A Double-Niched Evolutionary Algorithm and its Behavior on Polygon-Based Problems

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Abstract. Multi-modal multi-objective optimization problems are commonly seen in real-world applications. However, most existing researches focus on solving multi-objective optimization problems without multi-modal property or multi-modal optimization problems with single objective. In this paper, we propose a double-niched evolutionary algorithm for multi-modal multi-objective optimization. The proposed algorithm employs a niche sharing method to diversify the solution set in both the objective and decision spaces. We examine the behaviors of the proposed algorithm and its two variants as well as three other existing evolutionary optimizers on three types of polygon-based problems. Our experimental results suggest that the proposed algorithm is able to find multiple Pareto optimal solution sets in the decision space, even if the diversity requirements in the objective and decision spaces are inconsistent or there exist local optimal areas in the decision space.

Keywords: Evolutionary computation, multi-objective optimization, multi-modal optimization, niche, diversity

1 Introduction

There are many multi-objective optimization problems in real-world applications. Due to the conflicting nature of objectives, there is typically no single optimal solution to these problems, rather a Pareto optimal solution set. The image of the Pareto optimal solution set in the objective space is referred to as the Pareto front. The general task (in *a posteriori* situations) of a multi-objective optimizer is to find an approximate solution set not only close to but also well distributed on the Pareto front.

In view of this, a large number of multi-objective evolutionary algorithms (MOEAs) are designed to solve multi-objective optimization problems over the past two decades. The most typical MOEAs are the Pareto-based ones, in which the Pareto dominance relationship is adopted as the first selection criterion to distinguish well converged solutions, while a density-based second selection criterion is used to promote diversity in the objective space. The widely adopted density-based selection criteria are the crowding distance [1] and niche sharing [4] methods, to name a few.

On the other hand, the objective(s) of an optimization problem may have multi-modal property. For such an objective, there exist different optimal solutions which have the same objective value. This requires evolutionary algorithms to maintain diversity among solutions in the decision space to provide more options for the decision maker. Most existing researches focus on multi-modal single-objective optimization, where niche techniques, e.g., the fitness sharing [3] and crowding [12] methods, are usually employed to diversify the solution set.

Up to now, there are only a few researches on multi-modal multi-objective evolutionary optimization. How to maintain diversity in both the objective and decision spaces is a crucial issue for evolutionary algorithms to solve multi-modal multi-objective optimization problems. In this paper, we propose a Double-Niched Evolutionary Algorithm (DNEA), in which the niche sharing method is adopted in both the objective and decision spaces. We compared the proposed DNEA with three state-of-the-art designs on polygon-based problems, where the performance of the achieved solution sets in the objective space can be visually examined in the decision space. Besides a basic type of the polygon-based problems, we also adopted two other types to further investigate and discuss the behaviors of the competing algorithms on multi-modal multi-objective optimization.

The remainder of this paper is organized as follows. In Section 2, the related works on multi-modal multi-objective optimization problems and techniques for diversity maintenance are reviewed for the completeness of the presentation. The proposed DNEA is then described in detail in Section 3. Section 4 presents the experimental results and relevant discussions. Section 5 concludes the paper and provides future research directions.

2 Related Works

2.1 Multi-modal Multi-objective Optimization Problems

As defined in [7] recently, a multi-modal multi-objective optimization problem has more than one Pareto optimal solution sets. In other word, there are at least two similar feasible regions in the decision space corresponding to the same region of the objective space. Later, [13] gave a simple real-world example in the path-planning problem. The traveling time and the number of transfer stations are two objectives in this example. There may exist two different paths that have the same objective values. In such a situation, if an optimizer can provide both of the paths, the decision maker will have more options for other considerations (e.g. gas station).

