A Novel Multi-objective Orthogonal Simulated Annealing Algorithm for Solving Multi-objective Optimization Problems with a Large Number of Parameters

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Abstract. In this paper, a novel multi-objective orthogonal simulated annealing algorithm MOOSA using a generalized Pareto-based scale-independent fitness function and multi-objective intelligent generation mechanism (MOIGM) is proposed to efficiently solve multi-objective optimization problems with large parameters. Instead of generate-and-test methods, MOIGM makes use of a systematic reasoning ability of orthogonal experimental design to efficiently search for a set of Pareto solutions. It is shown empirically that MOOSA is comparable to some existing population-based algorithms in solving some multi-objective test functions with a large number of parameters.

1 Introduction

Many real-word applications usually involve simultaneous consideration of multiple performance criteria that are often incommensurable and conflict in nature. It is very rare for these applications to have a single solution, but rather a set of alternative solutions. These Pareto-optimal solutions are those for which no other solution can be found which improves along a particular objective without detriment to one or more other objectives. Multi-objective evolutionary algorithms (MOEAs) for solving multobjective optimization problems gain significant attention from many researchers in recent years [1]-[8]. These optimizers not only emphasize the convergence speed to the Pareto-optimal solutions, but also the diversity of solutions. Niching techniques, such as fitness sharing and mating restriction, are employed for finding uniformly distributed Pareto-optimal solutions [2]-[3], and elitism is incorporated for improving the convergence speed to the Pareto front [4].

In recent years, many MOEAs employing local search strategies for further improving convergence speed have been successively proposed [4]-[7]. Population-

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based MOEAs have a powerful ability to extensively explore candidate solutions in a whole search space and painstakingly exploit candidate solutions in a local region, in parallel. In the neighborhood of each individual, it is beneficial for MOEAs to use local search strategies to exploit better solutions. However, local search strategies increase computation time in each generation. In order to avoid wasting time in unnecessary local searches, MOEAs must choose good individuals from the population for further exploiting non-dominated solutions [8]. However, it is difficult to determine which individual is good for exploit.

Knowles and Corne [5] proposed a non-population based method, Pareto archived evolution strategy (PAES), to find a Pareto font. It employs a local search strategy for the generation of new candidate solutions, and utilizes elite set information to aid in the calculation of the solution quality. However, the local search strategy is based on generate-and-test methods that cannot efficiently solve large multi-objective optimization problems (MOOPs) with a large and complex search space.

Recently, an efficient sigle-objective orthogonal simulated annealing algorithm OSA is proposed [9]. High performance of OSA mainly arises from an intelligent generation mechanism (IGM) which applies orthogonal experimental design to speed up the search. IGM can efficiently generate a good candidate solution for next move of OSA by using a systematic reasoning method. In this paper, a novel multi-objective orthogonal simulated annealing algorithm MOOSA using a generalized Pareto-based scale-independent fitness function and multi-objective IGM (MOIGM) is proposed to efficiently solve multi-objective optimization problems with large parameters. Instead of generate-and-test methods, MOIGM makes use of a systematic reasoning ability of orthogonal experimental design to efficiently search for a set of Pareto solutions. It is shown empirically that MOOSA is comparable to some existing population-based algorithms in solving some multi-objective test functions [1] with a large number of parameters.

2 Orthogonal Experimental Design [9]

MOOSA with a multi-objective intelligently generation mechanism (MOIGM) is based on orthogonal experimental design (OED). The basic concepts of OED are briefly introduced in Section 2.1. The orthogonal array and factor analysis of OED used in MOIGM are described in Section 2.2.

2.1 Concepts of OED

An efficient way to study the effects of several factors simultaneously is to use OED based on orthogonal array and factor analysis [10], [11]. Many design experiments use OED for determining which combinations of factor levels to use for each experiment and for analyzing the experimental results. The factors are the variables (parameters), which affect the chosen response variables (objective functions), and a setting (or a discriminative value) of a factor is regarded as a level of the factor. The term ‘main effect' designates the effect on the response variable that one can trace to a design parameter [10].

