Diversity Assessment in Many-Objective Optimization

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***Abstract*—Maintaining diversity is one important aim of multiobjective optimization. However, diversity for many-objective optimization problems is less straightforward to define than for multiobjective optimization problems. Inspired by measures for biodiversity, we propose a new diversity metric for many-objective optimization, which is an accumulation of the dissimilarity in the population, where an L_p-norm-based ($p<1$) distance is adopted to measure the dissimilarity of solutions. Empirical results demonstrate our proposed metric can more accurately assess the diversity of solutions in various situations. We compare the diversity of the solutions obtained by four popular many-objective evolutionary algorithms using the proposed diversity metric on a large number of benchmark problems with two to ten objectives. The behaviors of different diversity maintenance methodologies in those algorithms are discussed in depth based on the experimental results. Finally, we show that the proposed diversity measure can also be employed for enhancing diversity maintenance or reference set generation in many-objective optimization.**

***Index Terms*—Diversity, evolutionary algorithm, many-objective optimization, metric.**

I. Introduction

Many-objective optimization [1] has become an active research topic in multiobjective evolutionary algorithms (MOEAs) [2], because of the challenges it poses to evolutionary algorithms and practicability in the real world [3]–[6]. Many-objective optimization problems (MaOPs) [1], [7], i.e., multiobjective optimization problems (MOPs) [8] with more than three objectives, are hard to be solved by most existing MOEAs [9], [10].

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None of the three main approaches, Pareto-, aggregation-, and performance indicator-based MOEAs is able to efficiently produce a solution set for MaOPs with satisfactory convergence and diversity [9]. The failure of Pareto-based MOEAs to converge on MaOPs comes from their ineffectiveness in distinguishing the quality of solutions when the number of objectives becomes large [11], [12], which is completely different from their efficiency on MOPs with two or three objectives (e.g., [13]), even though the speed of the nondominated sort for MaOPs has been improved by fast sorts [14]–[17]. Aggregation-based MOEAs such as MOEA/D [18] decompose an MaOP into a number of single-objective optimization problems using a set of predefined weight vectors, thereby avoiding the convergence problem. However, a limited number of weight vectors in the high-dimensional space lead to poor diversity for MaOPs [19], [20]. Indicator-based MOEAs use an indicator as their fitness function to optimize an MaOP, which can be classified into three categories (distance-, hypervolume-, and R2-based MOEAs) [10]. $I_{\varepsilon+}$ [21] is the earliest distance-based indicator that is used in indicator based evolutionary algorithm (IBEA) to improve convergence, but it is not a diversity indicator and leads to poor diversity [12]. In contrast, hypervolume evaluates both convergence and diversity [22], thus many hypervolume-based MOEAs [23]–[25] have been developed. Although the computational complexity for calculating the exact hypervolume has been lowered [26], [27], MOEAs rely on on-line hypervolume calculation have not been applied to MaOPs [28]. R2 [29] evaluates both convergence and diversity and R2-based MOEAs for MaOPs have been reported in [30] and [31].

Existing research on MaOPs can be roughly divided into four categories: 1) objective reduction [32], [33]; 2) incorporation of preferences [34]; 3) modified dominance relationships; and 4) introduction of additional selection criteria. In case there is a strong correlation between objectives, some objectives can be removed [35]. To this end, statistical machine techniques, such as feature selection [36], principal component analysis (PCA) [37], [38], and maximum variance unfolding (MVU) [39] can be employed for objective reduction. In practice, users are often interested in only a part of the Pareto optimal solutions [40]. Therefore, if user preferences are available, preference-based approaches can be designed [34], [41]–[43]. To improve the effectiveness in distinguishing solutions in many-objective optimization, several modified dominance relations [44]–[48] have been proposed. To accelerate the convergence of MOEAs (Pareto-, aggregation-, and performance indicator-based) for solving MaOPs, additional selection criteria have been introduced [49]. For example, non-dominated sorting genetic algorithm (NSGA)-III [50] employs a set of reference points to maintain population diversity, where the reference points can be considered as a set of preferred solutions. Knee point driven evolutionary algorithms [51] uses the distance of knee points to a hyperplane as an additional selection criterion. Two_Arch2 [52] adapts an L_p-norm distance-based selection criterion in addition to its $I_{\varepsilon+}$-based selection. The dual population paradigm [53] uses both Pareto- and aggregation-based techniques.

It is well recognized that performance indicators of MOEAs should be able to account for convergence, diversity, and uniformity of the solution set [22], [54], [55]. However, MaOPs may pose serious challenges to existing performance indicators in assessing convergence, diversity, and uniformity. For instance, ratio-based performance indicators such as error ratio [56] and ratio of nondominated individuals [57], and binary performance indicators, including C-metric [58] and purity [59], require dominance comparisons, which are less effective for MaOPs. In addition, distance-based performance indicators, e.g., maximum Pareto front error [56], generational distance (GD) [56], and GD_p [60] need to sample a large set of uniformly distributed reference points sampled from the true Pareto front, which is hard to guarantee for MaOPs. Note that some performance indicators are able to account for both convergence and diversity, such as hypervolume [22], R2 [29], inverted GD (IGD) [61], and averaged Hausdorff indicator Δ_p [62].

Unlike uniformity metrics such as distribution (UD) [57], spacing (SP) [63], and minimal SP [59], diversity is less straightforward to characterize mathematically. Existing diversity metrics view diversity from different perspectives. For examples, maximum spread (MS) [58] uses the spread of a solution set, whereas both number of distinct choices (NDC) [64] and entropy-based metric suggested in [65] employ divided grids in the objective space. By contrast, sigma diversity metric (SDM) [66] assigns several reference lines and diversity measure (DM) [67] adopts a reference set. In addition, there are some metrics that can assess both diversity and uniformity, such as Δ [68] and diversity comparison indicator (DCI) [55]. However, the above-mentioned metrics may encounter difficulties in assessing diversity for MaOPs due to the following two reasons. First, spread will no longer be able to fully characterize the diversity of the whole Pareto front in a high-dimensional space. Second, parameters in the diversity metrics are harder to specify for MaOPs.

