f_2(X,w), \cdots, f_p(X,w)\right)$ denotes the performance measure evaluated at the given decision variables X and random conditions w, we call it "simulation response value" in this paper. $y\left(X, f\left(X, w\right)\right)$ denotes the simulation objective output at the given decision variables X and random conditions w. $E\left[y\left(X, f\left(X, w\right)\right)|_X \right]$ denotes the expected simulation output by the given decision variables X, we call it "fitness value" in this paper. Note that $F(X)$ is not known explicitly, that is there is no analytical expression for $F(X)$.

The most serious problem is that a single experiment at the trial point x_k may have a simulation response value $f(x_k, w)$ which is very different from the expected simulation response $F(x_k)$, reduplicate simulation at x_k are necessary. Law and Kelton [15] suggest that at least three to five reduplicate simulation should be conducted at any experimental point in simulation studies. In reference [10], rather than the fixing reduplicate simulation times at a constant value, it is set to a variable value according to the following expressions.

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$$p_i = \frac{m}{\left\| X_i - X^* \right\|} = \begin{cases} 5 & if\ p_i \in (0,5] \\ 10 & if\ p_i \in (5,10] \\ 15 & if\ p_i \in (10,15] \\ 20 & if\ p_i \in (15,20] \\ 25 & if\ p_i \in (20,25] \\ 30 & if\ p_i \in (25,\infty) \end{cases} \quad (2)$$

Where p_i denotes the frequency of reduplicate simulation at the point of X_i, $\|\cdot\|$ is the vector norm and m is a parameter, X_i is the No i individual and X^* is the best individual among the current population.

Obviously, the current selection of reduplicate simulation times in simulation optimization was provided with some adaptability, it can select an appropriate reduplicate simulation times according to the distance between the trial individual and the current best individual. At the same time, there are some disadvantages in the current selection methods. (1) The complicacy of material problem has not been considered. The method presented by reference [9] is available to the simple optimization problem, but to the complex optimization problem, it is very difficult to get a considerable estimation to the fitness of trial point through such few reduplicate simulations, as a result, the final optimization solution is not correct. (2) The computing precision has not been considered in optimization process. The traditional algorithm didn't calculate the computing precision to the fitness of trial point after reduplicate simulations. If the computing precision is low (that is, the computing error is very big), then it will lead to the misdirection in optimization process and the incorrect result in the final solution. (3) The optimization of reduplicate simulation times has not been considered. For example, if it can get a considerable estimation to the fitness of the trial point which near the current best point through few reduplicates simulations, it is not necessary to run the latter simulations.

Considering the disadvantages of current selection of reduplicate simulation times in simulation optimization, this paper presents an adaptive selection of reduplicate simulation times in simulation optimization by using empirical knowledge. The paper is organized as follows. Section 2 summarizes some empirical knowledge from simulation optimization studies. Section 3 describes the method of this paper in detail. The method of this paper mainly consists of three steps: complexity estimation to the optimization problem, classified operation of trial point and adaptive selection of the reduplicate simulation times. In Section 4, the proposed method is illustrated by some numerical examples. Finally, the conclusions of this study are drawn with possible directions for subsequent studies.

2. Empirical Knowledge

Empirical knowledge from simulation optimization studies is an important source for the creation of accurate simulation models. Based on empirical knowledge, the well-known engineering principles help a lot in achieving time, cost and quality goals [11]. One way of creating a reasonable connection between optimization process simulations and reality is the integration of empirical knowledge. In general, combining empirical knowledge and process simulation can be done in following ways [12]: (1) Empirical knowledge is used for the development and calibration of simulation models, (2) results from process simulations are used for planning, designing and analyzing real experiments, and (3) process simulation and real experiments are performed in parallel (such as, online simulation).

This paper focuses on the use of empirical knowledge for the development and calibration of simulation models. We apply the following empirical knowledge to optimization process simulation: (1) In the process of simulation optimization, "shorter simulation time and higher computing precision" is an ideal effect. (2) Usually, for points further away from the optimal point the response surface is relatively flat; as the trial point gets closer to the optimum the curvature of the response surface becomes sharper [10]. (3) In order to get a better optimization effect, few reduplicate simulations is enough to the trial point in the relatively flat response surface; more reduplicate simulation should be applied to the trial point in the relatively sharp response surface [10]. (4) Commonly, more reduplicate simulation implies longer execution time. (5) It is expected that more reduplicate simulation would result in an average response of better quality (higher computing precision). (6) To the different optimization problem, the least reduplicate simulation times available to all trial points is different in a given precision. Generally, using data from replicated studies in simulation models improves the empirical basis of the model and can lead to better calibrations.