Actually, before the concept of multi-modal multi-objective optimization problems is proposed, there have been some researches on this topic. For instance, a map-based problem is proposed in [5], where the goal is find a location nearest to elementary school, junior-high school, convenience store, and railway station on a real-world map. Clearly, it is a four-objective optimization problem. Since the numbers of the aforementioned places are usually more than one on the map, there may exist several optimal locations that have the same objective values. In addition, a few real-world multi-objective optimization problems are also identified to multi-modal property in the literature [11].

In this study, we adopt the polygon-based problems [5] as test problems in the experiments. The polygon-based problems can be termed as an ideal version of the aforementioned map-based problems. The Pareto optimal sets of these problems are located in several regular polygons, which is relatively easy for investigating the behavior of an optimizer at the early stage of the research on multi-modal multi-objective optimization. Moreover, there have not been a widely accepted metric to simultaneously measure the convergence and diversity performances in both the objective and decision spaces of a solution set for multi-modal multi-objective optimization, whereas these performances in the polygon-based problems can be visually examined in a two-dimensional space. This is another important reason of adopting the polygon-based problems in this study.

2.2 Diversity Maintenance in the Objective and Decision Spaces

In early 70s and 80s, some classic niche techniques, e.g., the fitness sharing [3] and crowding [12] methods, have been proposed to manipulate the distribution of solutions in the decision space for multi-modal evolutionary optimization. In the fitness sharing method, individuals in the same neighborhood will degrade the fitness of each other, thereby discouraging the others occupying the same niche. In crowding methods, an offspring and its close parents compete with each other, and individuals with better fitness in the sparse areas are favored. There are a lot of other niche methods developed in the last two decades, e.g., clearing [10] and speciation [6]. However, all of above methods can only deal with single-objective optimization problems.

On the other hand, MOEA are developed to provide a diverse solution set in the objective space for multi-objective optimization. Non-dominated Sorting Genetic Algorithm II (NSGA-II) [1] is one of the most representative Pareto-based MOEAs. In NSGA-II, solutions with large crowding distances in the objective space are preferred in the environmental selection. Niched Pareto Genetic Algorithm (NPGA) [4] is another classic Pareto-based MOEA, where the fitness sharing method [3] is termed as the niche sharing method to promote diversity in the objective space. MOEA Based on Decomposition (MOEA/D) [14] is also found a promising alternative to solve multi-objective optimization problems. In MOEA/D, a number of scalarizing functions based on a set of well distributed reference vectors are used to guide the evolution. The diversity of solutions is ensured by the distribution of the reference vectors. In addition, indicator-based MOEAs [8, 15] and reference points-based MOEAs [9] are theoretically well-supported options.

There have been a few works on maintaining diversity in the decision space for multi-objective optimization. In [2], the Omni-optimizer was proposed by applying the crowding distance in the decision space. A decision space-based niching NSGA-II (DN-NSGA-II) in [7] was developed to search multiple Pareto optimal solution sets, which is similar to omni-optimizer. Very recently, a multi-objective particle swarm optimization algorithm with ring topology and special crowding distance [13] is proposed to obtain good distributions among the population.

In this paper, we propose a double-niched evolutionary algorithm for multi-modal multi-objective optimization. In the proposed algorithm, the niche sharing method is simultaneously employed for diversity maintenance in both the objective and decision spaces. We describe the proposed algorithm in detail in the next section.

3 A Double-Niched Evolutionary Algorithm

The general framework of DNEA is similar to other generational evolutionary algorithms. What makes DNEA special is its environmental selection operator, which is detailed in Algorithm 1.

Algorithm 1 Environmental Selection of DNEA

Require: N (population size), Q (candidate solution set), σ_{obj} (niche radius in the objective space), σ_{var} (niche radius in the decision space)

1: $F = F_1 \cup F_2 \cup ...F_k =$ *Nondominated_sort* (Q)
2: $P = F_1 \cup F_2 \cup ...F_{k-1}$
3: $N' = N - |P|$
4: **while** $|F_k| > N'$ **do**
5:     **for all** $\boldsymbol{x}_i \in F_k$ **do**
6:         calculate $f_{DS}(\boldsymbol{x}_i)$ according to σ_{obj} and σ_{var}
7:     **end for**
8:     $\boldsymbol{x}_{\max} = \arg \max_{\boldsymbol{x}_i \in F_k} f_{DS}(\boldsymbol{x}_i)$
9:     $F_k = F_k / \{\boldsymbol{x}_{\max}\}$
10: **end while**
11: $P = P \cup F_k$
12: **return** P