This paper aims to address the difficulties the existing diversity metrics encounter in many-objective optimization. We propose a new diversity metric inspired by a measure for biodiversity. We show that the proposed new diversity metric is able to more accurately measure the diversity of solutions in high-dimensional spaces. Furthermore, our results indicate that the proposed diversity metric can enhance the diversity performance of evolutionary algorithms for solving MaOPs replying on a predefined reference set or weight vectors.

The rest of this paper is organized as follows. The difficulties in assessing diversity for MaOPs are discussed in Section II. To address these difficulties, Section III presents a new diversity metric, together with empirical comparative analysis of its ability to measure diversity and the influence of convergence on the DM. In Section IV, we employ the proposed metric to assess the diversity performance of four popular MOEAs for MaOPs and discuss the theoretical rationale behind these empirical results. In Section V, the proposed DM is adopted for maintaining diversity or generating a reference set, which is shown to be able to enhance the diversity of solutions obtained by the MOEAs under comparison. Section VI concludes this paper.

II. Diversity in Evolutionary Multiobjective Optimization

Diversity is an important topic in multiobjective optimization, which provides decision makers information for choosing preferred solutions. When clear user preferences are not available, it is highly desirable that a limited number of solutions can be obtained that uniformly spread over the whole PF and are as diverse as possible. However, unlike convergence, a well established definition for diversity of solutions obtained by MOEAs still lacks.

Diversity and uniformity are two related aspects for evaluating the distribution of an obtained solution set. More often than not, researchers are confused about the meanings of these two measures. It should be stressed that a solution set with good uniformity does not necessarily mean that it also has good diversity, and vice versa. Generally speaking, solutions in a set with good uniformity should have the same dissimilarity with their neighbors, whereas solutions in a set with good diversity should provide decision makers the maximum amount of information. Mathematically, diversity and uniformity can be described as in (1) and (2), where X is a solution set and s is a solution in X. It is worth noting that dissimilarity$(s, X - s)$ is the dissimilarity of s to the rest of X (or the diversity contribution to X), which measures the different degree of s to other solutions in X. In the existing research, there are different metrics to describe the dissimilarity between solutions, such as various distances. Therefore, the sum of dissimilarity$(s, X-s)$ indicates the diversity of X, while the variance of dissimilarity$(s, X - s)$ specifies the uniformity

$$\mathrm{diversity}(X) = \sum_{s\in X} \mathrm{dissimilarity}(s, X - s) \tag{1}$$

$$\mathrm{unifomity}(X) = \operatorname*{var}_{s\in X}(\mathrm{dissimilarity}(s, X - s)). \tag{2}$$

In order to better understand (1) and (2), we use Fig. 1 to illustrate the differences between diversity and uniformity. Solution sets in panels A, B, D, and E of the figure show good uniformity but relatively poor diversity. Solutions in panels D and E are of obviously poor diversity, because they are distributed only in small parts of the whole PF. Solutions in panel B loses information of the boundary of the PF. Although solutions in panel A are distributed over the whole PF with perfect uniformity, there is redundancy in the information on each objective, resulting in worse diversity than those in panel C. From these examples, we can see that a solution set with good diversity means that it contains the maximum amount of information for decision makers.

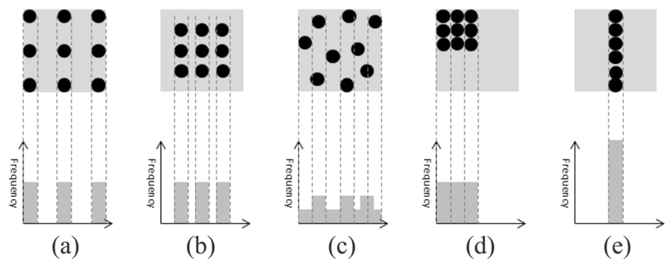

Fig. 1. Illustration of the differences between diversity and uniformity. (a) Good uniformity but relatively poor diversity. (b) Good uniformity but lack of the boundary. (c) Relatively poor uniformity but good diversity. (d) Good uniformity but poor diversity. (e) Good uniformity but extremely poor diversity.

TABLE I
EXISTING DIVERSITY METRICS AND THEIR CHARACTERISTICS

Metric	Mixed	Parameter Needed	Reference Needed
MS [58]	N	N	N
NDC [64]	N	Y	N
Entropy [65]	N	Y	N
SDM [66]	N	Y	Y
DM [67]	N	Y	Y
Δ [68]	Y	N	N
DCI [55]	Y	Y	N
Hypervolume [22]	Y	N	Y
IGD [61]	Y	N	Y
R2 [29]	Y	N	Y
Δ_p [62]	Y	N	Y

A. Challenges in Diversity Assessment for MaOPs

The high-dimensional objective space in MaOPs does not only make it very hard for decision makers to intuitively judge the diversity of the solution set, but also creates difficulties in quantitatively assessing the diversity. As we know, a solution set of a limited size can distribute only very sparsely in a high-dimensional space [69], which is known as "curse of dimensionality." In other words, a solution set of a limited size is hard to describe a PF in high dimensions, which causes trouble to decision makers in solving MaOPs. Therefore, diversity maintenance and assessment pose a serious challenge to many-objective optimization.

B. Existing Diversity Metrics

Existing diversity metrics can be divided into two classes: 1) mixed and 2) unmixed diversity metrics. Unmixed metrics measure the diversity only, but mixed metrics try to capture more aspects of the distribution of a solution set (convergence for instance).

Table I provides a summary of widely used existing diversity metrics.

The first five metrics are unmixed, which can characterize diversity only, and their disadvantages are obvious. MS [58] uses the spread of a solution set as a measure of diversity, which is incomplete to evaluate the diversity of the whole solution set. NDC [64] and entropy [65] divide the objective space into a number of grids (b divisions for each objective), NDC counts the number of grids having solutions in them and entropy calculates the entropy of all the nonempty grids. They both require a predetermined parameter b, which greatly affects the assessment result. SDM [66] assigns several reference lines to determine whether solutions are located near the lines by a distance threshold d, thus the diversity based on reference lines can be obtained. DM [67] uses the projection of the solution set to reference $(m-1)$-dimensional grids for measuring diversity, which requires both the number of grids and the reference set.

