Relation between Neighborhood Size and MOEA/D Performance on Many-Objective Problems

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Abstract. MOEA/D is a simple but powerful scalarizing function-based EMO algorithm. Its high search ability has been demonstrated for a wide variety of multiobjective problems. MOEA/D can be viewed as a cellular algorithm. Each cell has a different weight vector and a single solution. A certain number of the nearest cells are defined for each cell as its neighbors based on the Euclidean distance between weight vectors. A new solution is generated for each cell from current solutions in its neighboring cells. The generated solution is compared with the current solutions in the neighboring cells for solution replacement. In this paper, we examine the relation between the neighborhood size and the performance of MOEA/D. In order to examine the effect of local mating and local replacement separately, we use a variant of MOEA/D with two different neighborhoods: One is for local mating and the other is for local replacement. The performance of MOEA/D with various combinations of two neighborhoods is examined using the hypervolume in the objective space and a diversity measure in the decision space for many-objective problems. Experimental results show that MOEA/D with a large replacement neighborhood has high search ability in the objective space. However, it is also shown that small replacement and mating neighborhoods are beneficial for diversity maintenance in the decision space. It is also shown that the appropriate specification of two neighborhoods strongly depends on the problem.

Keywords: Evolutionary multiobjective optimization, many-objective problems, MOEA/D, neighborhood size.

1 Introduction

Evolutionary multiobjective optimization (EMO) has been successfully applied to various application fields [4], [5], [26]. Pareto dominance-based algorithms such as NSGA-II [6], SPEA [34] and SPEA2 [32] have frequently been used in the literature. Recently, a scalarizing function-based EMO algorithm called MOEA/D (Multi-Objective Evolutionary Algorithm based on Decomposition [30]) has rapidly increased the popularity due to its simplicity, high search ability, and computational efficiency. In MOEA/D, a multiobjective problem is decomposed into a number of single-objective problems using a scalarizing function with different weight vectors. Each single-objective problem optimizes the scalarizing function with a different

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weight vector. Since fitness evaluation for each individual is based on scalarizing function calculation, it can be efficiently performed even for many-objective problems. High search ability of MOEA/D has been repeatedly reported especially for difficult multiobjective problems in the literature [11], [21], [31].

The main feature of MOEA/D is the decomposition using a scalarizing function with different weight vectors (as its name explicitly shows). Thus the choice of an appropriate scalarizing function is important. Different scalarizing functions work well on different problems. Different scalarizing functions may be effective in different stages of evolution. Adaptive selection of a scalarizing function and the use of multiple scalarizing functions were examined [14], [15]. The population size is also an important parameter since it determines the granularity of weight vectors [13]. Actually the population size is the same as the number of weight vectors in MOEA/D.

Another important feature of MOEA/D is the use of a kind of a neighborhood structure defined by the Euclidean distance between weight vectors. By viewing each weight vector as a point in the weight vector space, MOEA/D can be explained as a cellular algorithm. Each cell has a different weight vector and a single solution. Each cell has a certain number of neighboring cells. A new solution for a cell is generated by choosing a pair of parents from the current solutions in its neighboring cells (i.e., local mating). The generated solution is compared with those solutions in the neighboring cells for solution replacement (i.e., local replacement).

The number of neighboring cells (i.e., neighborhood size) is an important user-definable parameter. However, the importance of its appropriate specification has not been stressed in the literature. This may be because MOEA/D on two-objective and three-objective problems usually has high search ability over a wide range of different specifications of the neighborhood size. In this paper, we demonstrate that its search ability for many-objective problems strongly depends on the neighborhood size. In order to examine the local mating and the local replacement separately, we use a variant of MOEA/D with two neighborhoods as in our former studies on MOEA/D [11], [13], [15]. A pair of parents is selected from a mating neighborhood, and the generated solution is compared with current solutions in a replacement neighborhood. Using such a variant, we examine various combinations of two neighborhoods (e.g., a small mating neighborhood and a large replacement neighborhood). Performance of MOEA/D with two neighborhoods is evaluated with respect to the hypervolume in the objective space and a diversity measure in the decision space.

This paper is organized as follows. First we explain a variant of MOEA/D with two neighborhoods in Section 2. In Section 3, we explain two types of many-objective test problems. One is many-objective knapsack problems, which are used to evaluate the search ability of MOEA/D in the objective space. The other is many-objective distance minimization problems, which are used to visually examine the diversity of solutions in the decision space. Performance measures in the objective space and diversity measures in the decision space are discussed in Section 4. Then we examine the relation between the performance of MOEA/D and the specifications of two neighborhoods through computational experiments in Section 5. Experimental results show that the performance of MOEA/D on many-objective knapsack problems strongly depends on the specifications of two neighborhoods. Different specifications are needed for hypervolume maximization in the objective space and diversity maximization in the decision space. Finally we conclude this paper in Section 6.

