Multimodal multi-objective optimization: A preliminary study

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Multimodal Multi-objective Optimization: A Preliminary Study

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***Abstract*—In real world applications, there are many multi-objective optimization problems. Most existing multi-objective optimization algorithms focus on improving the diversity, spread and convergence of the solutions in the objective space. Few works study the distribution of solutions in the decision space. In practical applications, some multi-objective problems have different Pareto sets with the same objective values and these problems are defined as multimodal multi-objective optimization problems. It is of great significance to provide all the Pareto sets for the decision maker. This paper describes the concept of multimodal multi-objective optimization problems in detail. Novel test functions are also designed to judge the performance of different algorithms. Moreover, some existing multi-objective algorithms are tested and compared. Finally, a decision space based niching multi-objective evolutionary algorithm is proposed to solve these problems. The experimental results suggest that existing multi-objective optimization algorithms fail to find all the Pareto sets while the proposed algorithm is able to find almost all the Pareto sets without deteriorating the distribution of solutions in the objective space.**

Keywords—Evolutionary algorithms; multimodal multi-objective optimization; niching

I. Introduction

Many optimization problems have two or more conflicting optimization objectives. Improvement of one objective will always lead to deterioration of the other objectives. These problems are usually called Multi-objective Optimization Problems (MOPs). It is impossible to find the best values of all objectives simultaneously. The multi-objective optimization algorithms try to find the best trade-off among different objectives. Instead of finding one single solution, MOPs need locating a set of non-dominated solutions. These solutions spread along the Pareto optimal tradeoff surface to provide more choices for decision makers. However, few multi-objective optimization algorithms focus on the distribution of solutions in decision space.

The decision space diversity has attracted several researchers' attention. Shir [1] changed the selection operator and diversity measure in CMA-ES [2] to enhance decision space diversity. Tahernezhad [3] adopted the innovative clustering-based scheme during the optimization cycle to obtain more diverse non-dominated vectors in the solution space. Ulrich [4] integrated decision space diversity into the hypervolume indicator so that these two set measures could be optimized simultaneously. Chan [5] applied Lebesgue Contribution and Neighbourhood Count on the evolutionary algorithm framework to maintain diversity in the parametric and the objective space. However, it is not enough only considering the diversity in decision space. These algorithms aims to improve the distribution of the obtained Pareto solutions by considering the diversity in the decision space, but do not intend to keep the solutions with the same objective values that have different decision values. In fact, the diversity and convergence of solutions in decision space should be considered simultaneously.

We try to introduce the niching method [6] into Multi-Objective Evolutionary Algorithm [7] to maintain different solutions corresponding to the same Pareto front point. Since there are too many Multi-Objective Evolutionary Algorithms, we take the NSGAII [8] as an example and design a decision space based niching NSGAII (DN-NSGAII) to solve this problem.

Niching methods allow solutions to evolve within local space. The first niching method was proposed by Cavicchio [9]. Subsequently other niching methods, such as crowding [10], fitness sharing [11], clearing [12] and speciation [13] were proposed. Niching methods promote the formation of sub-populations and maintain them. They are widely used in single objective multimodal problems. Qu [14] proposed distance based neighborhood differential evolution to solve single objective multimodal problems. Ring-topology based PSO was introduced by Li [15]. When niching methods are used in multi-objective optimization, they aim to enhance the diversity in objective space [16]. Niching methods were applied to multi-objective optimization by Hom [17] to spread its population out along the Pareto optimal tradeoff surface.

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However they are not used to maintain different solutions in decision space.

The rest of this paper is organized as follows. Section II introduces some multi-objective optimization definitions. The multimodal multi-objective optimization is described in detail in Section III with two novel test functions and one new indicator. A decision space based niching Multi-Objective Evolutionary Algorithm is proposed in Section IV. Section V presents the simulation results and discussions. Finally, the paper is concluded in Section VI.

