Adjusting Parallel Coordinates for Investigating Multi-Objective Search

Liangli Zhen[1,2], Miqing Li[2], Ran Cheng[2], Dezhong Peng[1] and Xin Yao[3,2]

[1] Machine Intelligence Laboratory, College of Computer Science, Sichuan University, Chengdu 610065, China
[2] CERCIA, School of Computer Science, University of Birmingham, Birmingham B15 2TT, U. K.
[3] Dept. of Computer Science and Engineering, Southern University of Science and Technology, Shenzhen 518055, China

llzhen@outlook.com, {limitsing, ranchengcn}@gmail.com, pengdz@scu.edu.cn, x.yao@cs.bham.ac.uk

Abstract. Visualizing a high-dimensional solution set over the evolution process is a viable way to investigate the search behavior of evolutionary multi-objective optimization. The parallel coordinates plot which scales well to the data dimensionality is frequently used to observe solution sets in multi-objective optimization. However, the solution sets in parallel coordinates are typically presented by the natural order of the optimized objectives, with rare information of the relation between these objectives and also the Pareto dominance relation between solutions. In this paper, we attempt to adjust parallel coordinates to incorporate this information. Systematic experiments have shown the effectiveness of the proposed method.

1 Introduction

Multi-objective optimization problems (MOPs), which involve several (conflicting) objectives to be optimized, widely exist in real-world applications [14]. Since the multiple objectives in an MOP can be in conflict with each other, there often exist a set of trade-off solutions, known as the Pareto optimal solutions. In order to solve such MOPs, a variety of multi-objective evolutionary algorithms (MOEAs) have been proposed, where the aim is to obtain (or approximate) the Pareto optimal solutions during one single run [3]. To investigate the search behavior of different MOEAs, the classic visualization technique, i.e., scatter plot, is used for the visualization of the population throughout the evolution process [11]. Despite that the scatter plot allows us to observe important information such as the shape and distribution of the candidate solutions and the conflict between objectives, its applicability is only limited to MOPs with two or three objectives.

With the aim of visualizing high-dimensional candidate solutions in evolutionary multi-objective search, another widely adopted visualization method is known the parallel coordinates [7], which places the objective axes parallel to each other rather than orthogonally such that an arbitrary number of dimensions can be displayed inside one 2D plane. Specifically, to show a solution set of an m-objective optimization problem,

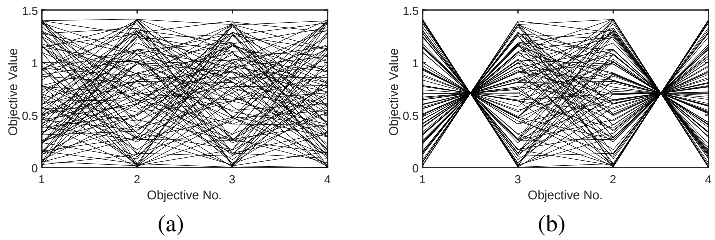


Fig. 1. Two different order of objective axes of a solution set in parallel coordinates.

parallel coordinates map them into a coordinate system with m parallel axes, typically vertical and equally spaced. One candidate solution is represented as a polyline with m vertices on these parallel axes, and the position on the ith axis corresponds to the value of the solution on the ith objective. Recently, the parallel coordinates plot has been dominantly used in high-dimensional data visualization [13], e.g., the multi-objective optimization with more than three objectives, in spite of the emergence of various visualization techniques [16, 15, 5, 6].

Despite its popularity, the parallel coordinates plot is not straightforward as the scatter plot to show the information contained in solution sets [13]. In a parallel coordinates plot, each vertical axis has at most two neighboring axes, and different order of objective axes provide different information about the conflict between objectives. The parallel coordinates plot only shows $(m-1)$ relationships of a total of C_m^2 relationships existing in m objectives. How to show the conflict between objectives clear becomes critical and challenging to the parallel coordinates plot. Take Fig. 1 as an example, which shows the parallel coordinates plots of two different order of the same solution set. In Fig. 1(a) where the order of objectives is f_1, f_2, f_3, and f_4, the conflict between any two adjacent objectives is mild. Conversely, in Fig. 1(b) where the order of objectives is f_1, f_3, f_2, f_4, the conflict between f_1 and f_3 and the conflict between f_2 and f_4 are intense, and imply that f_1 is negatively linear with f_3, and f_2 is negatively linear with f_4. Moreover, during the evolution process, the solutions are not mutually non-dominated, and the dominance relation between solutions are not considered in parallel coordinates plot makes the gradual improvement of the solution set invisible. In this paper, we aim to address these two problems in the parallel coordinates plot by adjusting parallel coordinates. The proposed parallel coordinates adjustment (APC) is capable of clearly presenting the relation between objectives and the dominance relation between candidate solutions.