In Algorithm 1, the solutions in the candidate solution set, Q, are first sorted to form several nondominated fronts, $F_1 \cup F_2 \cup ...F_k$, where k in F_k is the minimal value such that $|F_1| + |F_2| + ...|F_k| > N$ (N is the population size) (Line 1). This procedure is similar to that in NSGA-II [1]. Then, the first F_{k-1} nondominated fronts are combined into the new population, P (Line 2). $N' = N - |P|$ is the number of solutions remain to be chosen into P (Line 3). While $|F_k| > N'$, the double-sharing function, f_{DS}, of each solution in F_k is calculated as follows (Line

6):

$$f_{DS}(\boldsymbol{x}_i) = \sum_{\boldsymbol{x}_j \in F_k} Sh_{\mathrm{obj}}(i,j) + Sh_{\mathrm{var}}(i,j) \quad (1)$$

In this formulation, $Sh_{\mathrm{obj}}(i,j) = \max\{0, 1 - d_{\mathrm{obj}}(i,j)/\sigma_{\mathrm{obj}}\}$ and $Sh_{\mathrm{var}}(i,j) = \max\{0, 1 - d_{\mathrm{var}}(i,j)/\sigma_{\mathrm{var}}\}$, where $d_{\mathrm{obj}}(i,j)$ and σ_{obj} are the Euclidean distance between $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ and the niche radius in the objective space, respectively, and $d_{\mathrm{var}}(i,j)$ and σ_{var} have the similar meanings in the decision space. Then, the solution with the maximum value of the double-sharing function, $\boldsymbol{x}_{\max}$, is deleted from F_k (Line 9). Finally, the remaining solutions in F_k (where $|F_k| = N'$) are merged into P (Line 11).

Note that the settings of σ_{obj} and σ_{var} are non-trivial. Generally, the higher dimension of the objective (decision) space and the smaller population size, the larger value of σ_{obj} (σ_{var}). If σ_{obj} (σ_{var}) is too large (e.g. larger than the distance between any pair of solutions), boundary solutions are more likely to be selected. Conversely, if σ_{obj} (σ_{var}) is too small (e.g. smaller than the distance between any pair of solutions), then the solutions to be discarded are selected at random as the double-sharing function would assign zero to every solution. In both of the above situations, the algorithm would encounter diversity maintenance issues. In this study, since it is easy to choose the above values for polygon-based problems, we handle them as pre-specified fixed parameters. Developing a method to adaptively tune σ_{obj} and σ_{var} is an interesting future work.

It can be seen from Algorithm 1 and Eq. (1) that solutions located in sparse regions either in the objective space or in the decision space are preferred. A solution that is very close to others in the objective (decision) space but far away from others in the decision (objective) space still has a chance to be selected. This means that DNEA has a great potential to maintain diversity in both the objective and decision spaces.

In the following section, we investigate the performance of DNEA on the polygon-based problems to demonstrate its effectiveness. We also test two variants of DNEA as competing algorithms. The first is termed as $\mathrm{DNEA}_{\mathrm{obj}}$, where any Sh_{var} is set to zero. This means that $\mathrm{DNEA}_{\mathrm{obj}}$ only has the ability to maintain diversity in the objective space. In this situation, $\mathrm{DNEA}_{\mathrm{obj}}$ is almost equal to NPGA. Conversely, setting Sh_{obj} to zero, the second is termed as $\mathrm{DNEA}_{\mathrm{var}}$, which only focuses on diversity in the decision space.