II. MULTI-OBJECTIVE OPTIMIZATION

A. Multi-objective optimization

Without loss of generality, a multi-objective problem with n-dimensional decision variable vectors and m objectives can be defined as follows:

$$\begin{cases} \min \ \mathbf{y} = F(\mathbf{x}) = (f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_m(\mathbf{x})) \\ \text{s.t.} \quad g_i(\mathbf{x}) \le 0, \ i = 1, 2, \ldots, k \\ \qquad h_j(\mathbf{x}) = 0, \ j = 1, 2, \ldots, l \end{cases} \tag{1}$$

where $\boldsymbol{x} = (x_1, x_2 \ldots, x_n) \in \boldsymbol{X} \subset \boldsymbol{R}^n$ is n-dimensional decision vector; $\boldsymbol{X}$ is n-dimensional decision space; $\boldsymbol{y} = (y_1, y_2 \ldots, y_m) \in \boldsymbol{Y} \subset \boldsymbol{R}^m$ is m-dimensional objective vector; $\boldsymbol{Y}$ is m-dimensional objective space; $F(\boldsymbol{x})$ defines m functions mapping $\boldsymbol{X}$ to $\boldsymbol{Y}$. $g_i(\boldsymbol{x}) \le 0 (i = 1,2,\ldots,k)$ defines k inequality constraints; $h_i(\boldsymbol{x}) = 0 (j = 1,2,\ldots,l)$ defines l equality constraints.

B. Pareto set and Pareto front

Unlike single-objective optimization, it is hard to decide which solution is the best one in multi-objective optimization. Dominate relationship [18] is generally used when comparing different solutions of multi-objective optimization problems. Take minimization multi-objective optimization problem as an example, a feasible solution x_1 is said to dominate another feasible solution x_2 ($x_1 \succ x_2$), if and only if, $f_i(x_1) \le f_i(x_2)$ for $i = 1, \ldots, m$ and $f_j(x_1) < f_j(x_2)$ for at least one $j \in \{1, \ldots, m\}$. Non-dominated solutions are the feasible solutions which are not dominated by any other solution. In decision space the set of non-dominated solutions is called Pareto optimal Set (PS). In objective space, the set of points corresponding to PS is called Pareto Front (PF).

III. MULTIMODAL MULTI-OBJECTIVE OPTIMIZATION

There are many multi-objective optimization problems which have more than one Pareto set. In other word, there are at least two similar feasible regions in the decision space corresponding to the same region of the objective space. These problems can be defined as multimodal multi-objective optimization problems. As shown in Fig. 1, the same shape dots in the decision space correspond to the same shape points in the objective area. For example, the two pentagrams in decision space (the left coordinate system) correspond to the same pentagram in objective space (the right coordinate system). It is a new challenge to find all the Pareto optimal solutions in decision space simultaneously.

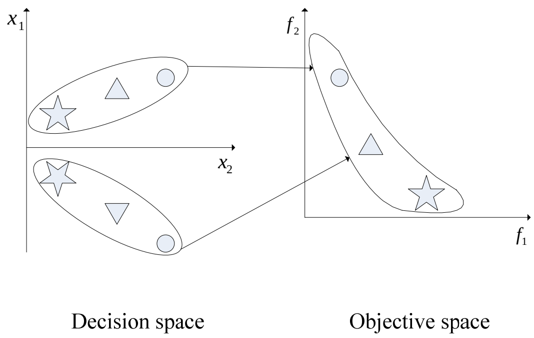


Fig 1. Multimodal multi-objective optimization problem

A. Difficulty analysis

Different solutions which correspond to the same point in objective space are difficult to maintain simultaneously. If one of the solutions in decision space has been obtained, the others are hard to be maintained. This situation is shown in Fig. 2. Both A_1 and A_2 in the decision space correspond to A' in the objective space. If we have obtained the solution A_1 in the decision space. A_2 has the same objective value with A_1. Assume that B is obtained in decision space, and B' is the point in objective space corresponding to B. The distance d_2 between A' and B' is too small. That is, A_1 and B are too crowded in the objective space. In the traditional multi-objective optimization algorithms, B will be deleted. However, in the decision space the distance d_1 between A_1 and B is relatively large. They are not crowded in the decision space. If we want to obtain both A_1 and A_2 at the same time, B should not be deleted. Solutions which are close to each other in the objective space may be far away from each other in the decision space.