2 MOEA/D with Two Neighborhoods

In MOEA/D [30], a multiobjective problem is decomposed into a number of single-objective problems using a scalarizing function with different weight vectors. A set of weight vectors satisfying the following two conditions is used in MOEA/D:

$$\lambda_1 + \lambda_2 + \cdots + \lambda_m = 1 \,, \tag{1}$$

$$\lambda_i \in \left\{0, \frac{1}{H}, \frac{2}{H}, ..., \frac{H}{H}\right\}, \; i = 1, 2, ..., m \,, \tag{2}$$

where H is a user-definable positive integer. The number of weight vectors can be calculated as $N = {}_{H+m-1}C_{m-1}$ (i.e., $N = C^{m-1}_{H+m-1}$ [30]). For example, we have 101 weight vectors for a two-objective problem when H = 100: $\boldsymbol{\lambda}$ = (0, 1), (0.01, 0.99), ..., (1, 0). In Fig. 1, we show 15 weight vectors for a three-objective problem when H = 4.

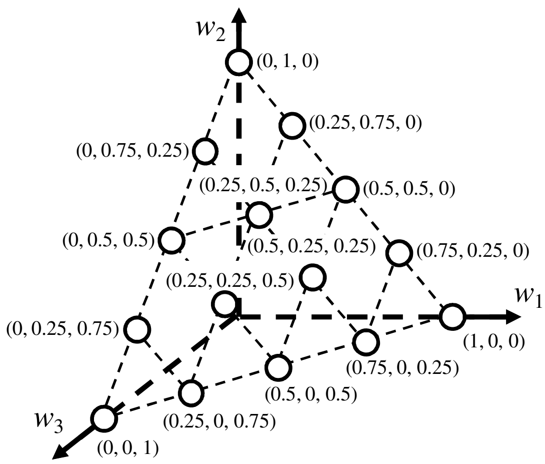


Fig. 1. A set of weight vectors for a three-objective problem (H = 4)

As a scalarizing function, we mainly use the weighted Tchebycheff in this paper. Only for many-objective knapsack problems with six and eight objectives, we use the weighted sum since better results were obtained from the weighted sum for those problems in our preliminary computational experiments (e.g., see [15]).

An m-objective maximization problem can be written as

$$\text{Maximize} \;\; \boldsymbol{f}(\boldsymbol{x}) = (f_1(\boldsymbol{x}), \; f_2(\boldsymbol{x}), \; ..., \; f_m(\boldsymbol{x})) \,, \tag{3}$$

where $\boldsymbol{f}(\boldsymbol{x})$ is the m-dimensional objective vector, $f_i(\boldsymbol{x})$ is the ith objective to be maximized, and $\boldsymbol{x}$ is the decision vector.

The weighted sum of the m objectives is written using a weight vector $\boldsymbol{\lambda}$ as

$$g^{WS}(\boldsymbol{x} \mid \boldsymbol{\lambda}) = \lambda_1 \cdot f_1(\boldsymbol{x}) + \lambda_2 \cdot f_2(\boldsymbol{x}) + \cdots + \lambda_m \cdot f_m(\boldsymbol{x}) . \tag{4}$$

The weighted Tchebycheff is written using a reference point $\boldsymbol{z}^* = (z_1^*, z_2^*, ..., z_m^*)$ and a weighted vector $\boldsymbol{\lambda}$ as follows:

$$g^{TE}(\boldsymbol{x} \mid \boldsymbol{\lambda}, \boldsymbol{z}^*) = \max_{i=1,2,...,m} \{\lambda_i \cdot \mid z_i^* - f_i(\boldsymbol{x}) \mid\} . \tag{5}$$

In Zhang and Li [30], the reference point $\boldsymbol{z}^*$ was specified for multiobjective knapsack problems (which are multiobjective maximization problems) as

$$z_i^* = 1.1 \cdot \max\{f_i(\boldsymbol{x}) \mid \boldsymbol{x} \in \Omega(t)\},\ i = 1, 2, ..., m , \tag{6}$$

where $\Omega(t)$ shows the tth population. We use this specification. For multiobjective function minimization problems, the following specification was used in [30]:

$$z_i^* = \min\{f_i(\mathbf{x}) \mid \mathbf{x} \in \Omega(t)\},\ i = 1, 2, ..., m . \tag{7}$$

We use this specification for multiobjective distance minimization problems.

As in our former studies [11], [13], [15], we implemented MOEA/D as a cellular algorithm with two neighborhoods. As shown in Fig. 1, a set of weight vectors can be viewed as a grid in the weight vector space where each weight vector corresponds to a cell. Each cell can be viewed as having a weight vector and a single solution.

Let N be the number of weight vectors, which is the same as the number of cells and the population size. We denote N weight vectors as $\boldsymbol{\lambda}^k$, $k = 1, 2, ..., N$ where $\boldsymbol{\lambda}^k$ is a weight vector assigned to the kth cell. In the original MOEA/D [30], each weight vectors has a set of neighbors. Our variant of MOEA/D has two sets of neighbors. That is, each cell has two sets of neighboring cells. One is for local mating and the other is for local replacement of solutions. As in the original MOEA/D [30], the definition of neighbors is based on the distance between weight vectors.