Orthogonal array is a factional factorial matrix, which assures a balanced comparison of levels of any factor or interaction of factors. In the context of experimental matrices, orthogonal means statistically independent. The array is called orthogonal because all columns can be evaluated independently of one another, and the main effect of one factor dose not bother the estimation of the main effect of another factor [11]. Factor analysis using the orthogonal array's tabulation of experimental results can allow the main effects to be rapidly estimated, without the fear of distortion of results by the effects of other factors. Factor analysis can evaluate the effects of solution factors on the evaluation function, rank the most effective factors, and determine the best level for each factor such that the evaluation function is optimized.

Orthogonal experimental design can provide near-optimal quality characteristics for a specific objective. Furthermore, there is a large saving in the experimental effort. OED uses well-planned and controlled experiments in which certain factors are systematically set and modified, and then main effect of factors on the response can be observed. OED specifies the procedure of drawing a representative sample of experiments with the intention of reaching a sound decision [10]. Therefore, OED using orthogonal array and factor analysis is regarded as a systematic reasoning method.

2.2 Orthogonal Array and Factor Analysis

The three-level orthogonal array (OA) used in intelligent generation mechanism is described as follows. Let there be N factors with three levels for each factor. The number of total experiments is 3^N for the popular "one-factor-at-once" study. All the optimization parameters are generally partitioned into N groups.

Table 1. Orthogonal array $L_9(3^4)$

	Factor i				
Experiment no. j	1	2	3	4	Fitness value f_j
1	1	1	1	1	f_1
2	1	2	2	2	f_2
3	1	3	3	3	f_3
4	2	1	2	3	f_4
5	2	2	3	1	f_5
6	2	3	1	2	f_6
7	3	1	3	2	f_7
8	3	2	1	3	f_8
9	3	3	2	1	f_9

One group is regarded as a factor. To use an OA of N factors with three levels, we obtain an integer $M = 3^{\lceil \log_3 (2N+1) \rceil}$, build a three-level OA $L_M(3^{(M-1)/2})$ with M rows and (M-1)/2 columns, use the first N columns, and ignore the other (M-1)/2-N columns. Table 1 illustrates an example of OA $L_9(3^4)$. OA can reduce the number of experiments for factor analysis. The number of OA experiments required to analyze all solution factors is only M, where $2N+1 \le M \le 6N-3$. An algorithm of constructing OA can be found in [12]. After proper tabulation of experimental results, the summarized data are analyzed using factor analysis to determine the relative effects of levels of various factors as follows.

Let f_j denote a fitness value of the combination corresponding to the experiment j, where $j = 1, \ldots, M$. Define the main effect of factor i with level k as S_{ik} where $i = 1, \ldots, N$ and $k = 1, 2, 3$:

$$S_{ik} = \sum_{j=1}^{M} f_j \cdot AF_j, \tag{1}$$

where $AF_j = 1$ if the level of factor i of experiment j is k; otherwise, $AF_j = 0$. Considering the case that the a fitness value is to be minimized, the level k is the best one when $S_{ik}=\min\{S_{i1}, S_{i2}, S_{i3}\}$. The main effect reveals the individual effect of a factor.

After the best one of three levels of each factor is determined, an intelligent combination consisting of all factors with the best levels can be easily derived. OED is effective for development design of efficient search for the intelligent combination of factor levels, which can yield a high-quality a fitness value compared with all values of 3^N combinations, and has a large probability that the reasoned value is superior to those of M representative combinations.

3 Multi-objective Orthogonal Simulated Annealing Algorithm MOOSA

MOOSA with MOIGM based on orthogonal experimental design (OED) can effectively solve intractable engineering problems comprising lots of parameters. A MOIGM uses a generalized Pareto-based scale-independent fitness function (GPSIFF) to efficiently evaluate the performance of solutions. GPSIFF evaluation procedure is described in Section 3.1. An MOIGM operation is briefly introduced in Section 3.2.A MOOSA using MOIGM is described in Section 3.3.

3.1 Use a Proposed GPSIFF

The fitness values for a set P of participant solutions to be evaluated are derived using a GPSIFF evaluation procedure at the same time in an objective space. GPSIFF makes direct use of general Pareto dominance relationship to obtain a single measurement of solutions. Simply, one solution has a higher score if it dominates more solutions. On the contrary, one solution has a lower score if more solutions dominate it.