3. Material Method

This paper performs the adaptive control to the reduplicate simulation of the optimization process through the adaptive selection of reduplicate simulation times. The method of this paper mainly consists of three steps. (1) Complexity estimation to the optimization problem. The main objective of this step is to find the minimal simulation times available to most trial points of given optimization problem in a given computing precision (such as 95%). (2) Classified operation of trial point. This step classifies the trial points into several parts according

to the distance between the trial point and the current best point. At the same time, it defines the different computing precision requirement to every parts of the trial points. (3) Adaptive selection of the reduplicate simulation times. This step achieves an appropriate reduplicate simulation times through the accumulation of reduplicate simulation times and the comparison of computing precision.

3.1 Complexity Estimation to Optimization Problems

According to the empirical knowledge "to the different optimization problem, the least reduplicate simulation times available to all trial points is different in a given precision", we should estimate the complexity of the optimization problem at first. The computing error of different reduplicate simulations is defined as following.

$$\varepsilon_{k_1,k_2} = \left| \frac{\overline{f_{k_2}(X,w)} - \overline{f_{k_1}(X,w)}}{\overline{f_{k_1}(X,w)}} \right| \tag{3}$$

Where X denotes the decision variables, w denotes the random variables, $\overline{f_{k_1}(X,w)}$ and $\overline{f_{k_2}(X,w)}$ denote the average response value of k_1 and k_2 replicate simulations at the decision variable X respectively. ε_{k_1,k_2} denotes the computing error of k_1 and k_2 replicate simulations at the decision variable X.

This paper classified the optimization problems into seven classes according to the conditions of table 1, the minimal simulation times available to most trial points of each class of optimization problem in a given computing precision $(1-\varepsilon)$ is listed in table 1. Noted that, the "Amount" in table 1 means the amount of trial points of random selection, the "Computing Error" means the computing error of different reduplicate simulation times, and the "Minimal Simulation Times" means the minimal simulation times that available to most trial points of this class optimization problem in a given computing precision $(1-\varepsilon)$.

3.2 Classified Operation of Trial Point

The author presents the following analysis based on the foregoing empirical knowledge (1)-(5). Usually, for points further away from the optimal point the response surface is relatively flat. So when you simulate the optimization process at these trial points repeatedly, the improvement of computing precision is not very distinct, but the increment of computing time is very remarkable. In this case, we can set a low computing precision to the reduplicate simulations of these trial points. In this way, the reduplicate simulation times will be decreased furthest and the computing time will be saved markedly. As the trial point gets closer to the optimum the curvature of the response surface becomes sharper. So when you simulate the optimization process at these trial points repeatedly, both the improvement of computing precision and the increment of computing time are very remarkable. In this case, we can set a high computing precision to the reduplicate simulations of these trial points. In this way, the accuracy of simulation optimization will be improved markedly through increment of reduplicate simulations.

Table 1: The classified condition and result of optimization problems

	Condition		Result
	Amount	Computing Error	Minimal Simulation Times
Class A	10,000	$\overline{\varepsilon_{1000,5000}} \le \varepsilon$	1000
Class B	10,000	$\overline{\varepsilon_{5000,10000}} \le \varepsilon$	5000
Class C	10,000	$\overline{\varepsilon_{10000,20000}} \le \varepsilon$	10,000
Class D	10,000	$\overline{\varepsilon_{20000,50000}} \le \varepsilon$	20,000
Class E	10,000	$\overline{\varepsilon_{50000,100000}} \le \varepsilon$	50,000
Class F	10,000	$\overline{\varepsilon_{100000,150000}} \le \varepsilon$	100,000
Class G	The problem of this class is too complex; we will study it in the future.		