When a solution is to be generated in a cell, a pair of solutions is randomly selected from its mating neighborhood. A new solution is generated by crossover and mutation. The generated solution for the cell is compared with current solutions in its replacement neighborhood. At each cell in the replacement neighborhood, the generated solution is evaluated using the weight vector in that cell. The solution replacement is performed when the generated solution is better than the current one in each cell. It should be noted that the comparison is based on the weight vector at each cell. Thus it is not likely that many current solutions are replaced with a single new solution even when we use a large replacement neighborhood. This is because a new solution is not likely to be evaluated as being better than current solutions at many cells with totally different weight vectors such as (0.2, 0.8), (0.5, 0.5) and (0.8, 0.2).

In the original version of MOEA/D, a parent outside the neighborhood can be probabilistically selected. In our variant, we always choose parents from the mating neighborhood. The upper bound on the number of replaced solutions with a new solution can be specified in the original MOEA/D. We do not use any upper bound on the number of replaced solutions in our variant. The original MOEA/D also has an option of using an archive population to store non-dominated solutions. We do not use any archive population. All of these settings in our variant are to clearly examine the effect of the neighborhood size on the performance of MOEA/D.

It is pointed out in several studies [10], [20], [23] that the recombination of similar parents improves the search ability of EMO algorithms on many-objective problems. This is because the current population of EMO algorithms has a large diversity in the decision space in the case of many objectives [20]. A good solution is not likely to be generated from a pair of totally different parents. MOEA/D has two nice properties as a many-objective optimizer: One is the scalarizing function-based efficient fitness evaluation, and the other is the local mating. It is shown in this paper that an appropriate specification of the mating neighborhood is important in the application of MOEA/D to difficult many-objective problems. The necessity of local replacement is also discussed with respect to the diversity in the decision space.

3 Many-Objective Test Problems

It has been pointed out in the literature that many-objective problems are difficult for Pareto dominance-based EMO algorithms [8], [19], [22]. When EMO algorithms are applied to many-objective problems, almost all solutions in the current population become non-dominated with each other within a small number of generations. This severely weakens the selection pressure of Pareto dominance-based fitness evaluation mechanisms towards the Pareto front. Various approaches have been proposed to increase the selection pressure [16], [17], [23]. EMO algorithms with other fitness evaluation mechanisms such as indicator-based EMO algorithms (e.g., SMS-EMOA [3]) and scalarizing function-based EMO algorithms (e.g., MOEA/D [30]) have been actively studied for many-objective problems. Currently evolutionary many-objective optimization is a hot topic in the EMO community [1], [2], [24], [35].

As test problems, we use two types of many-objective problems. One is knapsack problems, which are difficult many-objective problems for Pareto dominance-based EMO algorithms. The other is distance minimization problems, which are easy many-objective problems. We briefly explain those test problems.

We generated many-objective knapsack problems from the two-objective 500-item knapsack problem of Zitzler and Thiele [34]. This problem is written as follows:

$$\text{Maximize} \quad f_i(\boldsymbol{x}) = \sum_{j=1}^{n} p_{ij} x_j \,, \quad i = 1, 2, \tag{8}$$

$$\text{subject to} \quad \sum_{j=1}^{n} w_{ij} x_j \le c_i \,, \quad i = 1, 2, \tag{9}$$

$$x_j = 0 \text{ or } 1, \quad j = 1, 2, ..., n, \tag{10}$$

where n is the number of items (i.e., n = 500), $\boldsymbol{x}$ is a binary string, p_{ij} is the profit of item j according to knapsack i, w_{ij} is the weight of item j according to knapsack i, and c_i is the capacity of knapsack i. The value of each profit p_{ij} is a randomly specified integer in [10, 100]. This problem is referred to as the 2-500 problem in this paper.

We generated additional objectives $f_i(\boldsymbol{x})$ for i = 3, 4, ..., 8 by randomly specifying the value of the profit p_{ij} as an integer in [10, 100]. In this manner, we generated m-objective knapsack problems with up to eight objectives. Each of those test problems is referred to as the m-500 problem in this paper. It should be noted that all of those test problems have the same constraint conditions as the original 2-500 problem. That is, all of our multiobjective knapsack problems have the same feasible solution set. As a result, the Pareto optimal solutions of the original 2-500 problem are also Pareto optimal for the m-500 problems for m = 3, 4, ..., 8. This feature is used to visually examine the convergence and the diversity of solutions of many-objective knapsack problems by projecting them onto the two-dimensional objective space with $f_1(\boldsymbol{x})$ and $f_2(\boldsymbol{x})$. It has been demonstrated that randomly generated many-objective knapsack problems are difficult for Pareto dominance-based EMO algorithms [11], [23].