The rest of this paper is organized as follows. Section 2 provides the background, including a general definition of MOPs, concepts of Pareto dominance and Pareto optimal set, and some related work. Section 3 is devoted to the description of the proposed method. Section 4 provides some results of the investigation of MOEAs. Section 5 concludes the paper.

2 Background

A multi-objective optimization problem (MOP) can be generally formulated as a minimization problem and defined as follows:

$$\begin{aligned} \min \ & F(\mathbf{x}) = (f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_M(\mathbf{x}))^T \\ \text{s.t.} \ & \mathbf{x} \in \Omega, \end{aligned} \tag{1}$$

where $\mathbf{x} \in \mathbb{R}^n$ consists of n decision variables representing the values which are to be chosen in the optimization, $\Omega \subseteq \mathbb{R}^n$ is the decision space, and $F : \Omega \rightarrow \mathbb{R}^M$ consists of M (conflicting) objective functions $f_i : \mathbb{R}^n \rightarrow \mathbb{R}, (i = 1, \ldots, M)$.

For any two feasible solutions $\mathbf{a}$ and $\mathbf{b}$ of the MOP, it says that $\mathbf{a}$ is better than $\mathbf{b}$ if the following conditions hold:

$$\forall i \ f_i(\mathbf{a}) \leq f_i(\mathbf{b}) \ \text{ and } \ \exists j \ f_j(\mathbf{a}) < f_j(\mathbf{b}), \tag{2}$$

where $i, j \in \{1, 2, \ldots, M\}$. In other words, $\mathbf{a}$ is not worse than $\mathbf{b}$ on all objectives and $\mathbf{a}$ is better than $\mathbf{b}$ on at least one objective. We can also say that $\mathbf{a}$ dominates $\mathbf{b}$, and denote it as $\mathbf{a} \prec \mathbf{b}$. A solution that is not dominated by any other solutions is denoted as Pareto optimal. The set of the Pareto optimal solutions in the decision space is denoted as the Pareto set, and the corresponding outcome in objective space is denoted as the Pareto front. From the formulation in (1), we can see that the conflicts between objectives prevent us from having a single optimal solution but rather a Pareto set for an MOP.

MOEAs optimize MOPs by producing a solution set at each generation and evolving the candidate set gradually. The parallel coordinates plot is frequently used to view these high-dimensional solutions, but it suffers from the visual clutter problem [9]. To address this problem in parallel coordinates, Ankerst *et al.* proposed to reorder the axes such that similar dimensions are positioned close to each other [1]. They modeled the reordering of axes as a traveling salesman problem (TSP) and applied a heuristics to solve it. In [2], Artero *et al.* presented a method, called similarity-based attribute arrangement (SBAA), to select two dimensions with the largest similarity as the initial axes, and then to search for the dimensions which will be positioned to the left and the right of them. The SBAA method has a much lower computational complexity comparing with the previous methods. However, it may leads to some intense conflict between objectives being invisible. Actually, the most desirable order of the objectives should make the most conflicting information visible that every objective at most can only be placed adjacently with two other objectives.