The rest six metrics are unmixed, which evaluate more than diversity. Consequently, it is hard to single out the performance on diversity only from the value of these metrics. Δ assesses the distribution of the solution set [68]. Δ is a combination of the spread (measured by distances to the extreme points) and uniformity (measured by distances to the nearest neighbors). DCI [55] also employs a grid environment to assess both spread and uniformity, so the number of grids needs to be predefined. Hypervolume calculates the volume that the obtained solution set dominates respect to a reference point [70], but it cannot be applied to MaOPs in practice due to its prohibitively high computational complexity [27]. IGD is the average distance from a reference set (samplings on the true PF) to the obtained set. The idea of R2 is similar to IGD, where the reference set used is a set of weights, and the distance from the reference set to the solutions is calculated using the Tchebycheff function. Δ_p is the Hausdorff distance between the obtained solution set and the reference, which evaluates both convergence and diversity and has been applied to both MOPs [71], [72] and MaOPs [73]. However, a reference set is still needed to calculate Δ_p.

Ideally, a diversity metric should assess diversity only and should be independent of any parameters or references. The main reason is that parameters or references may reduce the level of objectivity. Unfortunately, none of the existing diversity metrics fully satisfy the above requirements.

III. PROPOSED PURE DIVERSITY METRIC

A widely accepted definition for diversity still lacks in the area of evolutionary multiobjective optimization. By contrast, measures for biodiversity has been extensively studied in biology. Among various measures for biodiversity, the PD has been proposed for measuring the diversity of species [74] as follows:

$$\mathrm{PD}(X) = \max_{s_i \in X}(\mathrm{PD}(X - s_i) + d(s_i, X - s_i)) \tag{3}$$

where

$$d(s, X) = \min_{s_i \in X}(\mathrm{dissimilarity}(s, s_i)). \tag{4}$$

In the above equations, $d(s_i, X-s_i)$ denotes the dissimilarity d from one species s_i to a community X.

We can find that (1) and (3) are equivalent except for the difference in the defining the sum, if s is viewed as a solution in the solution set X. In addition, (3) does not require any reference, nor any parameters. Thus, PD in (3) can be a promising measure for population diversity in multiobjective optimization.

Fig. 2 provides an illustrative example of how PD is calculated. In the left panel of the figure, solution s_i and other solutions $X - s_i$ are considered as two communities. Their diversity is the sum of diversity of $X - s_i$ (black dots) and the dissimilarity of s_i to $X - s_i$. With the recursion in (3), the

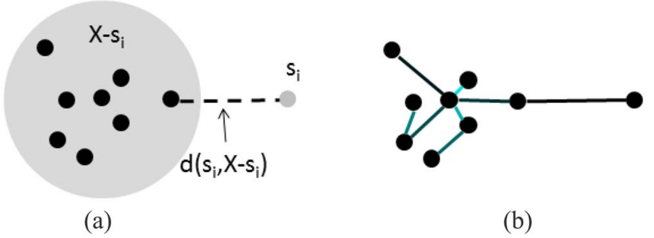

Fig. 2. Illustration of the PD metric. (a) $d(s_i, X - s_i)$ is calculated by the dissimilarity of s_i to its nearest neighbor. (b) PD value of X is the sum of the linked dissimilarity.

Algorithm 1 Pseudo Code for the Calculation of PD

Input: **D**-dissimilarity matrix of every two solutions.

1: Set D_{max} as the maximal element of $\mathbf{D}$.
2: $D_{max} = D_{max} + 1$, $PD = 0$.
3: Set the diagonal elements of $\mathbf{D}$ as D_{max}.
4: **for** $k = 1 : n - 1$ **do**
5: $\quad d = min(\mathbf{D}, [], 2)$. // Find the nearest neighbor to each solution according to $\mathbf{D}$ in each row.
6: $\quad$ Find solution i with the maximal d_i to its neighbor j.
7: $\quad$ **while** i and j is connected by previous assessed solutions **do**
8: $\quad\quad \mathbf{D}(i, j) = D_{max}$ and $\mathbf{D}(j, i) = D_{max}$. // Mark the connected subgraph.
9: $\quad\quad d = min(\mathbf{D}, [], 2)$.
10: $\quad\quad$ Find solution i with the maximal d_i to its neighbor j.
11: $\quad$ **end while**
12: $\quad PD = PD + d_i$.
13: $\quad \mathbf{D}(i, :) = -1$. // Mark the chosen solution i.
14: $\quad \mathbf{D}(j, i) = D_{max}$. // Mark the used dissimilarity d_i.
15: **end for**

Output: PD;

dissimilarity of every single solution to the whole population can be evaluated, with each solution being linked to its nearest unreplicated neighbor. Then, the sum of those dissimilarity results in the diversity of the whole population, which can be seen as the structure of X, as shown in panel B of Fig. 2 (where the darker lines are connected earlier than the lighter lines).

To calculate the value of PD of a population with n solutions, an $n \times n$ dissimilarity matrix $\mathbf{D}$ for every two solutions is needed. Details of the calculation of PD are given in Algorithm 1. In each accumulation, solution i with the maximal dissimilarity to its nearest unmarked neighbor j is chosen by line 5, where $d = \min(\mathbf{D}, [], 2)$ means the smallest elements along the second dimension (the row of $\mathbf{D}$). In order to avoid repeated choice of i, we update $\mathbf{D}(i, :)$ to -1. Furthermore, any connected subgraph is avoided in PD, because a connected subgraph implies the dissimilarity of those solutions is repeatedly evaluated. When i and j can be connected via previously assessed solutions, we let $\mathbf{D}(i, j) = D_{\max}$ and $\mathbf{D}(j, i) = D_{\max}$, thus dissimilarity i and j cannot be used. If we skip line 8 in Algorithm 1, the connected subgraphs cannot be linked by other solutions, the dissimilarity from the subgraphs cannot be measured.

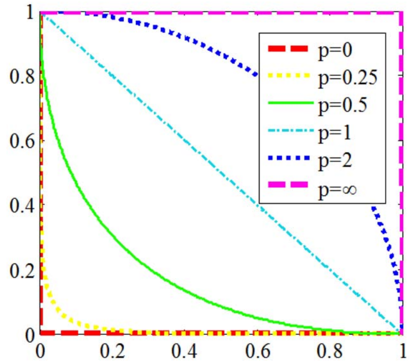

Fig. 3. Contour lines of different unit length L_p-norm. The smaller p is, the more sensitive L_p is to 0 in each dimension.