We also generated many-objective distance minimization problems with multiple Pareto regions to examine the behavior of EMO algorithms in a two-dimensional decision space [9], [12]. An example of a four-objective problem is shown in Fig. 2. All points in the shaded four squares are Pareto optimal solutions. The ith objective $f_i(\mathbf{x})$ is the minimum distance from a point $\mathbf{x}$ (i.e., solution $\mathbf{x}$) in the two-dimensional decision space to the ith vertexes of multiple polygons:

$$f_i(\mathbf{x}) = \min\{\mathrm{dis}(\mathbf{x}, \mathbf{a}_{i1}), \mathrm{dis}(\mathbf{x}, \mathbf{a}_{i2}), ..., \mathrm{dis}(\mathbf{x}, \mathbf{a}_{ik})\}\,,\ i = 1, 2, ..., m, \tag{11}$$

where dis($\mathbf{x}$, $\mathbf{a}_{ij}$) is the Euclidean distance between the two points $\mathbf{x}$ and $\mathbf{a}_{ij}$, $\mathbf{a}_{ij}$ shows the ith vertex of the jth polygon, k is the number of polygons (i.e., j = 1, 2, ..., k), and m is the number of objectives (i.e., the number of vertexes: i = 1, 2, ..., m). In Fig. 2, the four squares have exactly the same shape and the same size. Thus each square is mapped to the same Pareto front in the four-dimensional objective space.

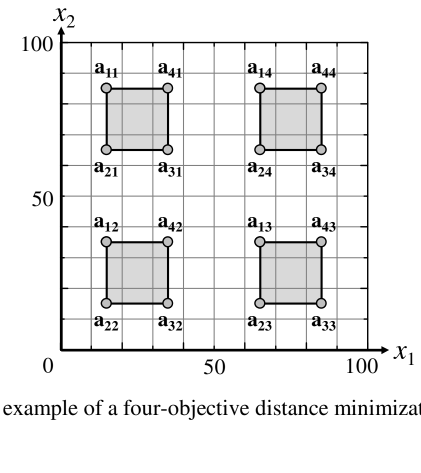


Fig. 2. An example of a four-objective distance minimization problem

In the same manner as in Fig. 2, we generated distance minimization problems with three, five and six objectives as shown in Fig. 3. We also generated four distance minimization problems with a single Pareto optimal region as shown in Fig. 4. In our test problems in Figs. 2-4, all points in each polygon are Pareto optimal solutions.

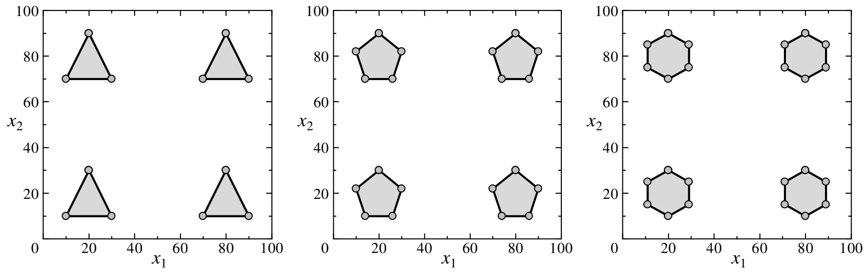


Fig. 3. Distance minimization problems with multiple Pareto optimal regions

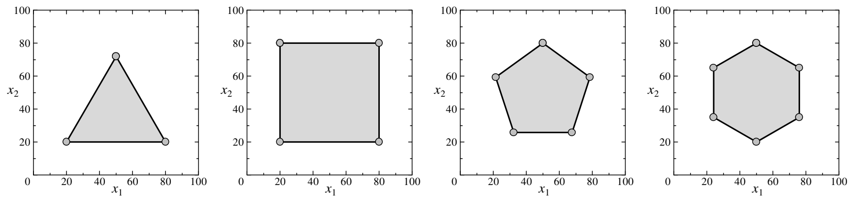


Fig. 4. Distance minimization problems with a single Pareto optimal region

4 Performance Measures and Diversity Measures

A number of performance measures have been proposed to evaluate a set of non-dominated solutions in the objective space [33]. We use the hypervolume measure, which has been frequently used in the literature.

With a few exceptions (e.g., Omni-Optimizer [7]), the decision space diversity has not been used in EMO algorithms. This is because the diversity maintenance in the objective space is very important in EMO algorithms. Recently, the importance of the diversity maintenance in the decision space was stressed in some studies [27]-[29] where the use of the Solow-Polasky diversity measure [25] was suggested. The use of a non-geometric binary crossover was proposed to directly increase the decision space diversity [18]. In this paper, we use the average distance between two solutions in the decision space as a diversity measure since its meaning can be easily understood. The distance between solutions of the knapsack problems (i.e., binary strings) is measured by the Hamming distance while the Euclidean distance is used for solutions of the distance minimization problems (i.e., two-dimensional real number vectors). Whereas we also calculated the Solow-Polasky diversity measure, we only report the average distance between solutions due to the page limitation.

