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Many-Objective Test Problems to Visually Examine the Behavior of Multiobjective Evolution in a Decision Space

Hisao Ishibuchi, Yasuhiro Hitotsuyanagi, Noritaka Tsukamoto and Yusuke Nojima

Department of Computer Science and Intelligent Systems, Graduate School of Engineering, Osaka Prefecture University, 1-1 Gakuen-cho, Naka-ku, Sakai, Osaka 599-8531, Japan
{hisaoi@, hitotsu@ci., nori@ci., nojima@}cs.osakafu-u.ac.jp

Abstract. Many-objective optimization is a hot issue in the EMO (evolutionary multiobjective optimization) community. Since almost all solutions in the current population are non-dominated with each other in many-objective EMO algorithms, we may need a different fitness evaluation scheme from the case of two and three objectives. One difficulty in the design of many-objective EMO algorithms is that we cannot visually observe the behavior of multiobjective evolution in the objective space with four or more objectives. In this paper, we propose the use of many-objective test problems in a two- or three-dimensional decision space to visually examine the behavior of multiobjective evolution. Such a visual examination helps us to understand the characteristic features of EMO algorithms for many-objective optimization. Good understanding of existing EMO algorithms may facilitates their modification and the development of new EMO algorithms for many-objective optimization.

Keywords: Evolutionary multiobjective optimization (EMO), many-objective optimization, multiobjective optimization problems, test problems.

1 Introduction

Evolutionary multiobjective optimization (EMO) has been a very active research area in the field of evolutionary computations [3], [5], [26]. A number of EMO algorithms have been proposed and successfully applied to various application tasks [1], [17], [18], [20]. Whereas well-known and frequently-used Pareto dominance-based EMO algorithms such as NSGA-II [6] and SPEA2 [30] work well on two-objective problems, their search ability is often severely degraded by the increase in the number of objectives as pointed out in the literature [4], [9]-[12], [19], [21], [23]-[25], [27], [32].

In the case of many-objective optimization, it is not easy to understand the behavior of multiobjective evolution by EMO algorithms. This is because we cannot visually monitor how a population of solutions is evolved in a high-dimensional objective space. This contrasts to the case of two objectives where we can visually show all solutions at each generation in a two-dimensional objective space in order to examine the move of a population from the initial generation to the final one. Such a visual examination helps us to understand the characteristic features of EMO algorithms such as the convergence-diversity balance and the uniformity of solutions along the

Pareto front. Better understanding of existing EMO algorithms may facilitates their modification and the development of new algorithms for many-objective optimization.

In this paper, we propose the use of many-objective test problems in a two- or three-dimensional decision space to visually examine the behavior of multiobjective evolution. A class of our test problems can be written in the following generic form:

$$\text{Minimize } \mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}),\ f_2(\mathbf{x}),\ ...,\ f_k(\mathbf{x}))\,, \tag{1}$$

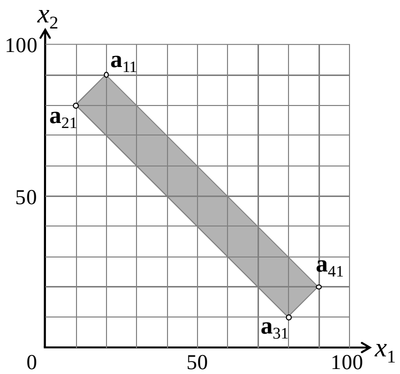
where $\mathbf{x}$ is a two- or three-dimensional decision vector (i.e., a point on a two- or three-dimensional decision space) and $f_i(\mathbf{x})$ is defined by the minimum distance from $\mathbf{x}$ to m points $\mathbf{a}_{i1}$, $\mathbf{a}_{i2}$, ..., $\mathbf{a}_{im}$ in the decision space:

$$f_i(\mathbf{x}) = \min\{\text{dis}(\mathbf{x}, \mathbf{a}_{i1}), \text{dis}(\mathbf{x}, \mathbf{a}_{i2}), ..., \text{dis}(\mathbf{x}, \mathbf{a}_{im})\}\,,\ i = 1, 2, ..., k. \tag{2}$$

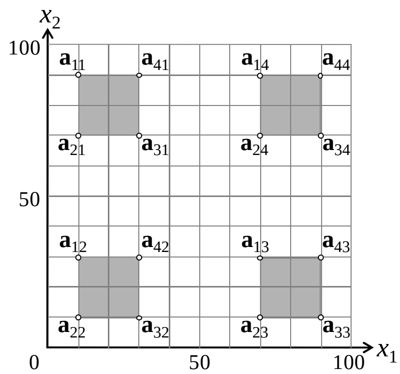
In this formulation, dis($\mathbf{x}$, $\mathbf{a}$) is a distance between the two points $\mathbf{x}$ and $\mathbf{a}$. We assume the use of the Euclidean distance throughout this paper.