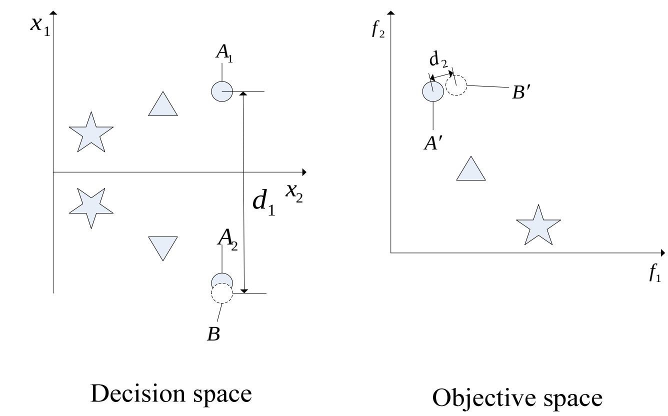


Fig 2. Difficulty to obtain all the Pareto sets

Considering only the distribution in decision space may obtain an incomplete PF. As mentioned above, if all the Pareto optimal solutions in decision space are wanted, the crowding distance in objective space should not be an indicator when creating mating pool. However, without this indicator, the diversity in objective space may be terrible. We want to obtain all the Pareto optimal solutions in decision space with high quality of obtained PF in objective space. It is not easy to consider the distribution in both decision and objective space simultaneously.

B. *Design of test functions*

Test functions have great significance for the theoretical research of the algorithm. They should be designed to simulate the real world application problems. There are several existing test functions to test the algorithmic ability to obtain diversified solutions in the decision space, such as Omni [19], EBN [20], Two-on-one [21], Superspheres [22] and so on. However, they are not consistent with the problem proposed in this paper. Therefore, new test functions are designed to test the algorithms' performance.

Without loss of generality, two bi-objective functions with two distinct Pareto sets are proposed. These two functions are constructed based on UF1 and UF3 [23] by the point symmetry and shift.

The design procedure of test function1 is as follows. The feasible solutions of the original function UF1 exist in space $0 \le x_1 \le 1$, $-1 \le x_2 \le 1$. First of all, though the symmetric extension of feasible region with $x_2 = 0$ as the axis of symmetry, feasible solutions exist in both $0 \le x_1 \le 1$, $-1 \le x_2 \le 1$ and $-1 \le x_1 \le 1$, $-1 \le x_2 \le 1$. For the scale of generality, the axis of symmetry is shifted from $x_2 = 0$ to $x_2 = 2$. Test function1 is named SS-UF1, which means symmetric and shifted UF1. More information about SS-UF1 is shown as follows.

SS-UF1

$$\begin{cases} f_1 = |x_1 - 2| \\ f_2 = 1 - \sqrt{|x_1 - 2|} + 2*(x_2 - \sin(6*\pi*|x_1 - 2| + \pi))^2 \end{cases} \tag{2}$$

where $1 \le x_1 \le 3$, $-1 \le x_2 \le 1$.

Its true PS is

$$\begin{cases} x_1 = x_1 \\ x_2 = \sin(6*\pi*|x_1 - 2| + \pi) \end{cases} \tag{3}$$

where $1 \le x_1 \le 3$.

Its true PF is

$$f_2 = 1 - \sqrt{f_1} \tag{4}$$

where $0 \le f_1 \le 1$.

Its true PS and PF are illustrated in Fig. 3.