This step classifies the trial points into several parts according to the distance between the trial point and the current best point. At the same time, it defines the different computing precision requirement to every parts of the trial points. The distance between the trial point and the current best point is defined in the following.

$$p_k = \frac{\left\| X_k - X^* \right\|}{\max\limits_{1 \le i \le n} \left\| X_i - X^* \right\|} \tag{4}$$

Where X_k denotes the number k trial point, X^* denotes the current best point, p_k denotes the distance between X_k and X^*, n denotes the amount of the current trial points. According to the classified condition as table 2, this paper classifies the trial points into four classes. The computing precision requirement of each class is listed in table 2.

Table 2: Classified condition and computing precision requirement of trial point

Class	Class one	Class two	Class three	Class four
Classified condition	$0 \le p_k < 0.1$	$0.1 \le p_k < 0.3$	$0.3 \le p_k < 0.6$	$0.6 \le p_k \le 1.0$
computing precision requirement	$1-\varepsilon$	$1-2\varepsilon$	$1-3\varepsilon$	$1-5\varepsilon$

3.3 Adaptive selection of the reduplicate simulation times

In the process of simulation optimization, "shorter simulation time and higher computing precision" is an ideal effect. In the guidance of this idea, this method decreases the reduplicate simulation times furthest within the computing precision requirement. This step achieves

an appropriate reduplicate simulation times through the accumulation of reduplicate simulation times and the comparison of computing precision. The material computational flow is in the following.

STEP1: let *Num* is the minimal simulation times that available to most trial points of the optimization problem in a given computing precision (95%), ε_0 is the computing precision requirement of the current trial point, $N = Num/10$, $\varepsilon_1 = 1-\varepsilon_0$, $I = 1$;

STEP2: $k_1 = I \times N$, $k_2 = (I+1) \times N$;

STEP3: IF $\overline{\varepsilon_{k_1,k_2}} \le \varepsilon_1$, THEN (GOTO STEP4), ELSE ($I = I+1$, GOTO STEP2);

STEP4: The reduplicate simulation times of this trial point is k_1 and the fitness estimation of this trial point is $\overline{f_{k_1}(X,w)}$.

4 Numerical examples

In order to testify the method of this paper, the author uses two numerical examples to test the validity of this method.

4.1 Watson Function

The Watson function incorporated with a stochastic term is as follows [13]:

$$F(X) = \min\left\{\sum_{i=1}^{29}\left[\sum_{j=2}^{9}(j-1)x_j\left(\frac{i}{29}\right)^{j-2} - \left(\sum_{j=1}^{9}x_j\left(\frac{i}{29}\right)^{j-1}\right)^2 - 1\right]^2 + x_1^2 + \left(x_2 - x_1^2 - 1\right)^2 + w\right\} \quad (8)$$

Where w follows the standard normal distribution truncated to the range of three standard deviations. The global optimization solution of Watson function is $F^*(X) = 1.3998E-6$.

At first, we should estimate the complexity of the Watson problem. Through repetitious selection of 10,000 initial points randomly, $\overline{\varepsilon_{10000,20000}} \le 0.01$ is accepted in Watson problem. So in the given computing precision 99%, Watson problem belongs to the problem of class C. That is, the minimal simulation time available to most trial points of Watson problem in the given computing precision 99% is 10,000 times.

At second, the author designs four different experimentation schemes to solve Watson problem. These experimentation schemes are designed as following: (1) simulate 1,000 times at every trial point repeatedly; (2) simulate 5,000 times at every trial point repeatedly; (3) simulate 10,000 times at every trial point repeatedly; (4) simulate applies the method of this paper. The computing result of these four experimentation schemes is displayed as table3 and figure1. Noted that, the "Simulation Result" in table3 means the global optimization solution solved by simulation optimization algorithm, the "Analysis Result" means the average of 20000 reduplicate simulations at the global optimization point solved by simulation optimization algorithm, the "Error" means the difference between "Simulation Result" and "Analysis Result". The computing formula of "Error" is displayed in the following:

$$Error = \left|\frac{Analysis\,result - Simulation\,result}{Analysis\,result}\right|.$$