Since m points ($\mathbf{a}_{i1}$, $\mathbf{a}_{i2}$, ..., $\mathbf{a}_{im}$) are used to define each objective $f_i(\mathbf{x})$, we need km points to define a k-objective test problem. As shown in this paper, we can generate various types of test problems in a two- or three-dimensional decision space using different combinations of those km points. For example, some test problems have small Pareto optimal regions while others have large ones. Some test problems have multiple equivalent Pareto optimal regions while others have disconnected ones. Two examples of our test problems are shown in Fig. 1. Fig. 1 (a) is a four-objective problem with a single rectangular Pareto optimal region (shaded area) while Fig. 1 (b) is a four-objective problem with four equivalent square Pareto optimal regions.

In this paper, first we briefly review related studies on many-objective test problems in Section 2. Next we show some interesting experimental results on our test problems with m = 1 (i.e., with a single Pareto optimal region) in Section 3. Then we discuss our test problems with m > 1 (i.e., with multiple Pareto optimal regions) and explain their usefulness in Section 4. Finally we conclude this paper in Section 5.



(a) Four-objective problem (m = 1 and k = 4).



(b) Four-objective problem (m = 4 and k = 4).

Fig. 1. Two examples of our test problems in Eq. (1) and Eq. (2).

2 Related Studies on Many-Objective Test Problems

One of the most frequently-used test problems in the EMO community is ZDT [29]. This is a set of six two-objective problems (ZDT1 to ZDT6). For many-objective optimization, seven test problems were proposed by Deb et al. [7], which are called DTLZ (DTLZ1 to DTLZ7). The main feature of the DTLZ problems is its scalability: The number of objectives can be arbitrarily specified. Two problems were added by Deb et al. [8]. Nine DTLZ problems have been frequently used in the literature [16].

Multiobjective 0/1 knapsack problems have also been used in many studies since Zitzler & Thiele [31]. They used nine problems with 250, 500 and 750 items and two, three and four objectives. In some studies [15], [16], [23], knapsack problems with more than four objectives have been generated to examine the performance of EMO algorithms for many-objective optimization. Other combinatorial optimization problems with many objectives (e.g., TSP [4], nurse scheduling [25], and job-shop scheduling [4]) have been also used as test problems in the literature [16].

The use of many-objective test problems in a two-dimensional decision space was proposed by Köppen & Yoshida [21]. They used a single regular polygon for problem definition. Thus their test problems can be viewed as a special case of our formulation with $m = 1$ (i.e., with a single Pareto optimal region). Singh et al. [24] used the same test problems as [21] to examine the performance of many-objective EMO algorithms. Some of our experiments in this paper have been motivated by [21] and [24].

On the other hand, Rudolph et al. [22] used two-objective test problems with multiple equivalent Pareto optimal subsets in a two-dimensional decision space. Each Pareto optimal subset was defined by two points as a line (or a curve) in the decision space. Thus their problems can be viewed as a special case of our formulation with $k = 2$ (i.e., our formulation is a general form of their test problems).

3 Results on Test Problems with a Single Pareto Region (m = 1)

As in Köppen & Yoshida [21], our test problems with a single Pareto optimal region (i.e., our test problems with $m = 1$) can be used to examine the distribution of solutions in a decision space for many-objective optimization. In our computational experiments, we used the following four EMO algorithms: NSGA-II [6], SPEA2 [30], MOEA/D [28] with the Tchebycheff (Chebyshev) function, and SMS-EMOA [27]. The first two are well-known and frequently-used Pareto dominance-based EMO algorithms. The other are recently-developed high-performance EMO algorithms with different fitness evaluation schemes: Scalarizing functions are used in MOEA/D for fitness evaluation while the hypervolume measure is used in SMS-EMOA.