3 Method

3.1 Reordering of objectives

In this section, we present an algorithm to arrange the order of objectives such that the most significant conflict (harmony) between objectives can be visualized. Since the conflict between objectives is local rather than global on the population from different generations, we need to re-evaluate the conflict between objectives during the evolution process. In this paper, we assess the conflict/harmony between two objectives according to the Spearman's rank correlation between the objectives of all candidate solutions. The Spearman's rank correlation coefficient is a nonparametric technique for evaluating the degree of rank correlation between two variables. It equals the Pearson correlation between the rank values of the two variables. Technically, the variables A and B are converted to rank variables r_A and r_B, respectively, according to the ranks of their observations. The Spearman's rank correlation coefficient is defined as

$$\rho(A, B) = \frac{cov(r_A, r_B)}{\sigma_{r_A} \sigma_{r_B}}, \tag{3}$$

where σ_{r_A} and σ_{r_B} are the standard deviation of r_A and r_B, respectively, and $cov(r_A, r_B)$ is the covariance of r_A and r_B. Intuitively, the Spearman's correlation between two variables will be high when observations have a similar rank between the two variables and low when observations have a dissimilar rank between the two variables. As it operates on the ranks of the data, the Spearman's correlation coefficient is appropriate for both continuous and discrete variables and is insensitive to the operations of translation/scaling on the data.

In the evolution process, the most conflicting/harmonious information between objectives is desirable for the users. For a solution set, we calculate the Spearman's rank correlation between objectives, and then we use the absolute values of the correlation to represent the harmony/conflict between two objectives. To arrange the order of these objectives in a parallel coordinates plot, we use a greedy strategy and propose an algorithm listed in Algorithm 1.

From the algorithm, we see that it consists of three stages: calculation of the Spearman's rank correlation, correlation sorting, and the arrangement of the order of objectives according to the sorted result. The third stage (Step 4 to Step 22) is the essential part of the proposed method. It handles a pair of two objectives at each iteration. It differs from the SBAA method, which iteratively adds one objective in one iteration. In our method, the two objectives may be both added in the system at one iteration as shown at Step 7. It may also add one objective at a time, as Step 11 and Step 14, if only one of the objectives at one side of a group and another objective is not joined in any group, as the conditions at Step 10 and Step 13. If both of the objectives are at the side of two different groups, the algorithm will merge these two groups by placing these two objectives adjacent. However, if both of these two objectives are at the side of the same group or one of the objectives has already connected to two other objectives, the algorithm will do nothing and go to the next step. Overall, after rearranging the order of objectives with Algorithm 1, the objective would be adjacent to the two objectives which have clearest (conflicting/harmonous) relation with except that these objectives have stronger relation with other objectives.

3.2 Involving dominance relation

Since the optimal solution of an MOP is a set of Pareto optimal vectors, the Pareto dominance relation between candidate solutions naturally becomes a criterion to distinguish different solutions. In the evolution process, the candidate solutions can be sorted into different levels according to the non-dominance relation by using the non-dominated

Algorithm 1 The proposed procedure of arranging the order of objectives in parallel coordinates

Require: The objective vectors of the solution sets $\mathbf{y}_i = f_i(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) \in \mathbb{R}^N, i \in \{1, \ldots, M\}$.
Ensure: The rearranged order of objectives.

$t \leftarrow 1$, $p(i) \leftarrow 0, i \in \{1, \ldots, M\}$; // t denotes the index of the current iteration, and $p(i)$ denotes the number of the connected adjacent objectives for the i-th objective.
Calculate the Spearman's rank correlation $R_{ij} \leftarrow \rho(\mathbf{y}_i, \mathbf{y}_j)$ via (3), **for all** $i > j \in \{1, \ldots, M\}$;
$list \leftarrow$ the sorting result on the absolute value of the correlation in descending order;
while exist one objective is not arranged **do**
  Denote two objectives whose correlation corresponding to the $list(t)$ as a and b;
  if $p(a) = 0$ and $p(b) = 0$ **then**
    Create a new group which includes a and b;
    $p(a) \leftarrow p(a) + 1$;
    $p(b) \leftarrow p(b) + 1$;
  else if $p(a) = 1$ and $p(b) = 0$ **then**
    Insert objective b to the same group with a;
    $p(b) \leftarrow p(b) + 1$;
  else if $p(a) = 0$ and $p(b) = 1$ **then**
    Insert objective a to the same group with b;
    $p(a) \leftarrow p(a) + 1$;
  else if $p(a) = 1$ and $p(b) = 1$ and a is not in the same group with b **then**
    Merge these two groups;
    $p(a) \leftarrow p(a) + 1$;
    $p(b) \leftarrow p(b) + 1$;
  end if
  $t \leftarrow t + 1$;
end while
return the order of the objectives in the group.

sorting approaches, such as the efficient non-dominated sorting method in [17]. We represent the candidate solutions with different colors according to their non-dominated levels such that the dominance relation can be easily observed. Fig. 2 shows an example of six solutions in a 3D objective space with parallel coordinates. From Fig. 2(a), it can be hard to observe the solutions which belong to the first non-dominated front, but we can easily do from Fig. 2(b) where the solutions with blue color lie in the first non-dominated front and the solutions with red color are located at the second non-dominated front.