4 Experiments

In this section, three types of polygon-based problems are first introduced. Then, the competing algorithms and the parameter settings are given. Finally, the performance of the competing algorithms are empirically evaluated and discussed.

4.1 Polygon-Based Problems

We adopt three types of polygon-based problems with 3 and 4 objectives in the experiments. There are four polygons in each problem. The details of them are described as follows.

Type I: The first type is a very basic one, where all the polygons have the same shape and size. The vertexes of triangles in the 3-objective problem of Type I are

$$\{A_1 = (20, 30), B_1 = (30, 10), C_1 = (10, 10),\\ A_2 = (80, 30), B_2 = (90, 10), C_2 = (70, 10),\\ A_3 = (80, 90), B_3 = (90, 70), C_3 = (70, 70),\\ A_4 = (20, 90), B_4 = (30, 70), C_4 = (10, 70)\}.$$

$A_iB_iC_i$, $i = 1, 2, 3, 4$ is the ith triangle. The three objectives to be minimized are formulated as follows:

$$\begin{aligned} f_1(\boldsymbol{x}) &= \min\{d(\boldsymbol{x}, A_i), i = 1, 2, 3, 4\} \\ f_2(\boldsymbol{x}) &= \min\{d(\boldsymbol{x}, B_i), i = 1, 2, 3, 4\} \\ f_3(\boldsymbol{x}) &= \min\{d(\boldsymbol{x}, C_i), i = 1, 2, 3, 4\} \end{aligned} \quad (2)$$

where $d(\boldsymbol{x}, X)$ is the Euclidean distance from a solution $\boldsymbol{x}$ to X (X is a vertex) in the decision space. Similarly, the objectives of the 4-objective problem of Type I can be defined. There are four rectangles with size of 20×20 in the 4-objective problem. Each polygon in these problems is a Pareto optimal region, and all the regions are mapped to the same Pareto front. Finding a uniformly distributed solution set in a polygon will lead to a well distributed approximate Pareto front.

Type II: The vertexes of polygons in Type II are the same as those in Type I. The difference is that $d(\boldsymbol{x}, X)$ is transformed into $d(\boldsymbol{x}, X)^{0.01}$ in the objectives in Type II. By such transformation, uniformly distributed solutions in the objective space are actually nonuniformly distributed in the decision space, and vice versa. By using the problems in Type II, we intend to investigate the behavior of each competing algorithm when the diversities in the objective and decision spaces are inconsistent.

Type III: For the problems in Type III, the size of polygons sequentially increases. To be specific, the vertexes of triangles in the 3-objective problem in Type III are

$$\{A_1 = (20, 30), B_1 = (30, 10), C_1 = (10, 10),\\ A_2 = (80, 30.02), B_2 = (90.01, 10), C_2 = (69.99, 10),\\ A_3 = (80, 90.2), B_3 = (90.1, 70), C_3 = (69.9, 70),\\ A_4 = (20, 92), B_4 = (31, 70), C_4 = (9, 70)\}.$$

The vertexes in the 4-objective problem are

$$\{A_1 = (10, 30), B_1 = (30, 30), C_1 = (30, 10), D_1 = (10, 10),\\ A_2 = (69.99, 30.01), B_2 = (90.01, 30.01), C_2 = (90.01, 9.99), D_2 = (69.99, 9.99),\\ A_3 = (69.9, 90.1), B_3 = (90.1, 90.1), C_3 = (90.1, 69.9), D_3 = (69.9, 69.9),\\ A_4 = (9, 91), B_4 = (31, 91), C_4 = (31, 69), D_4 = (9, 69)\}.$$

For the problems in Type III, only the first polygon is the true Pareto optimal region and all the other polygons are local optimal regions. This means that any solution located in the other polygons is dominated by a solution in the first polygon. By testing each competing algorithm on the problems in Type III, we expect to observe that whether the algorithm is trapped into the local optimal regions while maintaining diversity in the decision space.