5 Experimental Results

We applied our variant of MOEA/D, NSGA-II and SPEA2 to the 2-500, 4-500, 6-500 and 8-500 knapsack problems using the following parameter specifications:

Coding: Binary string of length 500 (i.e., 500-bit string),
Population size in NSGA-II and SPEA2: 200,
Population size in MOEA/D: 200 (2-500), 220 (4-500), 252 (6-500), 120 (8-500),
Termination condition: 200×2000 solution evaluations,
Parent selection: Random selection from the neighborhood (MOEA/D),
Binary tournament selection with replacement (NSGA-II and SPEA2),
Crossover: Uniform crossover (Probability: 0.8),
Mutation: Bit-flip mutation (Probability: 1/500),
Number of runs for each test problem: 100 runs.

In MOEA/D, we specified the size of the mating neighborhood as α% of the population size where α = 1, 2, 4, 6, 8, 10, 20, 40, 60, 80, 100. That is, these 11 specifications of α were examined. When α% of the population size was not an integer, the non-integer value was rounded down. For example, 1% of the population size 220 was handled as 2 by rounding down the calculated value 2.2. The same 11 specifications were also used for the replacement neighborhood. That is, the size of the replacement neighborhood was specified as β% of the population size where β = 1, 2, 4, 6, 8, 10, 20, 40, 60, 80, 100. All the 11×11 combinations were examined in our computational experiments.

The average value of the hypervolume of the final population over 100 runs of our variant of MOEA/D for each combination is summarized in Fig. 5. The origin of the objective space was used as a reference point in the hypervolume calculation. Good results were not obtained for many-objective knapsack problems by NSGA-II and SPEA2. For example, their results on the 8-500 problem were 1.10×10^{34} (NSGA-II) and 1.03×10^{34} (SPEA2) whereas the best result in Fig. 5 was 1.55×10^{34}. From Fig. 5, we can see that good results were obtained for all the four test problems when the size of the two neighborhoods was specified as follows: 2-10% of the population size for the mating neighborhood and 20-100% for the replacement neighborhood. We can also see from Fig. 5 that the sensitivity of the MOEA/D performance on the neighborhood size increases with the number of objectives. Whereas almost the same results were obtained from a wide range of parameter specifications for the 2-500 problem, very good results were obtained from only a few combinations for the 8-500 problem. These observations suggest that the use of appropriate neighborhoods is important in MOEA/D for many-objective knapsack problems. Fig. 5 also shows that the use of two different neighborhoods improves the performance of MOEA/D.

The average distance between solutions in the final population is summarized in Fig. 6. High average distances between solutions were obtained from a small mating neighborhood for all the six test problems independent of the size of the replacement neighborhood. We can see that there is no clear relation between the hypervolume in Fig. 5 and the decision space diversity in Fig. 6. In Fig. 7, we show the projection of a solution set onto the $f_1(\boldsymbol{x})$-$f_2(\boldsymbol{x})$ space obtained by a single run of MOEA/D with a different setting of two neighborhoods. We can see from Fig. 7 that a large diversity in the objective space was obtained from a small mating neighborhood.

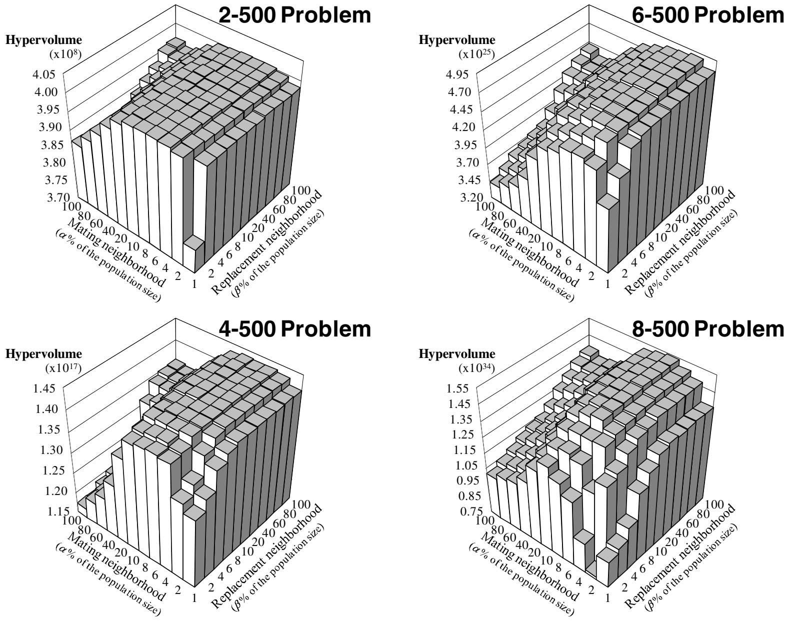


Fig. 5. Experimental results on the knapsack problems (Hypervolume measure)