With this simple color annotating method, we can obtain more information of the population, such as the number of individuals in different non-dominated front, how these candidates evolve, and the solutions at the boundaries. They are helpful for investigating the behavior of the MOEAs.

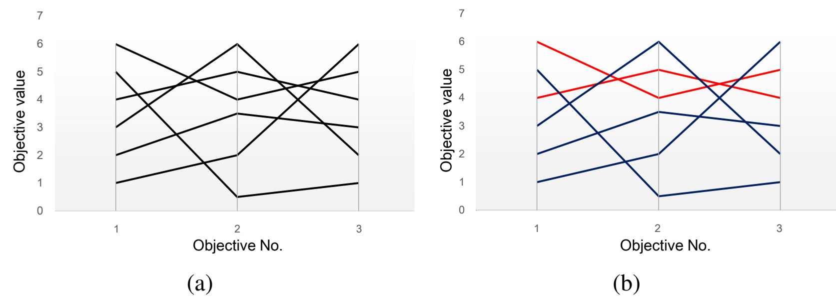


Fig. 2. Six solutions in 3D objective space with parallel coordinates plot. (a) presents the results without special colors about the dominance relation; (b) is the results with special colors according to the non-dominated levels of the solutions.

4 Results

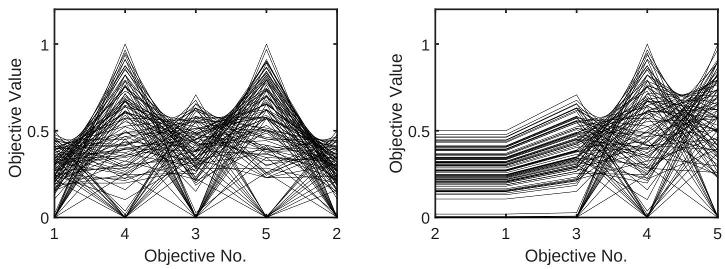
In order to demonstrate the main properties of the proposed method and illustrate how to use it to show solution sets and to investigate the search process of multi-objective optimization, a series of experiments are conducted on the test problems of DTLZ5(I,M) [4], multi-line distance minimization problem (ML-DMP) [13], and multi-point minimization problem (MP-DMP) [10, 8]. Specifically, the experiments to be conducted consist of two parts. In the first part, we demonstrate the result of the proposed method on rearranging the order of objectives for the solution sets of the DTLZ5(I,M) and ML-DMP via a many-objective optimizer, i.e., the strength Pareto evolutionary algorithm (SPEA2) [18] with the shift-based density estimation (SDE) [12] strategy (SPEA2+SDE)[4]. In the second part, we apply the proposed method to investigate the behavior of the SPEA2+SDE on the MP-DMP. The experimental setting is as follows: for the SPEA2+SDE, the maximum number of evaluation is used as the termination condition, which is set to 50000, 50000 and 100000 for the DTLZ5(I, M), MP-DMP, and ML-DMP, respectively, and the corresponding population sizes are 100, 100, and 200.

4.1 Visualization of solution sets

To analyze the conflict/harmony between objectives of a solution set, we conduct the experiment on the output of the SPEA2+SDE on DTLZ5(3, 5) problem, 5-objective ML-DMP, and 10-objective ML-DMP. From the definition of DTLZ5(I, M), we have that the first three objectives of DTLZ5(3, 5) are linear dependent. To evaluate the proposed method, we exchange the order of the objectives in DTLZ5(3, 5) to f_1, f_4, f_3, f_5, f_2. The solution set of the SPEA2+SDE on this problem is shown in Fig. 3(a), from which we can see that the conflict/harmony information between objectives is not easily visible. Fig. 4 shows two solution sets in decision space obtained by SPEA2+SDE on these two problems, respectively. The DL-DMP minimizes the distance of 2D points to a set