Table 3: Optimization Result of Watson function

Optimization Run			1	2	3	Average
Different experimentation schemes	No 1	Computing Time (S)	129.63	128.64	127.98	128.75
		Simulation Result	-0.4596	-0.4816	-1.6092	-0.8501
		Analysis Result	-0.6214	-0.5518	-1.2806	-0.8179
		Error	0.2604	0.1272	0.2566	0.2147
	No 2	Computing Time (S)	762.53	764.45	763.59	763.52
		Simulation Result	-0.4984	-1.5277	-0.6841	-0.9034
		Analysis Result	-0.6073	-1.6522	-0.5764	-0.9453
		Error	0.1793	0.0754	0.1868	0.1472
	No 3	Computing Time (S)	2220.80	2228.00	2226.59	2225.13
		Simulation Result	-1.2729	-0.5748	-0.5128	-0.7868
		Analysis Result	-1.388	-0.6944	-0.4437	-0.8420
		Error	0.0829	0.1722	0.1557	0.1369
	No 4	Computing Time (S)	2189.70	2196.30	2203.70	2196.57
		Simulation Result	-0.9785	-0.9119	-0.0573	-0.6492
		Analysis Result	-1.1016	-0.8433	-0.0664	-0.6703
		Error	0.1117	0.0813	0.1370	0.1100

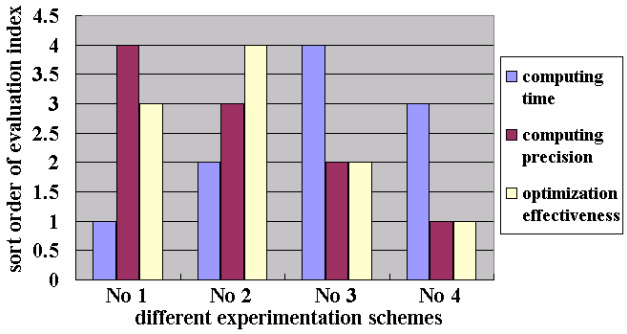

Fig.1. Sort order of optimization evaluation index of Watson function using different experimentation schemes

From figure 1, we can see that: along with the increase of the reduplicate simulation times, the computing time of optimization algorithm is longer and longer, the computing precision of optimization algorithm is higher and higher, and the global optimization solution is better and better. In the process of solving Watson problem, through the adaptive selection of reduplicate simulation times to the different trial points, the computing time is

decreasing and the global optimization solution is improving in the given computing precision.

4.2 Test function

Here we use the example of expectation model in reference [14].

$$\max f(X)=\int\left[(x_1-\varepsilon_1)\sin(4\pi x_2)+(x_3-\varepsilon_3)\sin(10\pi x_3)\right]\Phi(\varepsilon_1,\varepsilon_2,\varepsilon_3)\,d\varepsilon_1 d\varepsilon_2 d\varepsilon_3$$
$$subject\ to\quad 0\le x_i\le 5, i\in(1,2,3). \tag{9}$$

Where $\Phi(\varepsilon_1,\varepsilon_2,\varepsilon_3)$ is multi-normal probability distribution function, that is,

$$\Phi(\varepsilon_1,\varepsilon_2,\varepsilon_3)=(2\pi)^{-\frac{3}{2}}\|C\|^{-\frac{1}{2}}\exp\left\{-\frac{1}{2}(\varepsilon-\mu)^T C^{-1}(\varepsilon-\mu)\right\}$$

$$\varepsilon=\begin{pmatrix}\varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\end{pmatrix},\mu=\begin{pmatrix}\mu_1\\ \mu_2\\ \mu_3\end{pmatrix}=\begin{pmatrix}1\\ 2\\ 3\end{pmatrix},C=\begin{bmatrix}c_{11} & c_{12} & c_{13}\\ c_{21} & c_{22} & c_{23}\\ c_{31} & c_{32} & c_{33}\end{bmatrix}=\begin{bmatrix}2 & 1 & 1\\ 1 & 2 & 1\\ 1 & 1 & 2\end{bmatrix}.$$

At first, we should estimate the complexity of this expectation model problem. Through repetitious selection of 10,000 initial points randomly, $\overline{\varepsilon_{10000,20000}}\le 0.10$ is accepted in this expectation model problem. So in the given computing precision 90%, this expectation model problem belongs to the problem of class C. That is, the minimal simulation time that available to most trial points of this expectation model problem in the given computing precision 90% is 10,000 times.