Let a fitness value of a candidate solution be a tournament-like score obtained from all participant solutions in P. The fitness value of X can be given by the following score function:

$$\text{score}(X) = \{ p - q + c \mid p = |A|,\ q = |B|, c = |P| \ s.t.\ \ X \prec A, B \prec X, A \subseteq P \text{ and } B \subseteq P \}, \tag{2}$$

where $\prec$ stands for *domination*, c is the size of P, p is the number of solutions of a set A which can be dominated by X, and q is the number of solutions of a set B which can dominate X in the objective space. It is noted that the GPSIFF scores for the non-dominated solutions as well as dominated solutions are not always identical.

GPSIFF uses a pure Pareto-ranking fitness assignment strategy, which differs from the traditional Pareto-ranking methods, such as non-dominated sorting [16] and Zitzler and Thiele's method [1]. GPSIFF can assign discriminative fitness values to not only non-dominated individuals but also dominated ones.

3.2 Multi-objective Intelligently Generation Mechanism MOIGM

Consider a parametric optimization function of m parameters. According to a current solution $X=[x_1, \ldots, x_m]^T$ where x_i is a parameter value, an MOIGM generates two temporary solutions $X_1=[x_1^1, \ldots, x_m^1]^T$ and $X_2=[x_1^2, \ldots, x_m^2]^T$ from perturbing X, where x_i^1 and x_i^2 are generated by perturbing x_i as follows:

$$x_i^1 = x_i + \overline{x_i} \text{ and } x_i^2 = x_i - \overline{x_i},\ i=1, \ldots, m. \tag{3}$$

The values of $\overline{x}=[\overline{x_1}, \ldots, \overline{x_m}]^T$ are generated by Cauchy-Lorentz probability distribution [21].

Using the same division scheme for X, X_1, and X_2, partition all the m parameters into N non-overlapping groups with sizes l_i, $i=1, \ldots, N$, such that

$$\sum_{i=1}^{N} l_i = m. \tag{4}$$

The proper value of N is problem-dependent. The larger the value of N, the more efficient the MOIGM is if the interaction effects among groups are weak. If the existing interaction effect is not weak, the larger the value of l_i, the more accurate the estimated main effect is. Considering the trade-off, an efficient bi-objective division criterion is to minimize the interaction effects between groups and maximize the value of N. To efficiently use all columns of OA, N is generally specified as $N=(3^{\lfloor \log_3(2m+1) \rfloor}-1)/2$ and the used OA is $L_{2N+1}(3^N)$ excluding the study of intractable interaction effects. The N-1 cut points are randomly specified from the m-1 candidate cut points which separate solution parameters.

MOIGM employs an elite set E to hold a limited number of non-dominated solutions and aims at efficiently combining good parameters from solutions X, X_1, and X_2 to generate a good candidate solution $\overline{Q}$ for the next move. Let H be the number of objectives for the problem. How to perform an MOIGM operation on X with m parameters for a GPSIFF fitness value F and objective function values $f^1, \ldots, f^H$ is described as follows:

Step 1: Generate two temporary solutions X_1 and X_2 using X from Equ. (3).

Step 2: Adaptively divide each of X, X_1, and X_2 into N groups of parameters where each group is treated as a factor.

Step 3: Use the first N columns of an OA $L_M(3^{(M-1)/2})$, where $M = 3^{\lceil \log_3(2N+1) \rceil}$.

Step 4: Let levels 1, 2 and 3 of factor i represent the ith groups of X, X_1, and X_2, respectively.

Step 5: Add M combination experiments of the OA into E. Compute F_j and f^h of the generated combinations corresponding to the experiment j, where h=1, ...,H and j = 2, …, M. Note that F_j and f^h are the fitness value of $F(X)$ and the h^{th} objectives function value of $f(X)$, respectively.

Step 6: Compute the main effect S_{ik}^G using GPSIFF. Determine the best one of three levels of each factor based on the main effect S_{ik}^G, where i = 1, …, N and k = 1, 2, 3.

Step 7: The solution Q is formed using the combination of the best groups from the derived corresponding solutions.

Step 8: Compute the main effect S_{ik}^h using the one of objective fitness values. Determine the best one of three levels of each factor based on the main effect S_{ik}^h, where h = 1, …, H, i = 1, …, N and k = 1, 2, 3. The solutions Q^1, …, Q^H are formed.

Step 9: Add Q and Q^1, …, Q^H solutions into E. Recompute the value of F for all non-dominated solution in E.

Step 10: $\overline{Q}$ is selected from the best one of M-1 combination experiments except X, Q and Q^1, …, Q^H according the GPSIFF fitness value, except that $\overline{Q}$ is not equal X.