First we applied these EMO algorithms to a five-objective problem with five points at the vertices of a regular pentagon using the following setting:

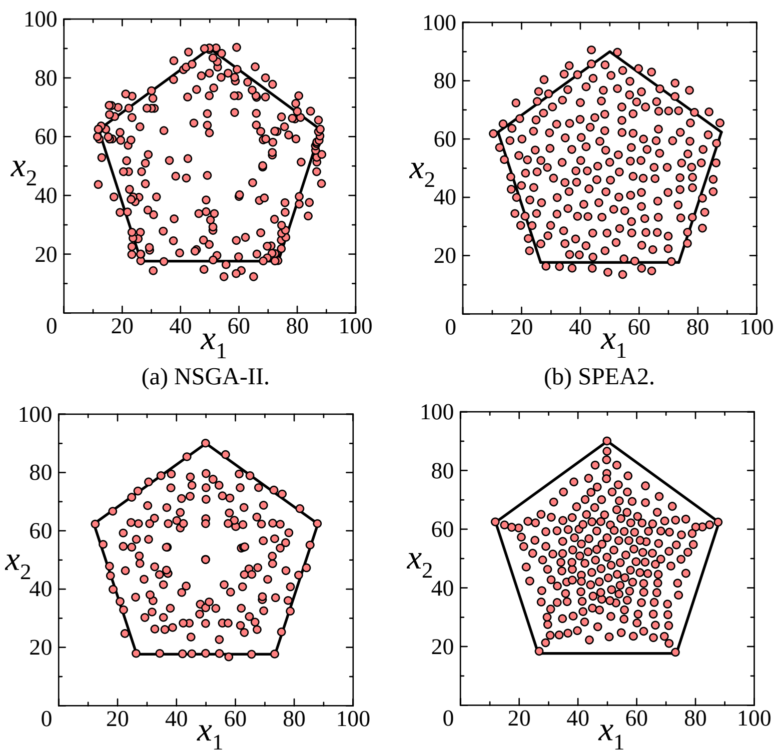
Population size: 200 (NSGA-II, SPEA2) and 210 (MOEA/D),
Total number of examined solutions (Termination conditions): 100,000,
Crossover probability: 1.0 (SBX with $\eta_c = 15$),
Mutation probability: 0.5 (Polynomial mutation with $\eta_m = 20$),

Reference point: Minimum value of each objective (MOEA/D)
Maximum value of each objective × 1.1 (SMS-EMOA).

In MOEA/D, the population size is the same as the number of weight vectors. Due to the combinatorial nature of uniformly distributed weight vectors, the population size cannot be arbitrarily specified (for details, see [28]). We used the closest integer to 200 among the possible values as the population size. The neighborhood size in MOEA/D was specified as 10% of the population size. The same termination condition (i.e., the examination of 100,000 solutions) was used for all algorithms whereas the computation time of SMS-EMOA was much longer than the other algorithms.

In Fig. 2, we show the final population in a single run of each algorithm. All points in the regular pentagon are Pareto optimal solutions. We can observe different characteristic features of each EMO algorithm in Fig. 2.

We can also generate test problems for examining both the convergence and the distribution of solutions. We show an example of such a test problem in Fig. 3 where a four-objective test problem was defined by four vertices of a long and thin rectangle.



(a) NSGA-II. (b) SPEA2.

(c) MOEA/D. (d) SMS-EMOA.

Fig. 2. The final population of a single run of each algorithm on the five-objective problem.

In the same manner as in Fig. 2, we applied the EMO algorithms to the four-objective test problem in Fig. 3. Each plot of Fig. 3 shows the final population in a single run of each algorithm. The Pareto optimal region is the inside of the slender rectangle. It looks difficult for NSGA-II and SPEA2 to converge all solutions into the Pareto optimal region (i.e., inside the slender rectangle including the boundary). On the other hand, good distributions of solutions were not obtained by MOEA/D.