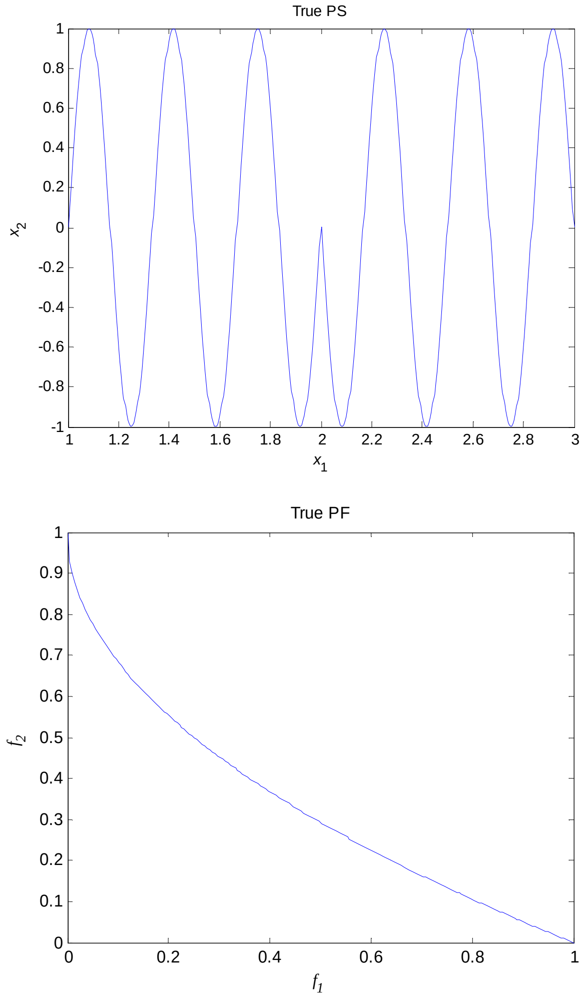


Fig. 3 Illustration of the true PS and PF of SS-UF1

The design procedure of test function 2 is as follows. The feasible solutions of the original function UF3 exist in $0 \le x_1 \le 1$, $0 \le x_2 \le 1$. Firstly, shift the feasible solutions two units to the positive direction of x_2 and maintain the original feasible solutions. In this way, feasible solutions exist in both $0 \le x_1 \le 1$, $0 \le x_2 \le 1$ and $0 \le x_1 \le 1$, $1 \le x_2 \le 2$. Test function2 is named S-UF3, which means shifted UF3. More information about S-UF3 is shown as follows.

$$
\begin{cases}
f_1 = x_1 \\
f_2 = \begin{cases}
1-\sqrt{x_1}+2*(4*(x_2-\sqrt{x_1})^2-2*\cos(\dfrac{20*(x_2-\sqrt{x_1})*\pi}{\sqrt{2}})+2)^2 & 0 \le x_2 \le 1 \\
1-\sqrt{x_1}+2*(4*(x_2-1-\sqrt{x_1})^2-2*\cos(\dfrac{20*(x_2-1-\sqrt{x_1})*\pi}{\sqrt{2}})+2)^2 & 1 < x_2 \le 2
\end{cases}
\end{cases}
\tag{5}
$$

where $0 \le x_1 \le 1$, $0 \le x_2 \le 2$.

Its true PS is

$$
\begin{cases}
x_2 = x_2 \\
x_1 = \begin{cases}
x_2^2 & 0 \le x_1 \le 1 \\
(x_2-1)^2 & 0 \le x_2 \le 2
\end{cases}
\end{cases}
\tag{6}
$$

Its true PF is

$$
f_2 = 1-\sqrt{f_1} \tag{7}
$$

where $0 \le f_1 \le 1$.

Its true PS and PF are illustrated in Fig. 4.

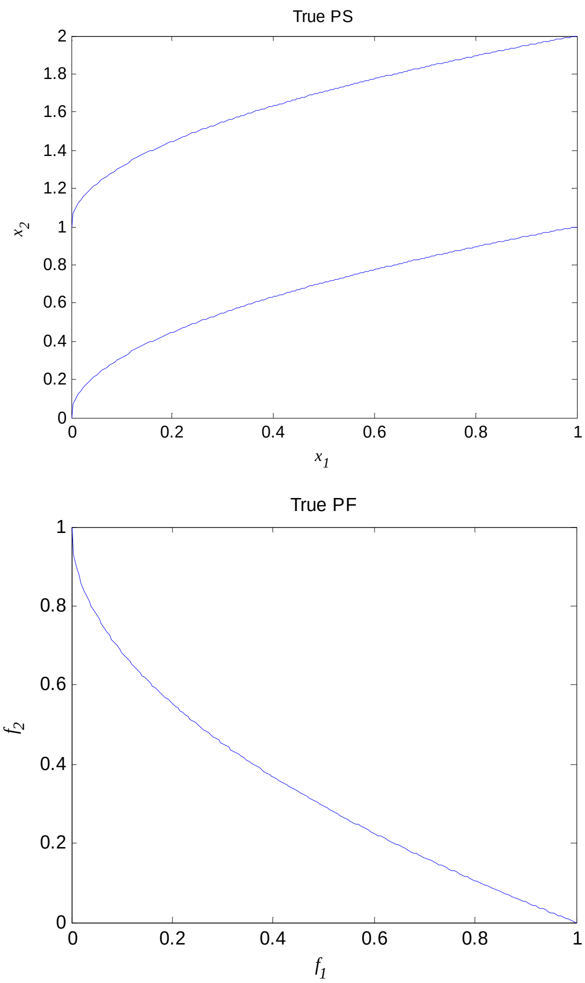
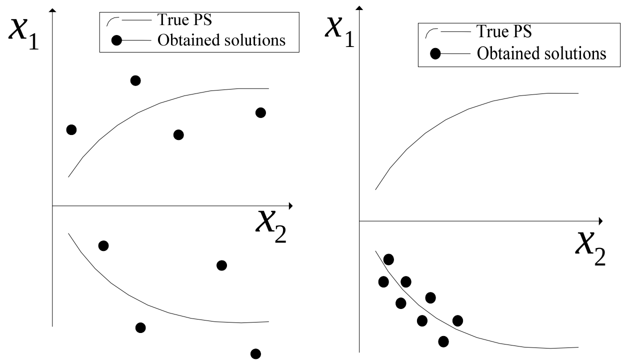