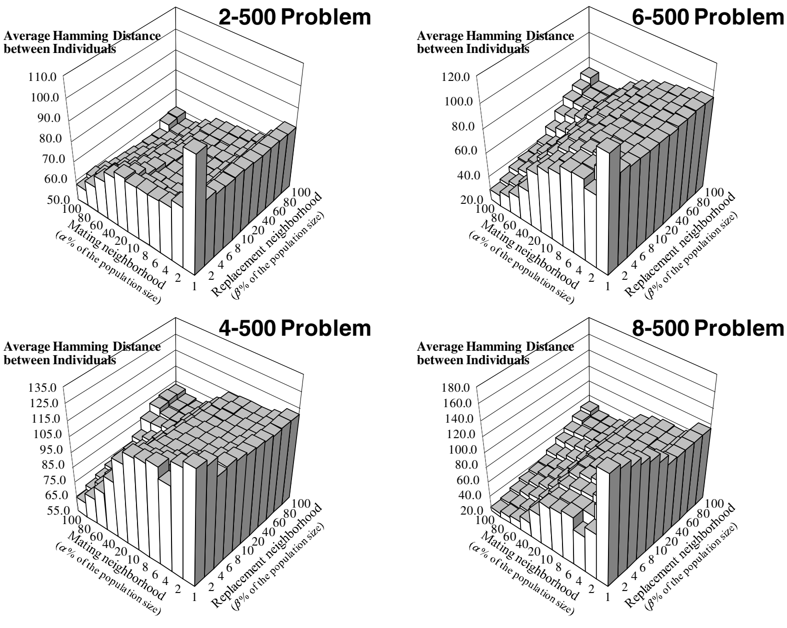
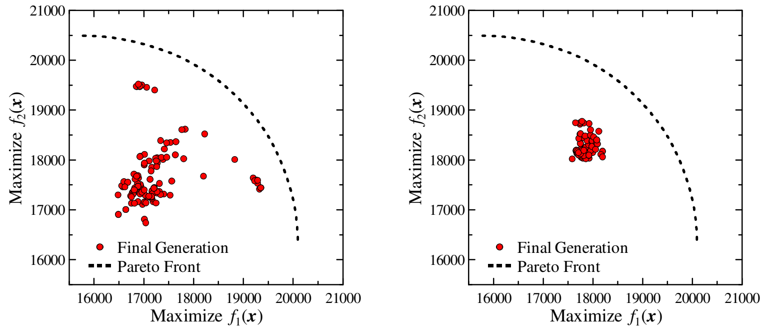


Fig. 6. Experimental results on the knapsack problems (Average Hamming distance)



(a) 1% mating and 100% replacement. (b) 100% mating and 1% replacement.

Fig. 7. Projection of a solution set obtained from a single run of MOEA/D with a different setting on the 8-500 problem. The dashed line shows the Pareto front of the 2-500 problem.

In Fig. 8 and Fig. 9, we show experimental results on the four test problems with a single Pareto optimal region in Fig. 4. Experimental results on the four test problems with four Pareto optimal regions in Fig. 2 and Fig. 3 are shown in Fig. 10 and Fig. 11. We can see that the four plots in each figure show somewhat similar patterns: Good results were almost always obtained from a small replacement neighborhood in Figs. 8-11. These observations are totally different from those for the knapsack problems.

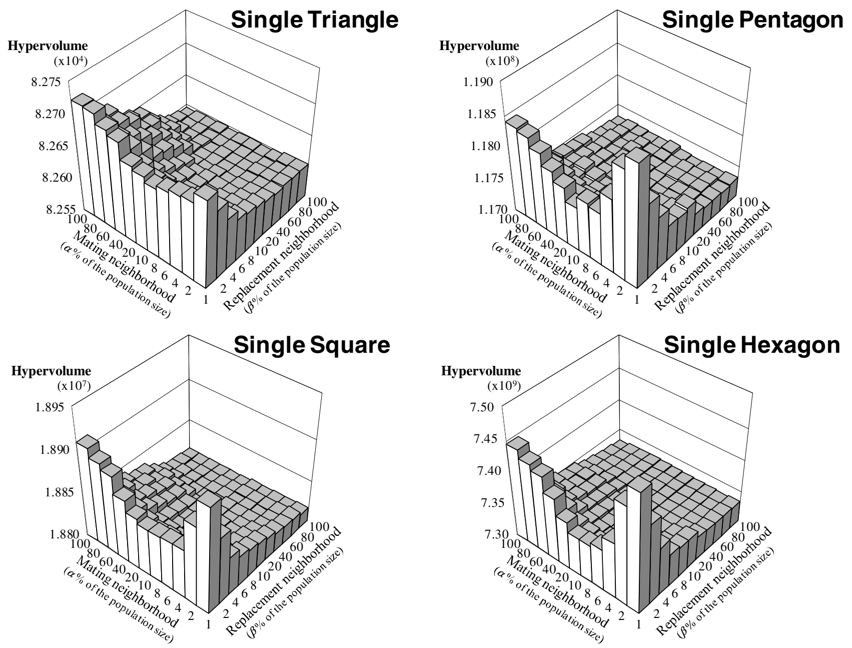


Fig. 8. Results on the minimization problems in Fig. 4 (Hypervolume measure)