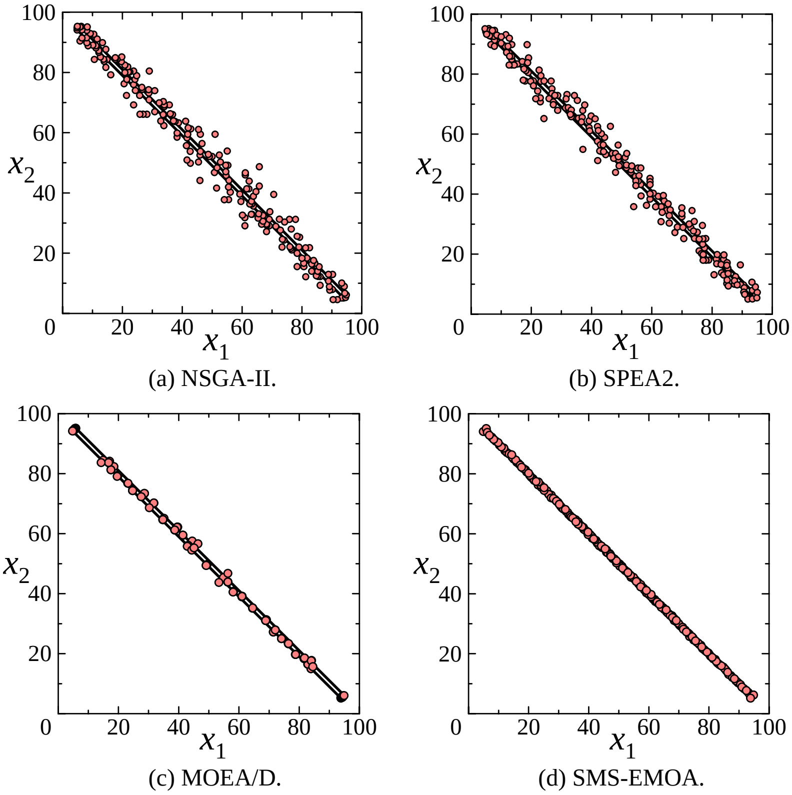
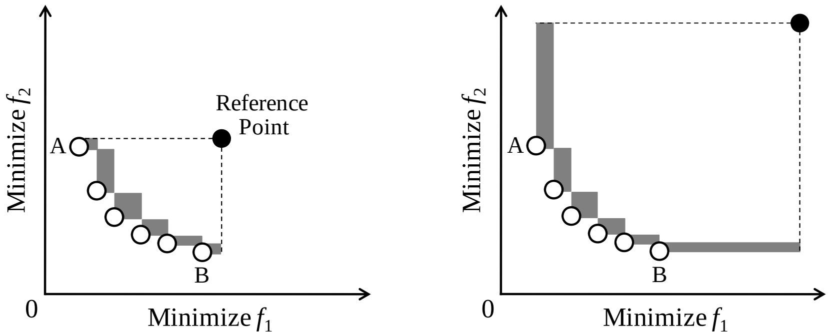


Fig. 3. The final population of a single run of each algorithm on the four-objective problem.

Our test problems can be also used to examine the effect of the location of a reference point on the hypervolume calculation. This effect has already been pointed out in some studies [2], [13], [14]. Explanations on this effect were, however, usually based on illustrations for two-objective problems such as Fig. 4. As shown in Fig. 4, the hypervolume contribution of the two extreme non-dominated solutions (i.e., non-dominated solutions with the best value for either objective: Points A and B in Fig. 4) strongly depends on the location of the reference point. The two plots in Fig. 4 show the same non-dominated solution set with different reference points. When the reference point is far from the Pareto front as in Fig. 4 (b), the two extreme solutions A and B have large hypervolume contributions as indicated by the two large shaded rectangles. On the other hand, if the reference point is close to the Pareto front as in Fig. 4 (a), the two extreme solutions A and B have small hypervolume contributions as indicated by the two small shaded rectangles. It should be noted that the hypervolume contribution of each of the other solutions is independent of the location of a reference point. Since the two extreme non-dominated solutions of a two-objective problem usually have the highest fitness values in most EMO algorithms, the location of a reference point has not a large effect on hypervolume-based EMO algorithms.



(a) Reference point close to the Pareto front. (b) Reference point far from the Pareto front.