4.2 Competing Algorithms and Parameter Settings

Besides the proposed DNEA and its two variants, DNEA_{obj} and DNEA_{var}, we applied three other algorithms, i.e., DN-NSGA-II, NSGA-II, and MOEA/D, to each test problem 30 times using the following specifications:

- Population size: 210 and 220 for 3- and 4-objective problems, respectively
- Population initialization: random values in $[0, 100]$ for each decision variable
- Termination condition: 300 generations
- Crossover probability: 1.0 (SBX with $\eta_c = 20$)
- Mutation probability: 0.5 (Polynomial mutation with $m = 20$)
- Niche radius in DNEA and its variants: $\sigma_{\text{obj}} = 0.06$ and $\sigma_{\text{var}} = 0.02$
- Neighborhood size in MOEA/D: 10% of the population size
- Crowding factor in DN-NSGA-II: half of the population size

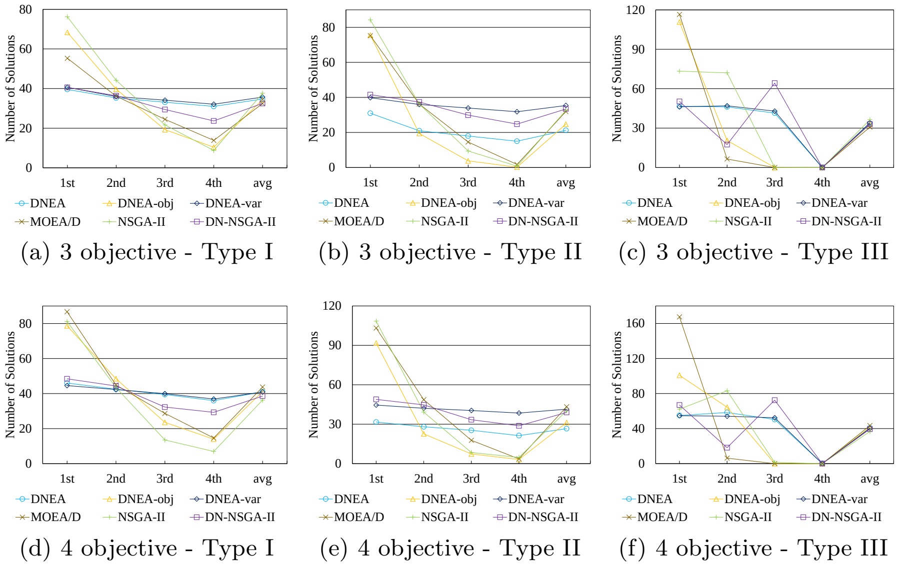
It is interesting to note that the competing algorithms can be classified into three categories. The first one is DNEA, which is designed to maintain diversity in both the objective and decision spaces. The second one includes DNEA_{obj} and the classic multi-objective optimizers, i.e., NSGA-II and MOEA/D. They only focus on diversity maintenance in the objective space. On the contrary, DNEA_{var} and DN-NSGA-II fall into the third one.

4.3 Results and Discussions

In this part, the performances of the competing algorithms are evaluated and discussed on the three types of polygon-based problems.

Results on Type I: In Fig. 1, we show the average number of solutions in the Pareto optimal regions achieved by each competing algorithms over 30 runs. In Fig.1(a), (b), (d) and (e), '1st' represents the average number of solutions in the polygon which contains the most solutions in each run. '2nd' represents that in the polygon which contains the second most solutions, and '3rd' and '4th' have the similar meanings. 'avg' indicates the average number of solutions in all the four polygons. Fig. 2 shows the final solution sets of each algorithm in a typical run in the decision space. In the typical run, the number of solutions in each polygon is the nearest to the average number over 30 runs. Note that the results in most other runs are similar to the typical one.