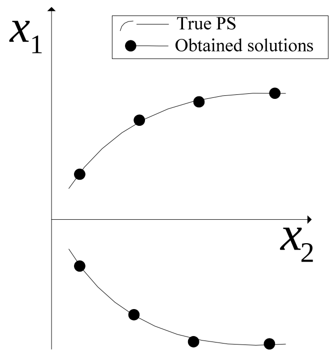
Fig. 4 Illustration of the true PS and PF of S-UF3

C. The indicator used to measure the qulity of obtained solurtions in the decision space

The indicator used to measure different algorithms should reflect both the diversity and the convergence in decision space. Most researchers only adopt the diversity indicator in decision space. However, the diversity in decision space doesn't guarantee their convergence to the true PS. This situation is shown in Fig. 5 (a), the diversity of obtained solutions is good, but the convergence of obtained solutions is poor. In this way, it is unreasonable to judge algorithms only by diversity in the decision space. Similarly, it is also unreasonable to judge algorithms simply by the convergence of their obtained solutions in the decision space (Fig. 5 (b)). The solutions we except to obtain should have both good diversity and convergence, which is shown in Fig. 5 (c). Therefore, both the diversity and the convergence of their obtained solutions should be considered.



(a) Good diversity poor convergence (b) Poor diversity good convergence



(c) Good diversity good convergence

Fig. 5 Diversity and convergence in the decision space

In this paper, we use Inverse Generational Distance (IGD) in decision space to judge obtained solutions. IGD is originally used in objective space to measure the distribution of obtained Pareto front points. IGD values represent the average distance (Euclidean distance) between the obtained solutions and reference solutions (true PF) in objective space. And a new indicator in the decision space (IGDX) is proposed by Zhou [24] to evaluate the diversity and convergence in the decision space. IGDX values represent the average distance (Euclidean distance) between the obtained solutions and reference solutions (true PS) in decision space. Let P^* denote a set of uniformly distributed points along the PS (in the decision space). Let O denote a set of obtained solutions, the IGDX can be calculated as the average distance from P^* to O:

$$IGDX(O,P^*) = \frac{\sum_{v\in P^*} d(v,O)}{\left|P^*\right|} \tag{8}$$

where $d(v,O)$ is the minimum Euclidean distance between v and the points in O. If P^* represents the PS well enough, IGDX can measure both the diversity and convergence in the decision space. A smaller IGDX value means the obtained solutions are closer to the true PS. As is shown in Fig. 6, the obtained solutions in (a) is closer to the reference PS than those in (b) and the IGDX of (a) is smaller than that of (b).