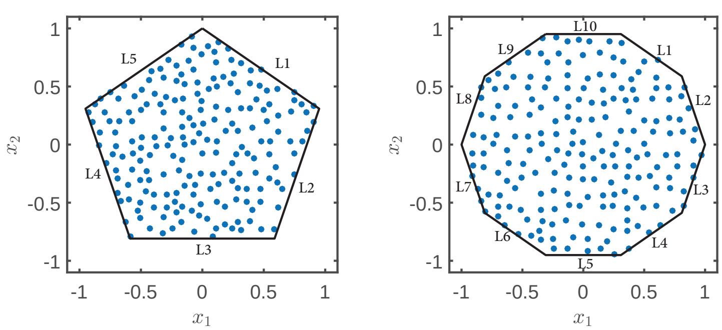
[4] SPEA2+SDE has shown its good performance on this problem [11].

of multiple straight lines, each of which passes through one edge of the given regular polygon. One feature of this problem is that these solutions are located in a regular polygon and their objective images are similar in the sense of Euclidean geometry. This allows us to observe the distribution of the solutions in the objective space via viewing them in the 2D decision space. We will use this feature of ML-DMP to analyze the results of the reordering of the objectives in parallel coordinates.



(a) (b)

Fig. 3. The solutions of the SPEA2+SDE for DTLZ5(3,5) with different order of objectives. The results before and after the rearranging of the order of objectives are shown at left and right, respectively.



(a) (b)

Fig. 4. The solutions of the SPEA2+SDE in the decision space for 5-objective ML-DMP and 10-objective ML-DMP at left and right, respectively.

Results on the DTLZ5(3, 5) problem From the definition of the DTLZ5(I, M) problem, we have that the first three objectives of DTLZ5(3, 5), i.e., f_1, f_2, and f_3, are linear dependent. The result after rearranging the order of objectives with the proposed method is shown in Fig. 3(b). We can see that the first three objectives are arranged in the adjacent positions, and it is consistent with our goal that placing the most conflicting/harmonious objectives in adjacent positions. Comparing with the result in Fig. 3(a), the result given by the proposed method provides important information between objectives that the first three objectives are harmonious, and the objectives f_3 and f_4 are conflicting, as well as f_4 and f_5.

Results on the 5-objective ML-DMP In Fig. 5(a) where the order of objectives is f_1, f_2, f_3, f_4, f_5, the conflict between any two adjacent objectives is rather mild. On the other hand, in Fig. 5(b) where the order of objectives is f_3, f_1, f_4, f_2, f_5, the conflicts between any two adjacent objectives are intense. Inspecting the result in Fig. 4(a), we find that the adjacent objectives automatically be rearranged by the proposed method are the most conflicting objectives, i.e, most of the points which are closer to L1 would be far away from L3 and L4, and most of the points which are closer to L2 would be far away from L4 and L5. This is caused by the fact that f_1 and f_3 are not completely conflicted. Similar situations hold for f_1 and f_4, f_4 and f_2, and f_2 and f_5. From Fig. 4(a) and Fig. 5(b), we obtain that the proposed method detects the most desirable information between objectives. This can bring some insights to the solution sets and the investigated MOEAs, which can be helpful to algorithm designers and decision makers.

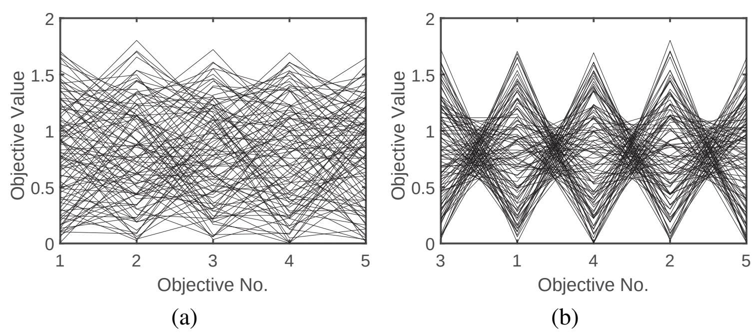


Fig. 5. The solution set of SPEA2+SDE on the 5-objective ML-DMP with different order of objective axes in parallel coordinates.