A. Dissimilarity

The evaluation of dissimilarity plays an important role in calculating PD. Usually, the distance between two solutions is adopted as their dissimilarity. Note however, that the Euclidean distance is not well suited for measuring neighborhood in a high-dimensional space [75], [76]. Since solutions of MaOPs are distributed in a high-dimensional objective space, the Euclidean distance (L_2-norm-based) is not suited for dissimilarity calculation in PD. To address this issue, L_p-norm-based distances have been suggested for diversity maintenance in solving MaOPs [52], [76], [77]. Fig. 3 illustrates the differences between various L_p-norm-based distances.

From Fig. 3 we can clearly see that the smaller p is, the more sensitive L_p is to 0 in each dimension. In contrast, the L_p-norm-based distance measures are not good for measuring dissimilarity of high-dimensional data for $p \geq 1$. Therefore, it is necessary to set $p < 1$ for measuring diversity in MaOPs. It has been shown that the effectiveness of the measure is not sensitive to p as long as $p < 1$ [75]. Therefore, p is not a parameter in PD and we set p to 0.1 in this paper.

B. Behavior Study

Indicators use a single scalar value to describe an m-dimensional distribution, thus some information will be lost no matter whichever indicator it is. Therefore, it is hoped that some key information is captured, although different indicators may capture different information. In the case that three extreme points of the PF $f_1 + f_2 + f_3 = 1$ are obtained, the values of diversity metrics vary with different solutions added to the set of three extreme points. Fig. 4 is the changing values of PD, MS, NDC ($b = 4$), and entropy ($b = 4$) when another solution from the PF is added to the set of three extreme points, where the color shows the size of metrics (the darker points have lower values than the lighter ones). If one solution is selected based on those metrics to increase diversity, the lighter parts in Fig. 4 have priority over the darker parts. Once the extreme points have been obtained, the MS value reaches its maximum. Thus, no solution is able to improve MS anymore. Although the middle part is promoted by NDC and entropy,

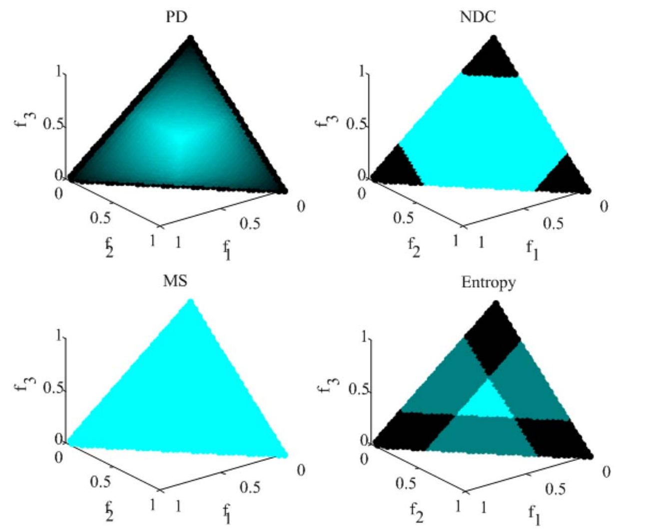

Fig. 4. Changing values of PD, MS, NDC ($b = 4$), and entropy ($b = 4$) when another solution from the PF $f_1 + f_2 + f_3 = 1$ is added to the set of three extreme points, where the color shows the size of metrics (the darker points have lower values than the lighter ones).

solutions cannot be distinguished within their grids. For PD, the middle part is promoted and the values change continuously. From Fig. 4, we find that PD can generally promote diverse solutions.

To further understand PD, we calculate the PD values of six sets of solutions with different PF distributions ($f_1 + f_2 + f_3 = 1$) shown in Fig. 5, where red dots are solutions, lines are the dissimilarity accumulated in PD, and the colors of lines denote the chosen order (the darker lines are chosen earlier than the lighter lines). From Fig. 5, we can see that set A spread very well over the whole PF, while sets B, C, and D do not. Thus, the diversity of sets B, C, and D should be worse than that of A, which is also reflected by the PD values.

Distinguishing sets A, E, and F from sets B, C, and D is the first step of PD, which comes from the aspect of spread. Further to spread to the whole PF, any repeated objective values are redundant to decision markers. Comparing A with E and F, we believe that A has better diversity than E and F, because A shows perfect uniformity. However, as the bar chart of the frequency of A shows, solutions in set A has many repeated objective values on f_1, whereas E has no repeated objective values on f_1. Fig. 6 also shows that A has repeated objective values on f_1, f_2, and f_3, but E does not. Therefore, E can provide more information to decision markers than A, which is therefore considered to have better diversity than A. The PD values of these solution sets indicate that it is able to detect the subtle differences in diversity between these solution sets.

So far we have revealed some promising properties of PD using illustrative examples. To further examine the usefulness of PD in diversity maintenance in many-objective optimization, we will perform a few additional experiments in the following, where we use an m-objective problem whose front can be characterized by $\sum_{i=1}^{m} f_i = 1$, as shown in Fig. 5. We use two different solution sets, one uniformly distributed set