At second, the author designs four different experimentation schemes to solve this expectation model problem. These experimentation schemes are designed as follows: (1) simulate 1,000 times at every trial point repeatedly; (2) simulate 5,000 times at every trial point repeatedly; (3) simulate 10,000 times at every trial point repeatedly; (4) simulate applies the method of this paper. The computing results of these four experimentation schemes are displayed in table4 and figure 2. The meaning of "Simulation Result", "Analysis Result" and "Error" in table 4 is the same as that of table 3.

From the figure 2, we can see that: with the increase of the reduplicate simulation times, the computing time of optimization algorithm is longer and longer, the computing precision of optimization algorithm is higher and higher, and the global optimization solution is better and better. In the process of solving this expectation model problem, through the adaptive selection of reduplicate simulation times to the different trial points, the computing time is decreasing and the global optimization solution is improving in the given computing precision.

Table 4: Optimization result of expectation model problem

Optimization Run			1	2	3	Average
Different experimentation schemes	No 1	Computing Time (S)	2949.6	2859.0	3015.0	2941.2
		Simulation Result	9.2119	9.1964	9.0164	9.1416
		Analysis Result	8.9636	8.9413	8.7979	8.9003
		Error	0.0277	0.0285	0.0248	0.0270
	No 2	Computing Time (S)	9135.3	9422.6	10122.0	9560.0
		Simulation Result	8.8635	9.0681	8.9383	8.9566
		Analysis Result	8.7188	8.9813	8.8148	8.8383
		Error	0.0166	0.0097	0.0140	0.0134
	No 3	Computing Time (S)	19654.0	18384.0	18681.0	18906.3
		Simulation Result	9.0775	9.0762	9.0475	9.0671
		Analysis Result	8.9826	9.0056	8.9707	8.9863
		Error	0.0106	0.0078	0.0086	0.0090
	No 4	Computing Time (S)	14925.0	13847.0	14410.0	14394
		Simulation Result	9.0847	9.0659	9.1022	9.0843
		Analysis Result	9.0029	8.9125	8.8975	8.9376
		Error	0.0091	0.0172	0.0230	0.0164

5. Result

In this paper, we present an adaptive selection of reduplicate simulation times in simulation optimization using empirical knowledge. The model is based on the empirical knowledge from simulation optimization practice. At first, the author summarizes some empirical knowledge from simulation optimization studies. At second, the author describes the method of this paper in detail. The method of this paper mainly consists of three steps: complexity estimation to optimization problem, classified operation of trial point and adaptive selection of the reduplicate simulation times. At third, the author uses two numerical examples to test the validity of this method. From the computing result of numerical examples we can see that, through the adaptive selection of reduplicate simulation times to the different trial points, the computing time is decreasing and the global optimization solution is improving with the given computing precision. In conclusion, the method of this paper is feasible, correct and valid.

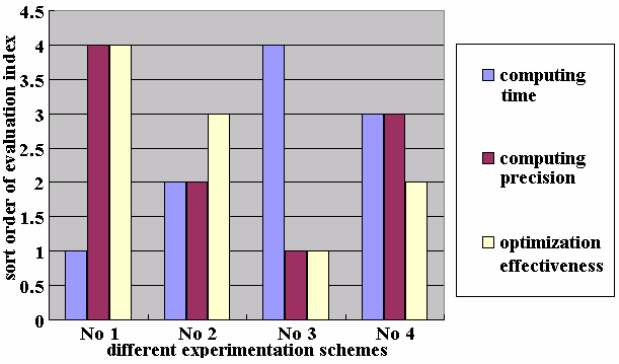

Fig.2. Sorting order of optimization evaluation index of expectation model problem using different experimentation schemes

We encounter several problems during modeling and integrating of empirical knowledge. Firstly, complexity estimation to the optimization problem is very difficult. As you know, the more trial points were estimated, the more reliable result will be get. But to a complex optimization, estimating enough trial points is not an easy thing. Secondly, the adaptive selection of the reduplicate simulation times need further study. The correctness and feasibility of this step is obviously from the theory aspects, but it is time-consuming in the practice aspects. These two points need further study in the future.

Finally, more methodological support for combining empirical knowledge and simulation modeling is needed. This could lead to a new and advanced type of experimental laboratory that uses process simulation as a virtual capability.

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