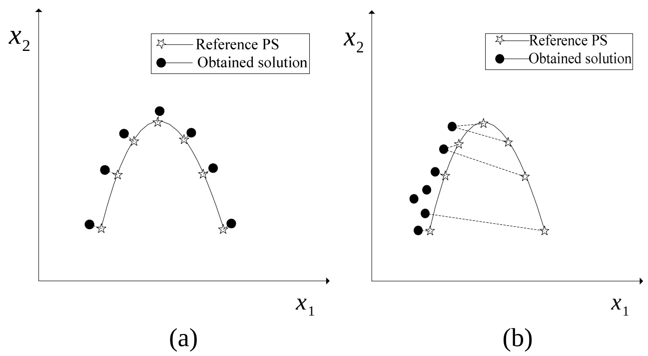


Fig. 6 Illustration of the IGDX

IV. Decision space based niching Multi-Objective Evolutionary Algorithm

In order to solve the multimodal multi-objective optimization problems, a decision space based niching method is proposed to be integrated into multi-objective evolutionary algorithms. Since the NSGAII [8] proposed by Deb is one of the most common used multi-objective evolutionary algorithms, we take it as an example in this paper. A fast nondominated sorting method is used to reduce the computational complexity. Besides, a selection operator is presented to select the best (with respect to fitness and spread in objective space) solutions. Is the NSGAII able to find all the PSs of problems proposed in this paper? It is tested on the test functions designed in Section III-C. The result is shown in Fig. 7. It is obvious that NSGAII cannot find all the Pareto optimal solutions. The reason is that the algorithm always delete crowded solutions in the objective space like B in the Fig. 2. It cannot obtain solutions like A_1 and A_2 simultaneously.

To maintain all the Pareto optimal solutions, two improvements are made. Firstly, niching method is used to create the mating pool. Secondly, selection operator is modified.

Niching method is used to create the mating pool. Only solutions in the same niche compete with each other. In this paper, crowding method [25] is used. The procedure to create the mating pool is described as follows. Firstly, a solution is randomly chosen from the population. Secondly, a constant number (crowding factor (CF)) of solutions are randomly selected in the left population. Thirdly, the distances (Euclidean distance) between the current solution and CF solutions are calculated and the closest one to the current solution is selected. Finally, add the superior one of the two solutions (current solution and the closest solution) to the mating pool. Repeat the four steps until the mating pool is full. Since the distance is calculated in the decision space, we call it decision space based niching NSGAII.

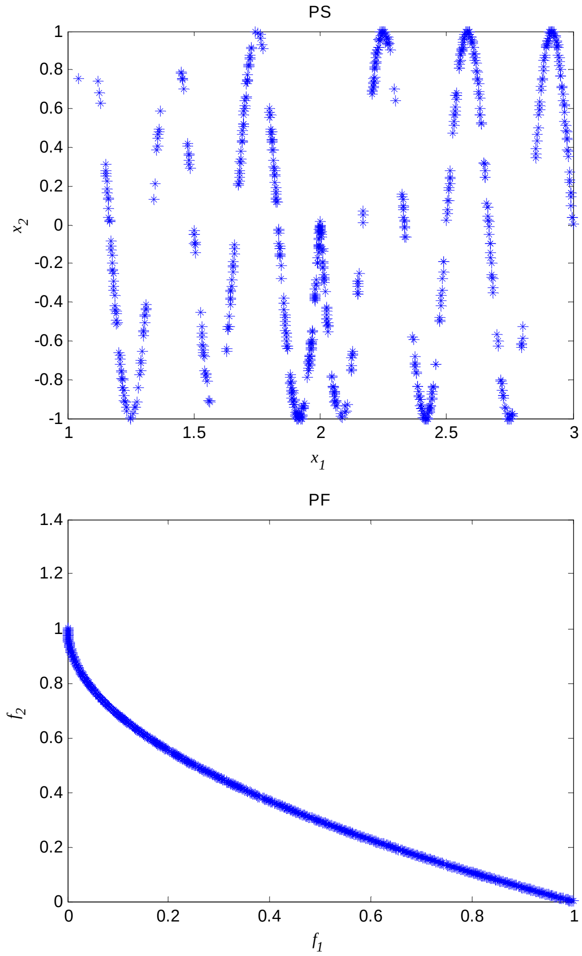


Fig. 7 The obtained PS and PF of NSGAII for SS_UF1

The original NSGAII selects solutions with respect to the nondominated sorting and the crowding in objective space. As it is analyzed above, the crowding in the objective space should not be considered to maintain different solutions corresponding to the same point in the objective space. The crowding in objective space is replaced with crowding in decision space.

The DN-NSGAII can find much more Pareto optimal solutions than NSGAII. We test it on SS_UF1. The result is shown in Fig. 8. Comparing Fig. 7 with Fig. 8, the obtained PS by DN-NSGAII is obviously better than the original NSGAII.