Results on the 10-objective ML-DMP In Fig. 6(a) where the order of objectives is f_1, f_2, f_3, f_4, f_5, f_6, f_7, f_8, f_9, f_{10}, the conflict between any two adjacent objectives is mild. In some area, the adjacent objectives are even harmonious, but they are not harmonious in the whole optimal region. In contrast, in Fig. 6(b) where the order of objectives is f_1, f_6, f_5, f_{10}, f_9, f_4, f_3, f_8, f_2, f_7, some pair of adjacent objectives are completely conflicting. From Fig. 4(b), we find that f_1 is negatively linear with f_6, i.e., any point which moves more closely to L1 would have a longer distance to L6 because these two lines are parallel and placed at two sides of optimal solutions. The objectives f_5 and f_{10}, f_9 and f_4, f_3 and f_8, f_2 and f_7 have similar relation. These five pairs of objectives are completely conflicting, respectively. It leads to the result in Fig. 6(b) that the lines of the solutions are intersected at one point between axes of Objective No. 1 and Objective No. 6, Objective No. 5 and Objective No. 10, Objective No.9 and Objective No. 4, Objective No. 3 and Objective No. 8, and Objective No. 2 and Objective No. 7, respectively. Moreover, three pairs of harmonious objectives, f_6 and f_5, f_{10} and f_9, f_4 and f_3, are then connected. These three pairs of objectives are the minimization distances to three pairs of adjacent lines as shown in Fig. 4(b). Finally, two conflicting objectives f_8 and f_2 are placed adjacent by the proposed method. The connected order of the objectives can be all shown with the value of the Spearman's rank correlation by the proposed algorithm, even through these conflicting/harmonious information between objectives are not easily observed by the user. Comparing with the result in Fig. 6(a), the result obtained by the proposed method is much clear for the algorithm designers and decision makers.

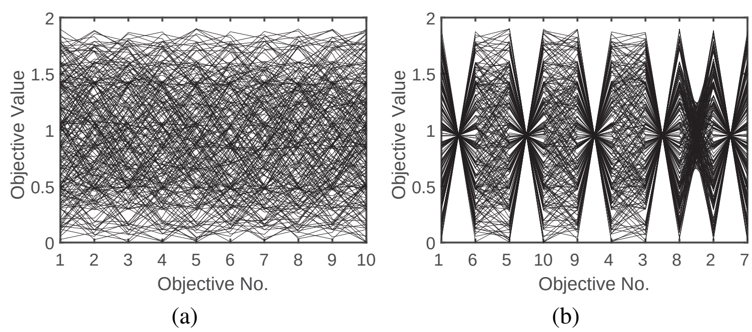
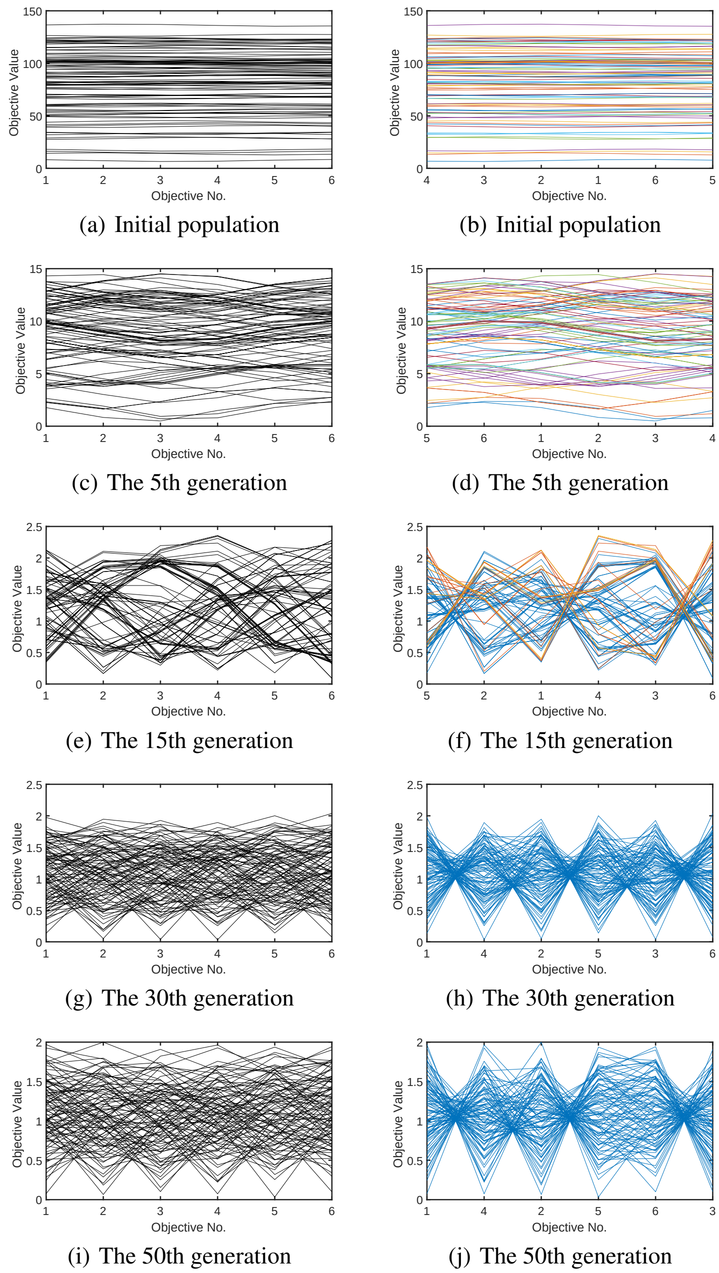