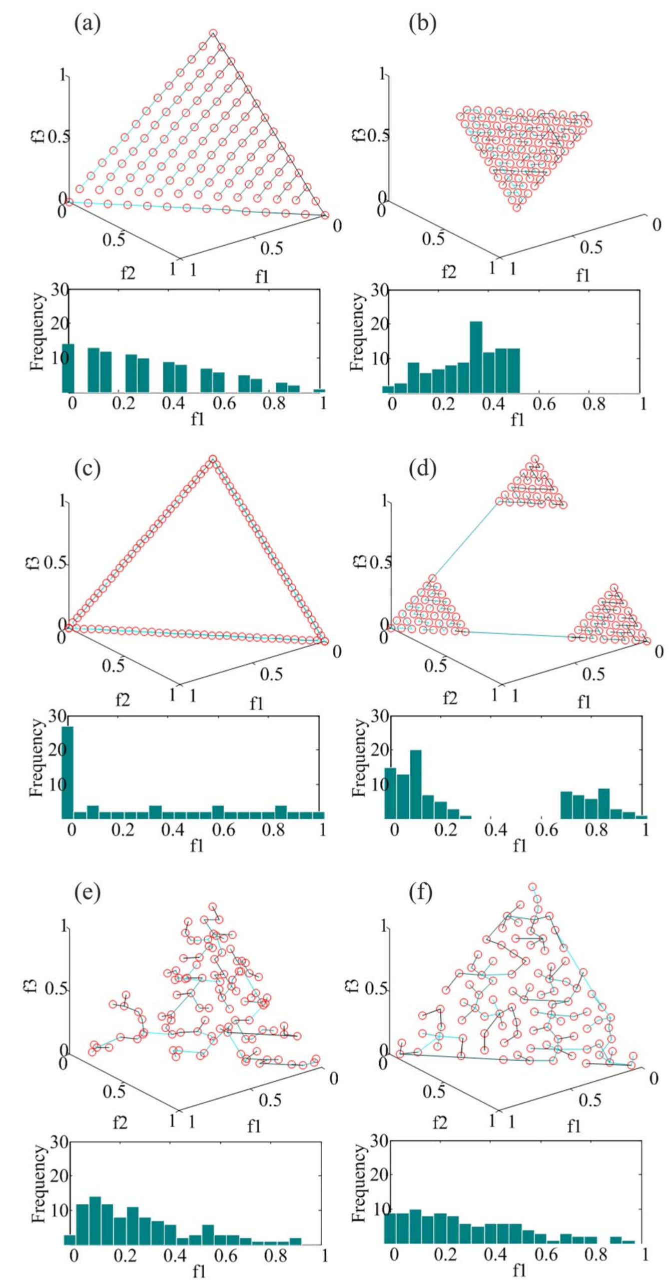

Fig. 5. Six different solution sets and their PD values. (a) PD = 8.1920e + 03. (b) PD = 4.5227e + 03. (c) PD = 5.2104e + 03. (d) PD = 5.0773e + 03. (e) PD = 1.5049e + 05. (f) PD = 2.5435e + 05.

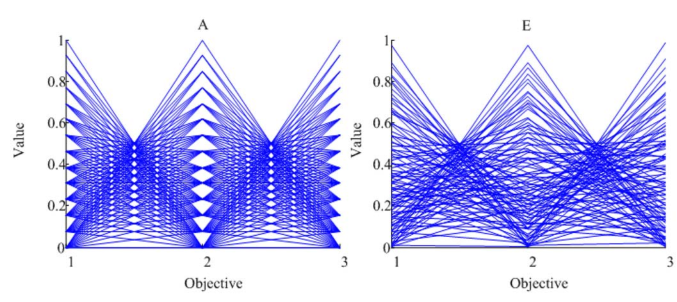

Fig. 6. Parallel coordinates of examples (a) and (e) in Fig. 5.

$U(n, m)$ denoted by A, and the other randomly distributed set $R(n, m)$ denoted as E, where n is the size of the set and m is the number of objectives.

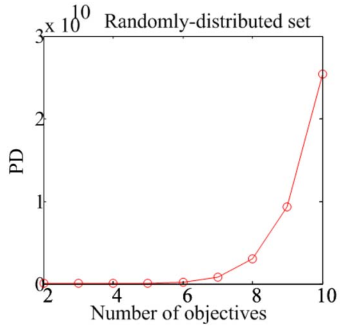

Fig. 7. Average PD values of a randomly distributed set with 100 solutions and different numbers of objectives.

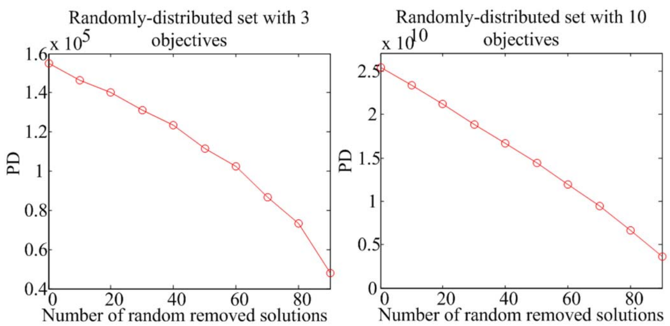

Fig. 8. Average PD values of randomly-distributed set with different numbers of dropped solutions for the 3 and 10-objective problems.

To show the influence of the number of objectives on PD, we conduct the following experiments.

1) Generate the test dataset $R(100, m)$ for 30 times for $m = [2, \ldots, 10]$, respectively.
2) Calculate their PD values.

Fig. 7 shows the average values of PD on a randomly distributed set with different numbers of objectives. Given a fixed number of solutions, the higher the dimension of the objective space, the more sparse the distribution of the solutions will be, the higher the degree of diversity will probably be. Therefore, MOEAs tend to achieve a set of solutions of a high degree of diversity but poor convergence [10]. Because of that poor balance of convergence and diversity, most MOEAs fail on many-objective optimization problems. That is the reason why the PD value increases dramatically with the increased number of objectives.

To show the effects of spread on PD, we conduct the following experiment.

1) Generate the test dataset $R(100, m)$ for 30 times for $m = 3, 10$, respectively.
2) Randomly remove different numbers of solutions in each dataset to change the spread, then calculate their PD values.

Fig. 8 shows the average PD values of randomly distributed sets with different numbers of solutions being removed for a 3- and 10-objective problems. As the number of solutions to be removed increases, the PD value decreases on all the test datasets with different numbers of objectives. The results show that PD is able to detect diversity loss resulting from the loss of solutions.

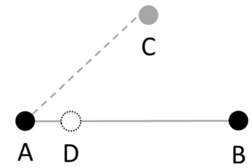

Fig. 9. Example of the effect of the number of solutions on PD.

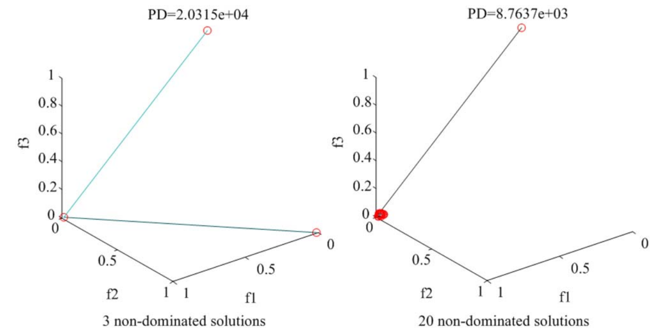

Fig. 10. PD values of two sets of 3 and 20 solutions.