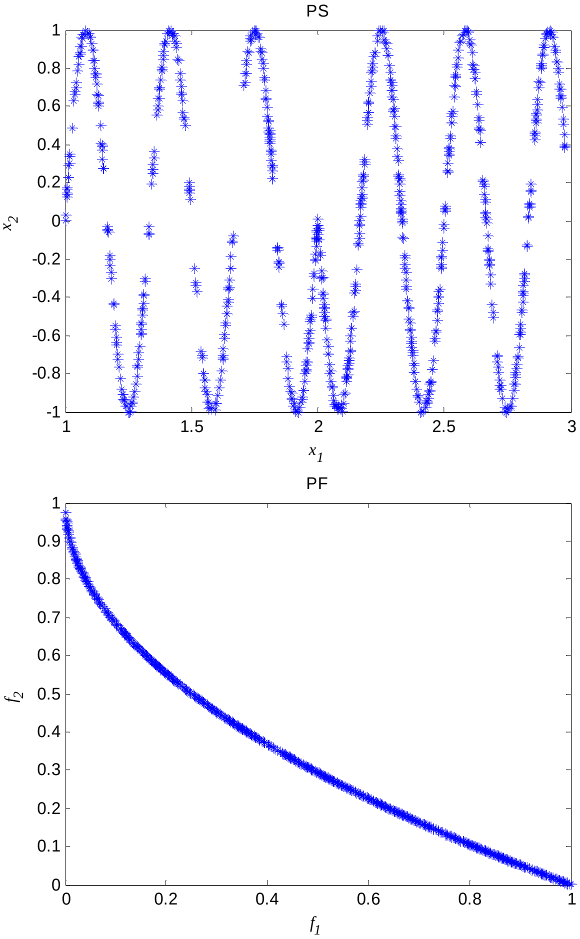


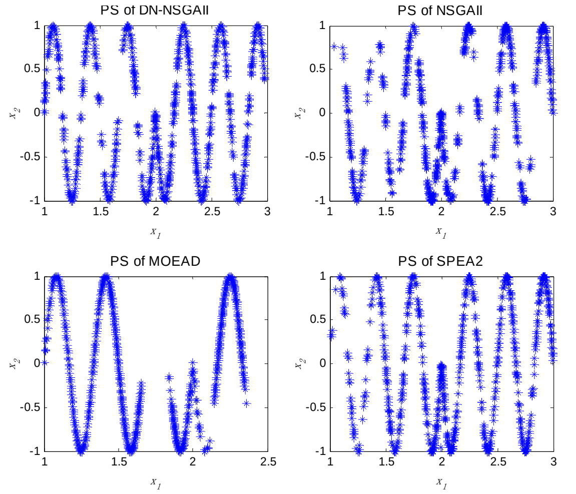
Fig. 8 The obtained PS and PF of DN-NSGAII for SS_UF1

V. Simulation Results

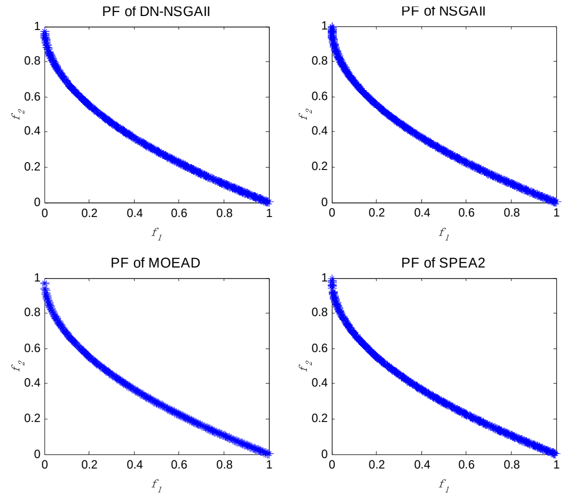
Four algorithms are tested on the two proposed novel test functions. They are DN-NSGAII, NSGAII [8], MOEAD [26] and SPEA2 [27]. The population size and generation number of all the four algorithms are set to 800 and 100 respectively.

The obtained PSs and PFs are shown in Fig. 9. Fig. 9 (a) and (c) show the four algorithms' obtained PS of the two test functions. Fig. 9 (b) and (d) show the four algorithms' obtained PF of the two test functions. The obtained PS of DN-NSGAII covers most of the true PS in both test functions, while other algorithms miss many parts of the true PS.