Fig. 6. The solution set of SPEA2+SDE on the 10-objective ML-DMP with different order of objective axes in parallel coordinates.

4.2 Investigation of search behavior

In this subsection, we demonstrate how to investigate the search behaviors of MOEAs using the proposed adjusted parallel coordinates method. To exemplify, we apply the SPEA2+SDE to solve a six-objective MP-DMP whose goal is to minimize the distance to the six vertexes of a polygon. The results are shown in Fig. 7, from which we have the following observations: 1) for the initial population, the individuals are fairly uniformly distributed in the whole objective space and they are sorted to many non-dominated fronts; 2) for the population in the 5th generation, the number of non-dominated fronts are fewer than that of the initial population; 3) in the 15th generation, the individuals are sorted into few non-dominated fronts and the conflict between f_3 and f_6, and the conflict between f_1 and f_4 are fairly intense; 4) in the 30th generation, the individuals are located in one non-dominated front, i.e., all of they are mutually non-dominated, and



(a) Initial population
(b) Initial population
(c) The 5th generation
(d) The 5th generation
(e) The 15th generation
(f) The 15th generation
(g) The 30th generation
(h) The 30th generation
(i) The 50th generation
(j) The 50th generation

Fig. 7. The populations of the SPEA2+SDE method on the 6-objective MP-DMP during the evolution process. The subplots at the left column are the results by using the original parallel coordinates, and the subplots at the right side are the results obtained by the proposed method.

the conflicts between f_1 and f_4, f_2 and f_5, f_3 and f_6 are more intense than those in the 15th generation; 5) in the 50th generation, the conflicts between f_1 and f_4, f_2 and f_5, f_3 and f_6 are very clear in the result obtained by the proposed method. In addition, the conflict/harmony between objectives changes which leads to the order of the objectives different during the evolution process (as shown in the right column of Fig. 7).

5 Conclusion

This paper focuses on adjusting parallel coordinates to investigate the search process of multi-objective optimization. It considers two aspects: 1) rearranging the order of objectives to make the relationships between objectives as clear as possible; 2) presenting the dominance relation between solutions to help us to know the evolution process. To demonstrate the effectiveness of the proposed method, a series of experiments have conducted on the solution sets or the population of the MOEAs on several benchmarks. It firstly illustrated how to use the proposed algorithm to reorder the objectives of mutually non-dominated solution sets. Then, the proposed method with objectives reordering and dominance relation denoting program is further used to investigate the search behavior of MOEAs. The experiments have shown that the proposed method can be helpful in investigating evolutionary multi-objective search. In the future, we would like to investigate how to extract more useful information from the solution sets or the population during the evolution process and then present this information in the parallel coordinates.

Acknowledgment

This work was supported in part by the National Natural Science Foundation of China under grants 61432012, 61329302, and the Engineering and Physical Sciences Research Council (EPSRC) of U.K. under grant EP/J017515/1.

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