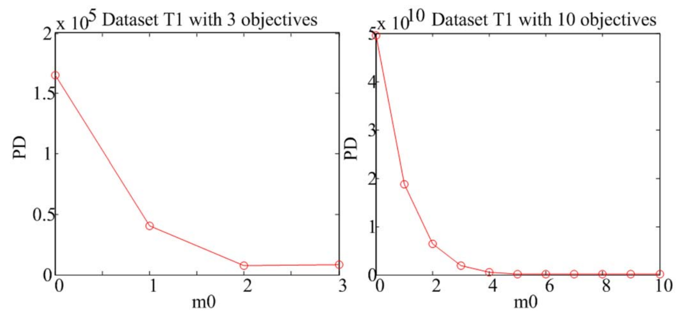

Fig. 11. Average PD values of dataset $T1(n, m, m_0)$ with three and ten objectives.

Taking Fig. 9 as an example, when solution C is added to set A, B, the PD value increases due to the dissimilarity of A and C. However, when solution D is added to set A, B, the PD value is not improved, because there is no more dissimilarity added. Therefore, we find that the number of solutions is not directly related to PD. The PD value increases only if the additional solutions bring more dissimilarity to the solution set, which can be shown in Fig. 10. Even the set of three solutions can have a larger PD value than the set of 20 solutions, because the former spreads more widely than the latter.

To study the impact of solutions having repeated objective values on PD, we conduct the following experiments.

1) Generate datasets $U(n, m)$ and $R(n, m)$ for $m = 3, 10$, respectively, where $n = C_{m+q-1}^{q}$. For 3- and 10-objective problems, n equals 105 and 220, respectively.
2) Construct datasets $T1(n, m, m_0)$ with m_0 objectives from $U(n, m)$ and other objectives randomly sampled for 30 independent times, where m_0 increases from 1 to m. Calculate their PD values.
3) Construct datasets $T2(n, m, K)$ with K randomly sampled from $U(n, m)$ and $n - K$ randomly-sampled from $R(n, m)$ for 30 independent times, where K increases with a step of ten solutions. Calculate their PD values.

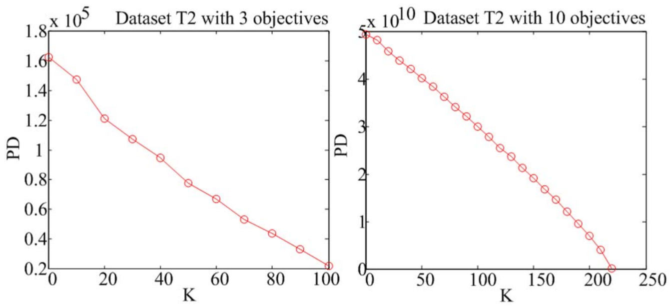

Fig. 12. Average PD values of dataset $T2(n, m, K)$ with three and ten objectives.

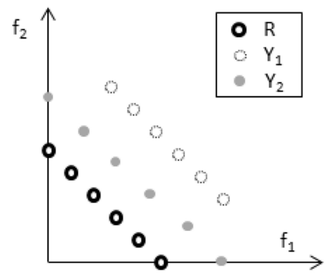

Fig. 13. Illustration of sets Y_1 and Y_2.

Fig. 11 shows the average PD values of dataset $T1(n, m, m_0)$ with three and ten objectives. When m_0 increases, the diversity of $T1$ decreases, because there are more objectives having repeated values. As expected, the PD values decrease as m_0 increases. Fig. 12 shows the average PD values of dataset $T2(n, m, K)$ with three and ten objectives. As K increases, there will be more solutions with repeated objective values, which decrease the diversity. Therefore, the PD value drops as K grows.

Solution sets with different degrees of convergence might have an impact on PD, because they might have different spreads. Taking a sampling set R from a true PF as an example, sets $Y_1(g) = R + g$ and $Y_2(g) = Rg$ are dominated by R as shown in Fig. 13. Y_1 is shifted from R, the dissimilarity between solutions is not changed from R. Therefore, the PD value of Y_1 equals to that of R. However, the scale of Y_2 is changed from R, Y_2 has a larger spread than R, the dissimilarity between solutions is g times as much as R, thus, the PD value of Y_2 is g times as much as R.

From the above example in Fig. 13, it is clear that PD is a sole metric that measures diversity only, which cannot show any information about convergence. Convergence and diversity are two important aspects to evaluate the obtained solution set of MOPs. Unlike the mixed metrics such as IGD, sole metrics such as GD and PD cannot compare solution sets for convergence and diversity at the same time. Sole metrics play a role of analyzing the reason why a solution set has poor performance. For example, Y_2 has an IGD value worse than R, which is hard to know the reason only from the IGD value. With the values of GD and PD, we can know that Y_2 distributes far from the true PF and has a larger spread than the true PF. As mentioned in [78], metrics compress the solution set into a single value to capture a certain characteristic. Multiple metrics should be employed to analyze the experimental results. Therefore, a combination of sole metrics for convergence and diversity as well as mixed metrics should be adopted to objectively evaluate solution sets, for instance, the combinations (GD, IGD, PD) and (Δ_p, PD) are highly recommended.

IV. Diversity Assessment of MOEAs Using Proposed Metric

Not much work has been reported on comparing the diversity maintenance performance of existing MOEAs. In this section, we use the proposed metric, PD to analyze the diversity maintenance performance of four MOEAs for solving MaOPs.

A. Test Problems and MOEAs Under Comparison

DTLZ [79] and WFG [80] are two widely used MaOP test suites. We study the diversity of MOEAs on those problems with 2–10 objectives. The simulation includes four MOEAs for solving MaOPs, including Two_Arch2 [52], NSGA-III [50], IBEA (with $I_{\varepsilon+}$) [21], and MOEA/D ($T = 50$) [18]. These MOEAs represent four different approaches in solving MaOPs. Two_Arch2 is a hybrid method combining Pareto dominance and performance indicators; NSGA-III is a Pareto dominance-based method with an additional mechanism for maintaining diversity with respect to a reference set; IBEA is a performance indicator-based algorithm, and MOEA/D is a decomposition approach. To conduct a fair comparison, we use the same crossover (SBX with $\eta = 15$) and mutation (polynomial mutation with $\eta = 15$) for the compared MOEAs. 30 independent runs are performed for each MOEA with a maximum of 90 000 function evaluations.