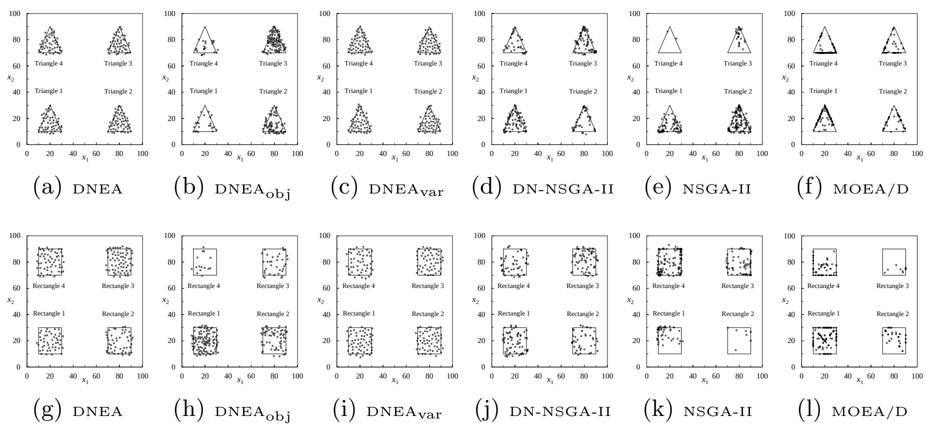
From Fig. 1(a) and (d), we can see that the difference between '1st' and '4th' obtained by DNEA_{obj}, NSGA-II, and MOEA/D is larger than the others, which means that most of the solutions achieved by these algorithms concentrate on one or two polygons. This can be also visually observed from the distribution of solutions in the decision space in Fig. 2. Thus, DNEA_{obj}, NSGA-II, and MOEA/D fail to get multiple Pareto optimal solution sets. On the other hand, the difference between '1st' and '4th' obtained by DNEA, DNEA_{var}, and DN-NSGA-II in Fig. 1 are relatively small. This suggests that the solutions are almost equally assigned to each polygon, which can be also observed in Fig. 2. From these observations, we can conclude that DNEA, DNEA_{var}, and DN-NSGA-II have a good ability to maintain diversity in the decision space. It is worth noting



(a) 3 objective - Type I (b) 3 objective - Type II (c) 3 objective - Type III

(d) 4 objective - Type I (e) 4 objective - Type II (f) 4 objective - Type III

Fig. 1. The average number of solutions in each polygon.



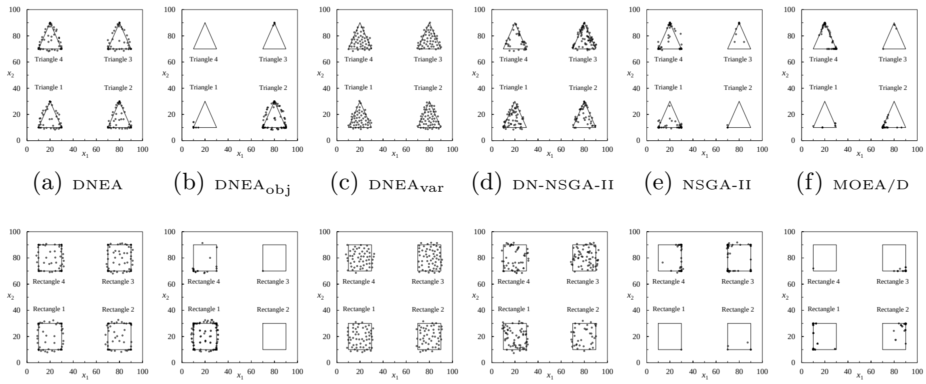
(a) DNEA (b) DNEA_{obj} (c) DNEA_{var} (d) DN-NSGA-II (e) NSGA-II (f) MOEA/D

(g) DNEA (h) DNEA_{obj} (i) DNEA_{var} (j) DN-NSGA-II (k) NSGA-II (l) MOEA/D

Fig. 2. The final solution sets in the decision space on the polygon-based problem in Type I (a-f and g-l show the results on the 3- and 4-objective problems, respectively).

that the difference between "1st" and "4th" of DN-NSGA-II is a bit larger than DNEA and DNEA_{var} in Fig. 1(a) and (d), and the distribution of solutions of DN-NSGA-II is not as good as those of DNEA and DNEA_{var} in Fig. 2. This indicates that the niche sharing method could perform better than the crowding distance method in maintaining diversity.