For an MOIGM operation, the number of objective function evaluations is M+H which includes M-1 evaluations for combinations of OA experiments, one for the evaluation of Q, *and* H evaluations for Q^1, …, Q^H.

3.3 Procedure of MOOSA

MOOSA is based on a simulated annealing algorithm (SA) for solving multi-objective optimization problems. There are four choices must be made in implementing a SA algorithm for solving an optimization problem: 1) solution representation, 2) objective function definition, 3) design of the generation mechanism, and 4) design of a cooling schedule. The choices 1 and 2 are problem-dependent. Designing an efficient generation mechanism plays an important role in developing SA algorithms. Generally, there are four parameters to be specified in designing the cooling schedule: 1) an initial temperature T_0, 2) a temperature update rule and 3) a stopping criterion of the SA algorithm.

MOOSA employs an elite set E which maintains the non-dominated solutions and MOIGM to efficiently search for a good candidate solution for the next move. Let a variable value N_s be the number of trials with the same solution X, a constant $\overline{N_s}$ be the max number of trials with the same solution. Without lose of generality, consider the case that the fitness value $F(X)$ and H objective function values f^1, …, f^H are to be minimized. The proposed MOOSA is described as follows:

Step 1: (Initialization) Randomly generate an initial solution X and compute $F(X)$ and f^1, …, f^H. Initialize the temperature $T=T_0$, $N_T=N_0$, and cooling rate CR. $Count=0$, $N_s=0$.
Step 2: (Update Elitism) Remove the dominated solutions in E.
Step 3: (Selection) If the solution X is not improved during $\overline{N_s}$ iterations (i.e. $N_s=\overline{N_s}$), randomly select a solution X from E and reset $N_s=0$.
Step 4: (Generation) Perform an MOIGM operation using X to generate a candidate solution $\overline{Q}$. Set $\overline{X}=X$.
Step 5: (Acceptance criterion) Accept $\overline{Q}$ to be the new solution X with probability $P(\overline{Q})$:

$$P(\overline{Q}) = \begin{cases} 1 & ,if\,(F(\overline{Q}) > F(X)) \\ \min\left(\exp(\frac{f^1(X) - f^1(\overline{Q})}{T}), \cdots, \exp(\frac{f^H(X) - f^H(\overline{Q})}{T}) \right) & ,if\,(F(\overline{Q}) \le F(X)) \end{cases} \quad (5)$$

If a new solution X is equal to an old solution $\overline{X}$, increase the value of N_s by one.
Step 6: (Decreasing temperature) Let the new values of T be $CR\times T$.
Step 7: (Termination test) If a pre-specified stopping condition is satisfied, stop the algorithm. Otherwise, go to Step 2.

Let G be the number of iterations. The complexity of MOOSA is $G\times(M+H)$ function evaluations.

4 Simulation Results

The coverage ratio of two non-dominated solution sets, A and B, obtained by two algorithms is used for performance comparison of the two algorithms, which is defined as follows [1]:

$$C(A,B) = \frac{\left|\{a \in A; b \in B; b \succeq a\}\right|}{\left|B\right|}, \quad (6)$$

where $b \succeq a$ means that b is weakly dominated by a. The value $C(A,B)=1$ means that all solutions in B are weakly dominated by A. On the contrary, $C(A,B)=0$ denotes that none of solutions in B is weakly dominated by A. Because the C measure considers the weakly dominance relationship between two sets A and B, $C(A, B)$ is not necessarily equal to $1-C(B,A)$.

Recently, Deb [18] has identified several problem features that may cause difficulties for multi-objective algorithms in converging to the Pareto-optimal front and maintaining population diversity in the current Pareto front. These features are multimodality, deception, isolated optima and collateral noise, which also cause difficulties in single-objective GAs. Following the guidelines, Zitzler et al. [1] constructed six test problems ZDT_1-ZDT_6 involving these features, and investigated the performance of various popular MOEAs. The empirical results demonstrated that SPEA outperforms

NSGA [7], VEGA [13], NPGA [2], HLGA [14] and FFGA [22] in small-scale problems. Each of the test functions is structured in the same manner and consists of three functions f_1, g, h [18]:

$$\text{Minimize } F(X) = (f_1(X), f_2(X)), \quad (7)$$
$$\text{subject to } f_2(X) = g(x_2, \dots, x_m)\cdot h(f_1(x_1), g(x_2, \dots, x_m)),$$
$$\text{where } X = [x_1, x_2, \dots, x_m]^T.$$

where f_1 is a function consisted of the first decision variable x_1 only, g is a function of the remaining m-1 variables, and the two variables of the function h are the function values of f_1 and g. These test problems are listed in Table 2. ZDT_5 is excluded because MOOSA uses real numbers for encoding.