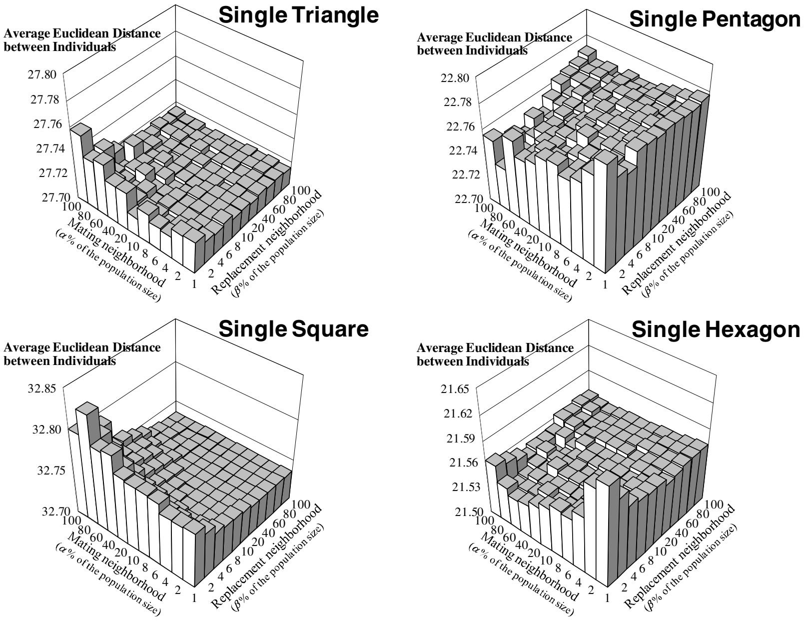


Fig. 9. Results on the minimization problems in Fig. 4 (Average distance)

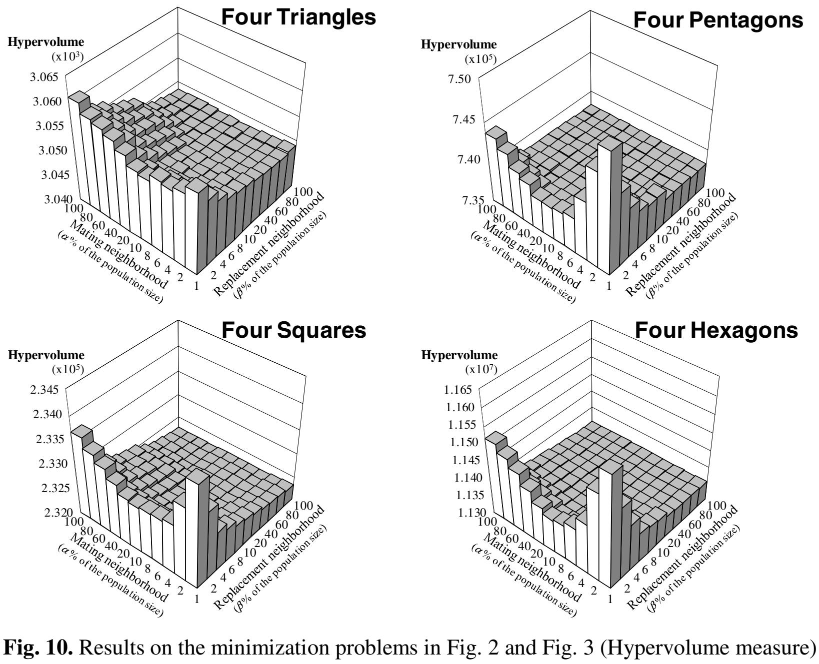


Fig. 10. Results on the minimization problems in Fig. 2 and Fig. 3 (Hypervolume measure)

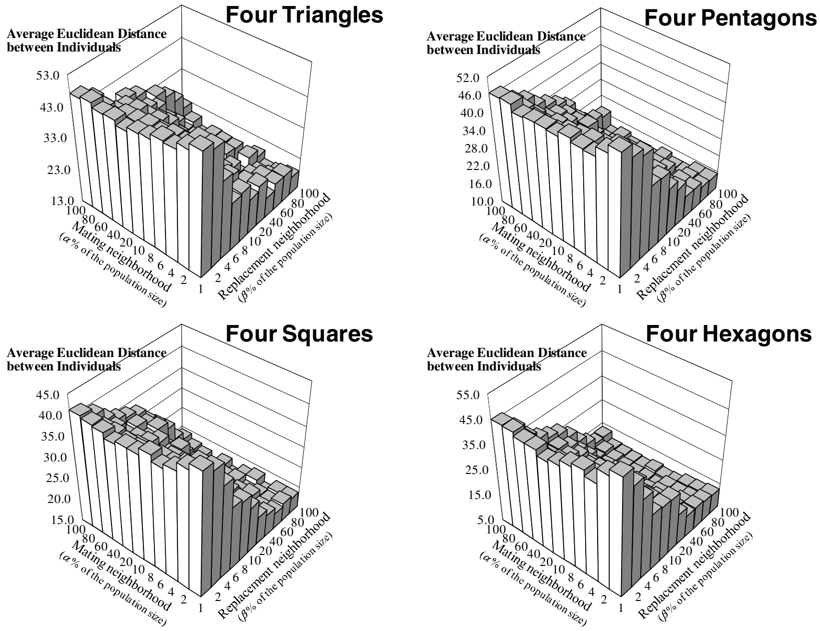
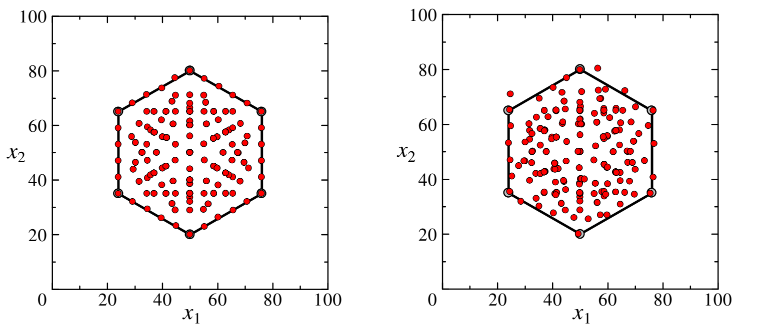