B. Performance of MOEAs in Terms of PD

Each MOEA obtains a total of 100 solutions for comparison on the DTLZ and WFG problems. The PD values of Two_Arch2, NSGA-III, IBEA, and MOEA/D on the problems with 2–10 objectives are shown in Figs. 14 and 15.

In Figs. 14 and 15, IBEA (with $I_{\varepsilon+}$) has the worst PD values on all low-dimensional problems. IBEA exhibits a clear advantage on convergence over others in solving MaOPs [12]. However, the diversity of the solution set obtained by IBEA is poor, because there is hardly any explicit diversity maintenance mechanism in IBEA. As shown in Fig. 16, IBEA performs the worst in terms of diversity on two multimodal MaOPs, DTLZ1, and DTLZ3, as the solutions it has achieved cannot spread over the whole PF. For other MaOPs, the solutions achieved by IBEA spread randomly on the whole PF and the resulting PD values keep increasing as the number of objectives increases, as shown in Fig. 7.

MOEA/D and NSGA-III perform differently from IBEA, as illustrated in Figs. 14–16. On the multimodal test functions, DTLZ1 and DTLZ3, the PD values of the solution sets obtained by MOEA/D and NSGA-III are better than that of the solutions achieved by IBEA because their solutions have better spread than those of IBEA. On the other MaOPs, MOEA/D, and NSGA-III perform worse in terms of PD values than IBEA, which can be attributed to the fact that their solutions contain many repeated objective values, which is clearly

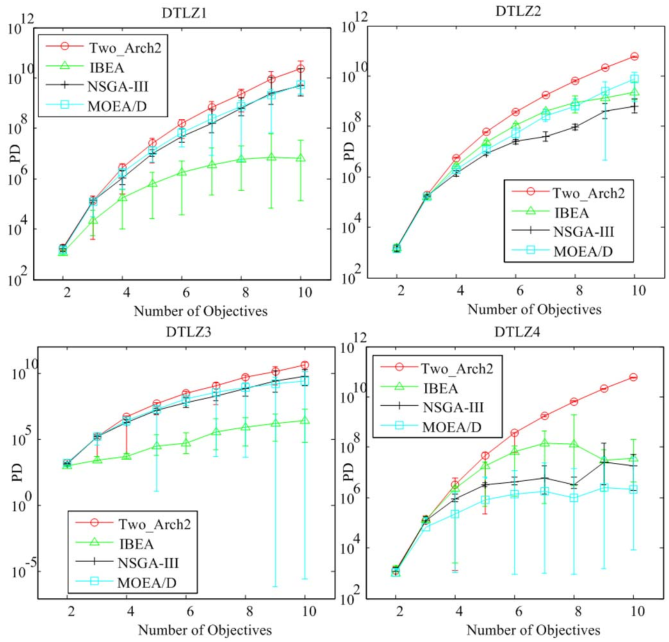

Fig. 14. PD values of Two_Arch2, NSGA-III, IBEA, and MOEA/D on the DTLZ problems with 2–10 objectives.

observed in Fig. 16. Note that both MOEA/D and NSGA-III rely on a similar diversity maintenance mechanism. The former is based on a predefined set of weight vectors, whereas the latter is based on reference points. As a result, the diversity performance of both algorithms heavily depends on the predefined reference set. Very typically, these reference sets contain a large number of solutions having repeated values on each objective, which degrades the diversity in terms of PD values.

By contrast, Two_Arch2 performs relatively poorly in terms of the PD values on 2- or 3-objective MOPs but performs the best in terms of the PD values on MaOPs having more than three objectives, as shown in Figs. 14 and 15. This is due to the fact that Two_Arch2 adopts a different mechanism for diversity maintenance from MOEA/D and NSGA-III. The L_p-norm-based diversity maintenance mechanism without any reference set that Two_Arch2 employs can avoid the disadvantages of the reference set based diversity maintenance mechanism both MOEA/D and NSGA-III use. Note, however, that Two_Arch2 is not best suited for solving MOPs with 2–3 objectives.

To show the diversity changes during the search of MOEAs in solving MaOPs, Fig. 17 plots the average PD values over the generations of Two_Arch2, NSGA-III, IBEA, and MOEA/D on DTLZ1 with ten objectives. At the very beginning, the four algorithms all have a large PD value, because the solutions they obtain are distributed randomly in the high-dimensional space, resulting in good diversity in terms of PD. In the late generations, the population converge toward the true PF, reducing the PD values. It is noticed that IBEA performs the worst in terms of the PD value during the whole evolutionary research, while Two_Arch2 obtains the best PD value. NSGA-III and MOEA/D show similar PD values that are better than those of IBEA but worse than Two_Arch2.