Results on Type II: Similar to Fig. 2, Fig. 3 shows the results of each competing algorithm on the polygon-based problems in Type II.



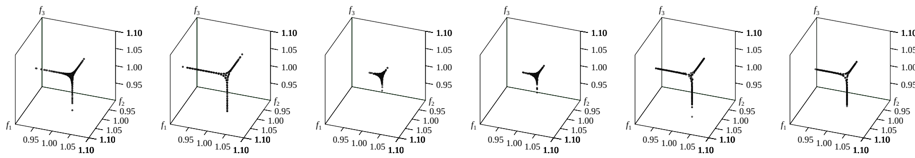
(a) DNEA (b) DNEA_{obj} (c) DNEA_{var} (d) DN-NSGA-II (e) NSGA-II (f) MOEA/D

(g) DNEA (h) DNEA_{obj} (i) DNEA_{var} (j) DN-NSGA-II (k) NSGA-II (l) MOEA/D

Fig. 3. The final solution sets in the decision space on the polygon-based problem in Type II (a-f and g-l show the results on the 3- and 4-objective problems, respectively).

The results in Fig. 1(b) and (e) are similar to those in Fig. 1(a) and (d), however, the average numbers of solutions in the polygons achieved by DNEA and DNEA_{obj} are smaller than the others. We speculate that the reason is the deterioration of the convergence ability for the complicated Pareto fronts by the enhancement of the diversification ability in those algorithms. From Fig. 3, we can see that only DNEA find all vertexes of all polygons. The solutions achieved by DNEA_{obj}, NSGA-II, and MOEA/D only concentrate on several vertexes due to the same reason when handling with the problems in Type I. The behaviors of DNEA_{var} and DN-NSGA-II are much the same as those in Fig. 2, since they only consider diversity in the decision space.

For further investigation, we show the non-dominated solutions in the objective space obtained by each algorithm on the 3-objective problem in the typical run in Fig. 4. It can be seen from Fig. 4 that the solutions obtained by DNEA_{var} and DN-NSGA-II focus on small areas. This observation suggests that they cannot maintain a good diversity in the objective space for the problems in Type II, although the distribution of their solutions looks uniform in the decision space in Fig. 3. The solutions obtained by DNEA, DNEA_{obj}, NSGA-II, and MOEA/D are widely spread in the objective space. However, as we have observed in Fig. 3, only DNEA can achieve solution sets with large diversity in the decision space. Similar results can be also observed on the 4-objective problem, where they are not presented due to space limits.



(a) DNEA (b) DNEA_{obj} (c) DNEA_{var} (d) DN-NSGA-II (e) NSGA-II (f) MOEA/D

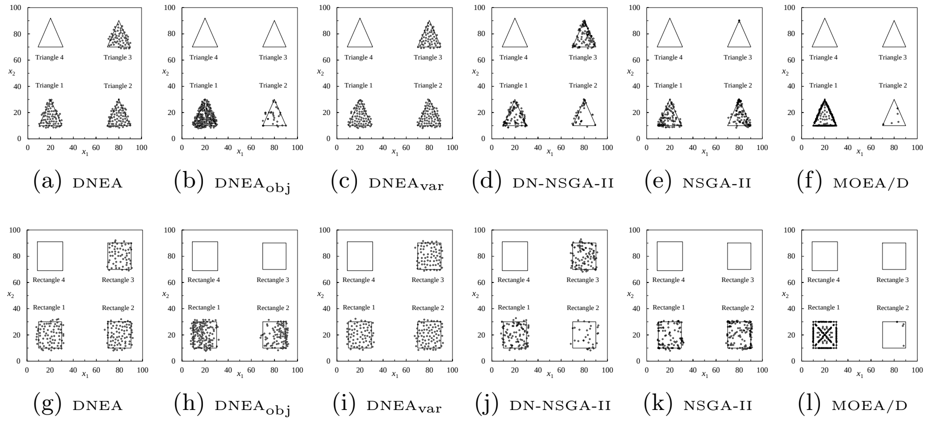
Fig. 4. The Pareto fronts on the 3-objective polygon-based problem in Type II shown by the 3D coordinates.