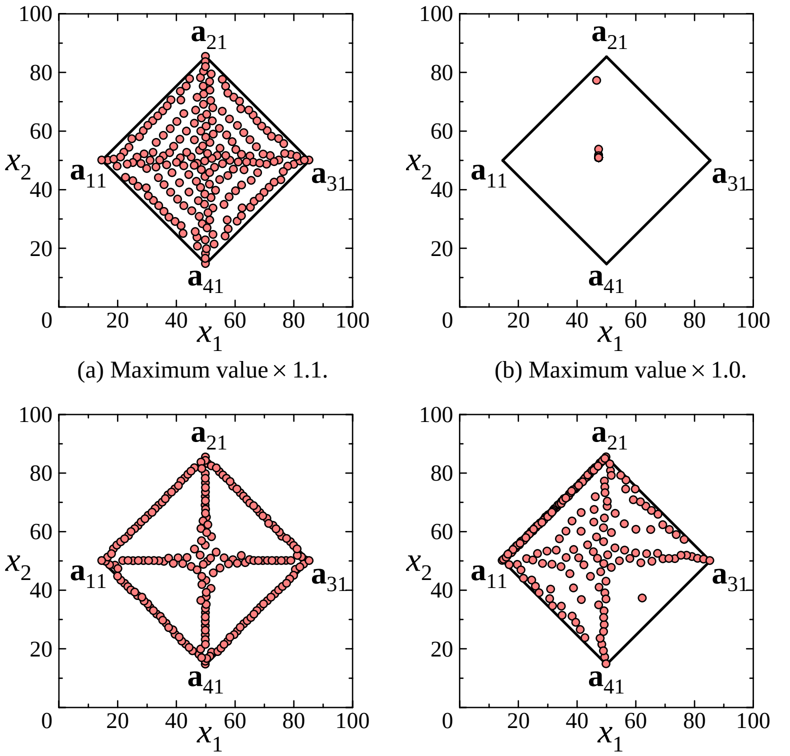
Fig. 4. Illustration of the hypervolume contribution of each non-dominated solution.

On the contrarily, in the case of multiobjective problems with more than two objectives, the location of a reference point has a dominant effect as shown in our experimental results on a four-objective problem in Fig. 5 using the hypervolume-based EMO algorithm: SMS-EMOA [27]. In our computational experiments, we specified the reference point using the maximum value of each objective over all solutions in the current population as follows: "*The i-th element of the reference point = The maximum value of the i-th objective* $\times\ \alpha$" where α is a pre-specified positive constant.

We performed computational experiments using various specifications of the value of α in order to examine the effect of the location of the reference point on the behavior of SMS-EMOA. In Fig. 5, we show the final population of a single run of SMS-EMOA using each of the following specifications of α:

(a) The maximum value of each objective × 1.1 (i.e., $\alpha = 1.1$),
(b) The maximum value of each objective × 1.0 (i.e., $\alpha = 1.0$),
(c) The maximum value of each objective × 10 (i.e., $\alpha = 10$),
(d) $f_1(\mathbf{x})$ and $f_2(\mathbf{x})$: The maximum value of each objective × 1.1 (i.e., $\alpha = 1.1$),
$f_3(\mathbf{x})$ and $f_4(\mathbf{x})$: The maximum value of each objective × 10 (i.e., $\alpha = 10$).

When a reference point is too close to the Pareto front, good solution sets were not obtained as shown in Fig. 5 (b). Good result was obtained in Fig. 5 (a) with $\alpha = 1.1$. By increasing the value of α (i.e., by increasing the distance of a reference point to the Pareto front), solutions moved to the lines between two points as shown in Fig. 5 (c). In Fig. 5 (d), $f_3(\mathbf{x})$ and $f_4(\mathbf{x})$ are distances from a solution $\mathbf{x}$ to the right and bottom points, respectively (while $f_1(\mathbf{x})$ and $f_2(\mathbf{x})$ are distances from a solution $\mathbf{x}$ to the left and top points, respectively). Many solutions are along the line between the left and top points (i.e., $\mathbf{a}_{11}$ and $\mathbf{a}_{21}$) for which the smaller value of α was used in our computational experiment in Fig 5 (d).



(a) Maximum value × 1.1.

(b) Maximum value × 1.0.

(c) Maximum value × 10.

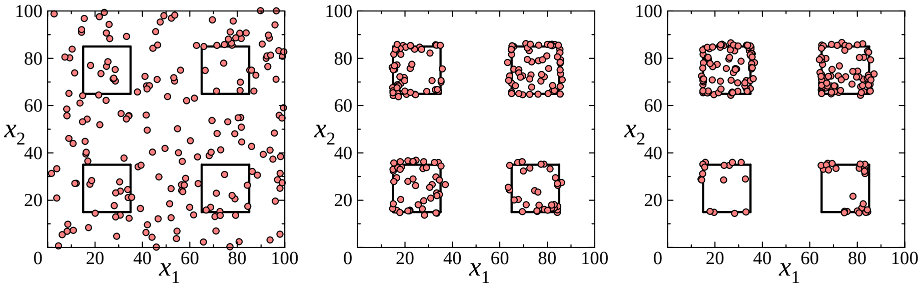
(d) f_1 and f_2: × 1.1, and f_3 and f_4: × 10.