Table 2. Test problems.

Test Problems	Objective functions	Domain x_i	Optimal solutions
ZDT_1	$f_1(X) = x_1$ $f_2(X) = g(X)\times h(f_1(X), g(X))$ $g(X) = 1 + 9\cdot\sum_{i=2}^{m} x_i/(m-1)$ $h(f_1(X), g(X)) = 1 - \sqrt{f_1/g}$	$x_i \in [0, 1]$, $i = 1,\cdots,m.$	$x_1 \in [0, 1]$, $x_i = 0$, $i = 2,\cdots,m.$
ZDT_2	$f_1(X) = x_1$ $f_2(X) = g(X)\times h(f_1(X), g(X))$ $g(X) = 1 + 9\cdot\sum_{i=2}^{m} x_i/(m-1)$ $h(f_1(X), g(X)) = 1 - (f_1(X)/g(X))^2$	$x_i \in [0, 1]$, $i = 1,\cdots,m.$	$x_1 \in [0, 1]$, $x_i = 0$, $i = 2,\cdots,m.$
ZDT_3	$f_1 = x_1$ $f_2(X) = g(X)\times h(f_1(X), g(X))$ $g(X) = 1 + 9\cdot\sum_{i=2}^{m} x_i/(m-1)$ $h(f_1(X), g(X)) = 1 - \sqrt{f_1(X)/g(X)} - (\frac{f_1(X)}{g(X)})\sin(10\pi x_1)$	$x_i \in [0, 1]$, $i = 1,\cdots,m.$	$x_1 \in [0, 1]$, $x_i = 0$, $i = 2,\cdots,m.$
ZDT_4	$f_1 = x_1$ $f_2(X) = g(X)\times h(f_1(X), g(X))$ $g(X) = 1 + 10(m-1) + \sum_{i=2}^{m}(x_i^2 - 10\cos(4\pi x_i))$ $h(f_1(X), g(X)) = 1 - \sqrt{f_1(X)/g(X)}$	$x_1 \in [0, 1]$, $x_i \in [-5, 5]$, $i=2,\cdots,m.$	$x_1 \in [0, 1]$, $x_i = 0$, $i = 2,\cdots,m.$
ZDT_6	$f_1 = 1 - \exp(-4x_1)\sin^6(6\pi x_1)$ $f_2(X) = g(X)\times h(f_1(X), g(X))$ $g(X) = 1 + 9\cdot((\sum_{i=2}^{m} x_i)/(n-1))^{0.25}$ $h(f_1(X), g(X)) = 1 - (f_1(X)/g(x))^2$	$x_i \in [0, 1]$, $i = 1,\cdots,m.$	$x_1 \in [0, 1]$, $x_i = 0$, $i = 2,\cdots,m.$

There are m parameters in each test problem. Each parameter in chromosomes is represented by 30 bits. The experiments in Zitzler's study indicate that the test problems ZDT_4 and ZDT_6 cause difficulties to evolve a well-distributed Pareto-optimal front. In their experiments, the reports are absent about the test problems with a large number of parameters. As a result, the extended test problems with a large number of parameters (m=63) are further tested in order to compare the performance of various algorithms in solving large MOOPs. Thirty independent runs were performed using the same fitness evaluations for various algorithms, N_{eval} = 25000. The parameter settings of VEGA, NPGA, NSGAII [24] and SPEA2 [23] are the same in [1], summarized as follows: the generations is 250, the crossover rate is 0.8, the mutation rate is 0.1, t_{dom}=10, the sharing factor σ_{share} is 0.4886, and the population size is 100. The population size and the external population size of SPEA2 are 80 and 20. Let the parameters of MOOSA be $\overline{N_s}$=10, CR=0.99, T_0=150.

The direct comparisons of each independent run between MOOSA and all compared MOEAs based on the C metric for 30 runs are depicted in Fig. 1. The average numbers of non-dominated solutions for various algorithms is shown in Table 3.