From the above-mentioned observations, we can conclude that maintaining diversity in both the objective and decision spaces is necessary for solving the problems in Type II. This motivates us to think that when the requirements of diversity in the objective and decision spaces are conflict, should we consider them equally, or make a trade-off between them? The proposed DNEA in this study belongs to the former way. Developing methods in the latter way will be a interesting future work.

Results on Type III: In the same manner as in the previous two subsections, the results on the polygon-based problems in Type III are shown in Figs. 1(c) and (f) and 5. The meaning of the results in Fig. 1(c) and (f) is a little different from those in Figs. 1(a), (b), (d), and (e). In Fig. 1(c) and (f), '1st', '2nd', '3rd', and '4th' indicate the first, second, third, and fourth polygon, respectively (only the first polygon is the true Pareto optimal solution set). Since the polygons in the Type III problems have different sizes, it is better to count the solutions in each polygon separately.

It can be seen from Figs. 1(c) and (f) and 5 that most of the solutions achieved by DNEA_{obj}, NSGA-II, and MOEA/D locate in the first and second polygons. Especially, almost all of the solutions achieved by MOEA/D are in the first polygon. The reason is that the scarlarizing function employed in MOEA/D provides a much larger selection pressure towards the Pareto front than the Pareto dominance criterion used in the other algorithms. The behaviors of DNEA and DNEA_{var} are nearly the same, where the solutions are equally assigned to the first three polygons. The solutions achieved by DN-NSGA-II also locate in the first three polygons, however, the number of solutions in the second polygon is smaller than those in the first and third polygons for unknown reason.

These observations indicate that maintaining diversity in the decision space can lead to more solutions in the local optimal areas than that in the objective space. However, such algorithms like DNEA, DNEA_{var}, and DN-NSGA-II are not trapped in these local optimal areas. They can also provide a well-distributed



(a) DNEA (b) DNEA_{obj} (c) DNEA_{var} (d) DN-NSGA-II (e) NSGA-II (f) MOEA/D

(g) DNEA (h) DNEA_{obj} (i) DNEA_{var} (j) DN-NSGA-II (k) NSGA-II (l) MOEA/D

Fig. 5. The final solution sets in the decision space on the polygon-based problem in Type III (a-f and g-l show the results on the 3- and 4-objective problems, respectively).

Pareto optimal solution set in the first polygon (i.e., the true Pareto optimal solution set). The question is that whether the solutions in the local optimal areas are necessary in a real-world application. If such solutions are actually needed for the decision maker, how to achieve them is another question. For example, the solutions in the fourth polygon may be needed in some situations, however, none of the algorithms can achieve them. Controlling the number of solutions in each local optimal region is another interesting future work.

5 Conclusions

In this paper, we proposed a double-niched evolutionary algorithm, i.e., DNEA, for multi-modal multi-objective optimization. In DNEA, a double sharing function is employed to estimate the density of a solution in both the objective and decision spaces. We introduced three types of polygon-based problems and applied DNEA, its variants, DN-NSGA-II, NSGA-II, and MOEA/D to them. In computational experiments, we have the following observations: (1) Diversity maintenance in the decision space is necessary to find multiple Pareto optimal solution sets. (2) Diversities in the objective and decision spaces should be simultaneously considered if they are inconsistent. (3) Promoting diversity in the decision space leads to more solutions in local Pareto optimal regions. Besides the future works mentioned in Subsection 4.3, balance between convergence and diversity in the decision space is certainly interesting for our future research.

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