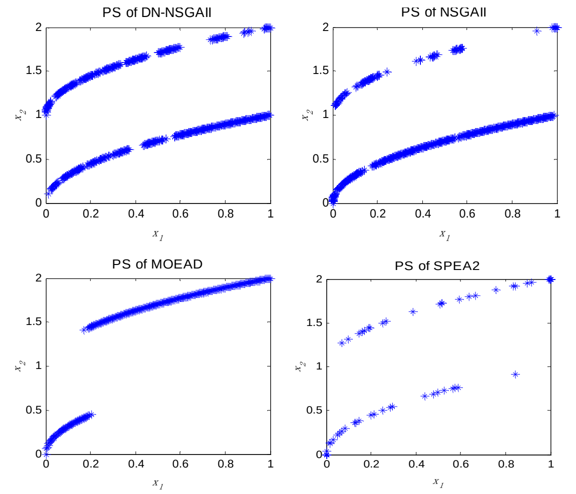
Hypervolume (HV) and IGD are used to measure their obtained PFs, and IGDX is used to measure their obtained PSs. The simulation results are shown in Table I-III. The results in the tables are all the average values of running 50 times. The higher HV and lower IGD mean the obtained PF is closer to the true PF, and the lower IGDX means the obtained PS is closer to the true PS. We can see that IGDX of DN-NSGAII is



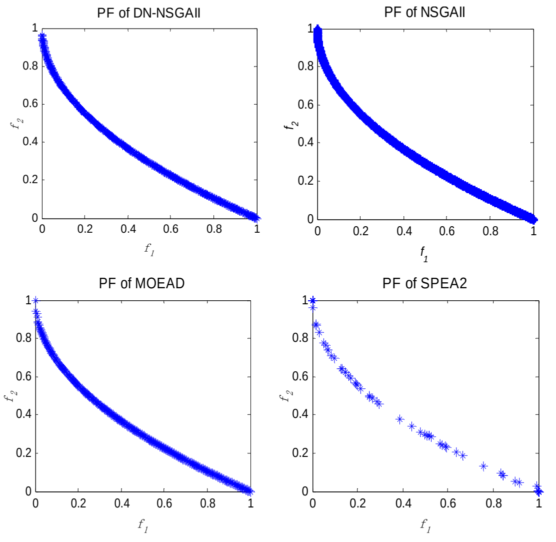
(a) Obtained PS of SS-UF1



(b) Obtained PF of SS-UF1



(c) Obtained PS of S-UF3



(d) Obtained PF of S-UF3

Fig. 9 Obtained PSs and PFs of test functions

TABLE I. IGDX OF THE FOUR ALGORITHMS

Algorithm / Test function	DN-NSGAII	NSGAII	MOEAD	SPEA2
SS-UF1	**0.0192**	0.0422	0.1648	0.0392
S-UF3	**0.0209**	0.0229	0.2974	0.0346

TABLE II. IGD OF THE FOUR ALGORITHMS

Algorithm / Test function	DN-NSGAII	NSGAII	MOEAD	SPEA2
SS-UF1	7.1799e-4	**5.9082e-4**	6.6112e-4	0.0022
S-UF3	0.0018	6.1077e-4	**5.7942e-4**	0.0155

TABLE III. HV OF THE FOUR ALGORITHMS

Algorithm / Test function	DN-NSGAII	NSGAII	MOEAD	SPEA2
SS-UF1	3.6652	**3.6658**	3.6655	3.6635
S-UF3	3.6441	3.6633	**3.6656**	3.6413

the lowest. From this point DN-NSGAII obtains the best PS. Although the HV and IGD of DN-NSGAII are not highest, they are close to the highest.

VI. CONCLUSION

This paper proposes a new challenge in multi-objective optimization. The difficulties to overcome the challenge are analyzed in detail. Two test functions are designed and three indictors are adopted to compare the performance of four algorithms. Finally a decision space based niching Multi-Objective Evolutionary Algorithm is proposed. Results show that the commonly used multi-objective optimizations fail to find all the Pareto optimal solutions, while DN-NSGAII can obtain more Pareto optimal solutions without deteriorating the PF.

DN-NSGAII will be further improved and novel high-dimension multimodal multi-objective test functions will be designed in the future. In addition, the proposed algorithm will be applied to real world problems.

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