Fig. 11. Results on the minimization problems in Fig. 2 and Fig. 3 (Average distance)

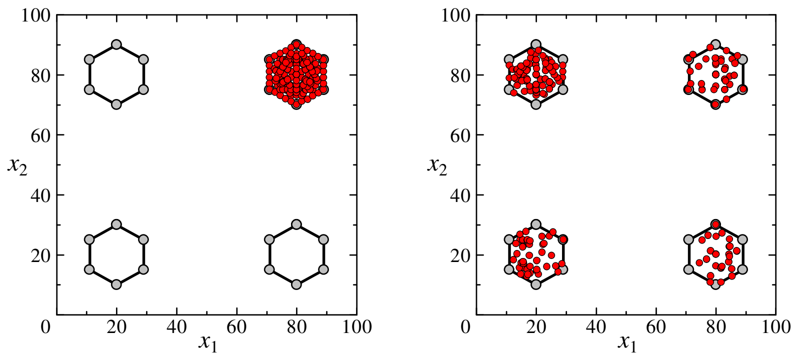


(a) 1% mating and 100% replacement. (b) 100% mating and 1% replacement.

Fig. 12. A solution set from a single run with a different setting (Single hexagon)

In Fig. 12 and Fig. 13, we show an obtained solution set from a single run of MOEA/D with a different setting. Whereas the result in Fig. 12 (a) looks nice, a higher hypervolume value was obtained from a small replacement neighborhood in Fig. 12 (b) as shown in Fig. 8. Fig. 13 clearly shows that a much larger diversity in the decision space was obtained from a small replacement neighborhood (see Fig. 11).

The average hypervolume values 1.08×10^7 and 1.18×10^7 were obtained for the four-hexagon problem by NSGA-II and SPEA2, respectively, while the best result by MOEA/D was 1.16×10^7 in Fig. 10. These results show that our distance minimization problems are not difficult for Pareto dominance-based EMO algorithms.



(a) 1% mating and 100% replacement. (b) 100% mating and 1% replacement.

Fig. 13. A solution set from a single run with a different setting (Four hexagons)

6 Conclusions

In this paper, we explained the relation between the performance of MOEA/D on many-objective problems and the specification of the size of the two neighborhoods (one is for local mating and the other is for local replacement). For many-objective knapsack problems, we obtained the following observations:

(1) Good results with respect to the hypervolume measure were obtained from the following combinations: The mating neighborhood size was 2-10% of the population size and the replacement neighborhood size was 20-100%. The larger the replacement neighborhood was, the better the performance of MOEA/D was.

(2) Good results with respect to the decision space diversity were obtained when the mating neighborhood size was 1% of the population size. The smaller the mating neighborhood was, the larger the decision space diversity was.

Different results were obtained for the distance minimization problems as follows:

(3) Good results with respect to both the hypervolume measure and the decision space diversity were obtained when the replacement neighborhood size was 1%. The smaller the replacement neighborhood was, the better the performance was.

(4) The best results with respect to both the hypervolume measure and the decision space diversity were obtained for the five-objective and six-objective problems when the size of the two neighborhoods was specified as 1% of the population size (whereas the worst results were obtained from this setting for the knapsack problems with respect to the hypervolume measure).

We can see from these observations that an appropriate specification of the two neighborhoods is totally problem-dependent. Moreover, good specifications for the hypervolume maximization are not always good for the decision space diversity maximization. For difficult many-objective problems, high selection pressure toward the Pareto front is needed for efficient search. Thus a large replacement neighborhood is beneficial for MOEA/D. For easy many-objective problems, high selection pressure is not needed. So a large replacement neighborhood is not needed. One potential disadvantage of a large replacement neighborhood is the increase in computation load, which should be further discussed in future studies.

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