Table 3. The average number of non-dominated solutions for 30 runs of various algorithms.

	MOOSA	SPEA2	NSGAII	NPGA	VEGA
ZDT_1	174.53	68.23	61.73	16.33	13.90
ZDT_2	194.93	40.53	35.33	9.16	5.53
ZDT_3	100.30	78.87	65.20	17.10	12.60
ZDT_4	4.90	4.83	3.83	6.10	4.80
ZDT_6	21.17	9.90	9.57	6.90	5.27

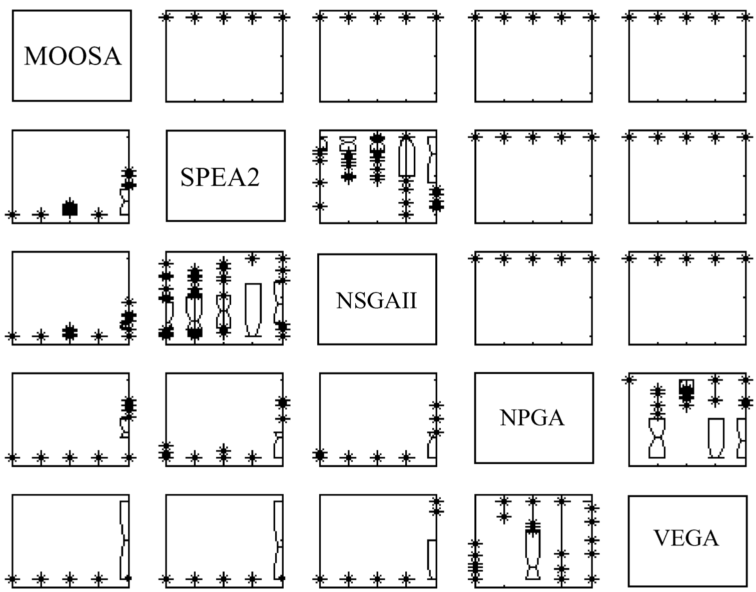

Fig. 1. Box plots based on the cover metric for multi-objective parametric problems. The leftmost box plot relates to ZDT_1, the rightmost to ZDT_6. Each rectangle refers to algorithm A associated with the corresponding row and algorithm B associated with the corresponding column and gives six box plots representing the distribution of the cover metric $C(A, B)$. The scale is 0 at the bottom and 1 at the top per rectangle.

For test problems ZDT_1, ZDT_2 and ZDT_3, MOOSA, SPEA2 and NSGAII evolved well-distributed Pareto fronts, and MOOSA is very close to the Pareto-optimal fronts. For the multimodal test problem ZDT_4, only MOOSA obtained a better Pareto front which is much closer to the Pareto-optimal front than those of the other algorithms. The well-distributed non-dominated solutions resulted from that OGM has well-distributed by-products which are candidate non-dominated solutions at that time. For ZDT_6, MOOSA also obtained a widely distributed front and MOOSA's solutions dominate all the solutions obtained by the other algorithms. Finally, it can be observed from [1] and our experiments that when the number of parameters increases, difficulties may arise in evolving a well-distributed non-dominated front. Moreover, it is observed that VEGA obtained some excel solutions in the objective f_1 in some runs of ZDT_2 and ZDT_6. This phenomenon agrees with [19], [20] that VEGA may converge to solution champion solutions only.

As shown in Table 3, the average number of non-dominated solutions obtained by MOOSA are more than the one obtained by others algorithms. As shown in Fig. 1, the quality of solutions obtained by MOOSA is superior to those of SPEA2, NSGAII, NPGA, and VEGA in terms of the number of non-dominated solutions, the distance between the obtained Pareto front and Pareto-optimal front, and the distribution of solutions.

5 Conclusions

In this paper, a novel multi-objective orthogonal simulated annealing algorithm MOOSA using the generalized Pareto-based scale-independent fitness function and orthogonal experimental design-based multi-objective intelligently generation mechanism (MOIGM) is proposed to efficiently solve multi-objective optimization problems (MOOPs) with a large number of parameters. The performance of MOOSA mainly rises from MOIGM. It uses uniform samples and systematic reason methods instead of generate-and-test methods, and thus MOOSA can efficiently find out a set of Pareto-solutions. It was also shown through the test functions that the performance of MOOSA is superior to some existing MOEAs in a limited computation time.

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