Fig. 5. Experimental results of SMS-EMOA with different specifications of a reference point.

4 Results on Test Problems with Multiple Pareto Regions (*m* > 1)

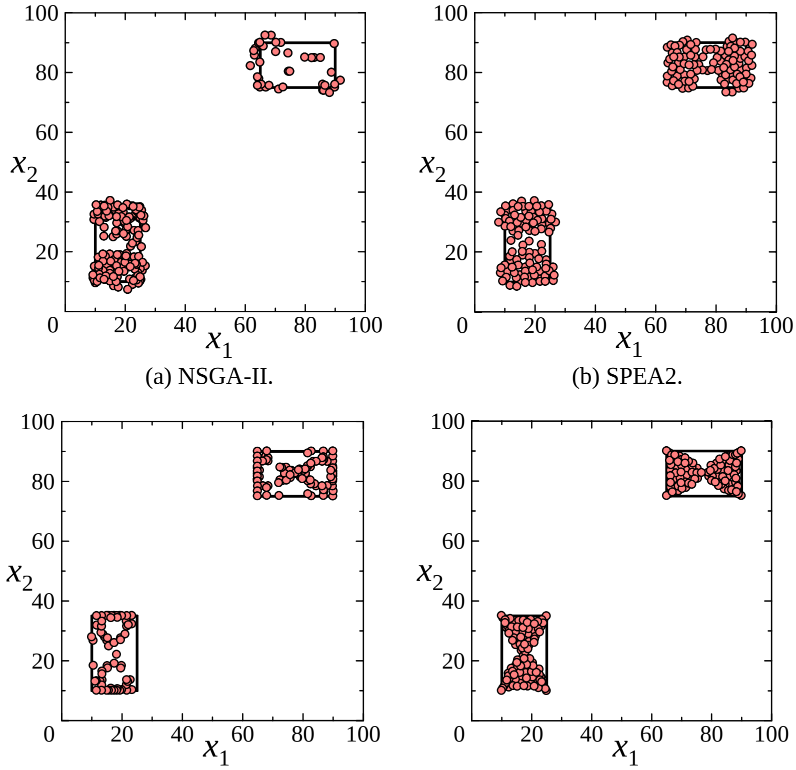
Using multiple polygons with the same shape, we can generate multiobjective problems with multiple equivalent Pareto optimal regions as shown in Fig. 1 (b) in Section 1. In Fig. 6, we show experimental results of a single run of NSGA-II on the four-objective problem in Fig. 1 (b). Fig. 6 shows a randomly generated initial population (a) and two intermediate populations (b) and (c). From the three plots in Fig. 6, we can see that every solution quickly moved to one of the four squares within the first 10 generations. Then they continued to move in the four squares. We performed computational experiments many times. In some runs, solutions converged to one or two squares. In other runs, all the four squares had at least one solution even after 500 generations. That is, final results were totally different in each run.

We can also generate test problems with disconnected Pareto regions by using multiple polygons with different shapes. In Fig. 7, we show experimental results on such a test problem. Each plot of Fig. 7 is the final population in a single run of each algorithm on the four-objective test problem with two rectangles. Since the two rectangles in Fig. 7 are not equivalent, solutions did not converge into one rectangle.



(a) Initial population. (b) 10th generation. (c) 20th generation.

Fig. 6. Experimental results of a single run of NSGA-II on the four-objective problem.



(a) NSGA-II. (b) SPEA2.

(c) MOEA/D. (d) SMS-EMOA.

Fig. 7. Results of a single run on a four-objective problem with disconnected Pareto regions.

Since the distribution in the decision space has not been taken into account in the design of almost all EMO algorithms, our intention is not to say which EMO algorithm is the best using our test problems but to visually examine the behavior of each EMO algorithm for many-objective optimization problems. However, performance measures for solution sets in the decision space may be an interesting research issue.

5 Conclusions

We proposed the use of many-objective test problems in a two- or three-dimensional decision space in order to visually examine multiobjective evolution for many-objective problems. Our test problems can be viewed as a generalized version of single polygon problems of Köppen & Yoshida [21] and multi-line (or multi-curve) problems of Rudolph et al. [22]. It is the main advantage of our test problems (and test problems in [21], [22]) that we can visually examine multiobjective evolution in the decision space. Whereas we generated test problems in a two-dimensional decision space for visual examination, it is also easy to generate test problems in a high-dimensional space by specifying multiple points with the required dimensionality.

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