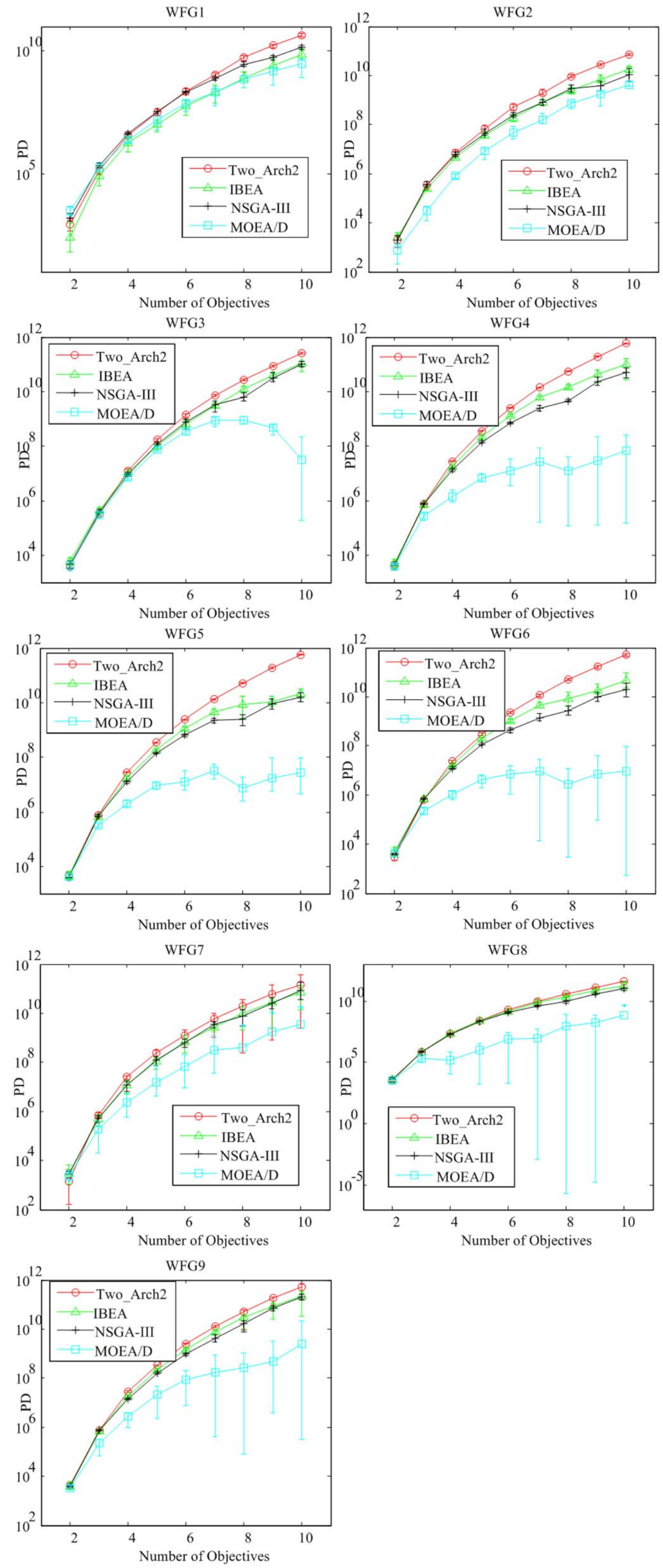

Fig. 15. PD values of Two_Arch2, NSGA-III, IBEA, and MOEA/D on the WFG problems with 2–10 objectives.

V. PD-Based Diversity Maintenance and Reference Set Generation

The above empirical results suggest that PD is an effective and subject diversity metric independent of a reference set.

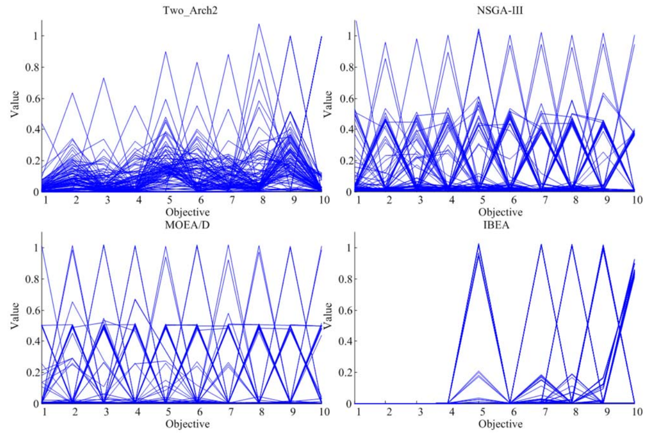

Fig. 16. Parallel coordinates of the solution set with the best PD values by Two_Arch2, NSGA-III, IBEA, and MOEA/D on DTLZ1 with ten objectives.

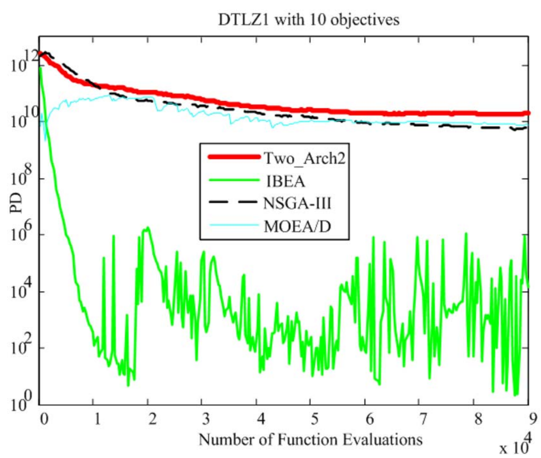

Fig. 17. Average PD values over generations of Two_Arch2, NSGA-III, IBEA, and MOEA/D on DTLZ1 with ten objectives.

In this section, we test the idea of using PD for diversity maintenance in selection, where n solutions need to be selected from a population (P_c) having N candidate solutions. The PD-based selection in essence chooses the solution having the maximal degree of dissimilarity to the selected population in each iteration. The details of the PD-based diversity maintenance scheme are given in Algorithm 2.

A. Simulation for PD-Based Diversity Maintenance Scheme

In this section, we simulate the situation that MOEAs may encounter in maintaining diversity. We assume the PF is defined by $\sum_{i=1}^{m} f_i = 1$, set P with n randomly generated solutions on the PF is considered to be the parent set, and set Q with $3n$ random samplings is viewed as the variations of P. We employ the PD-based diversity maintenance scheme on $P \cup Q$ to select n solutions P_n as the parent set for the next generation for 30 times. We compare the PD values of P and P_n in Table II, where the results are analyzed using Wilcoxon signed-rank tests [81]. In the population with 100 solutions, the PD-based diversity maintenance mechanism significantly improves the diversity of the population for the next generation except for the 2-objective case, because of the small number of objectives and the small population size n. When the population size n increases to 200, the improvement becomes greater than the case of $n = 100$. To conclude, the PD-based diversity maintenance scheme is effective for MOEAs in solving MaOPs.

Algorithm 2 Pseudo Code of the PD-Based Diversity Maintenance Scheme

Input: P_c-population of N candidates, $\mathbf{D}$-dissimilarity matrix of P_c, n-required size.

Set the index set of P_c as $I_c = [1 : N]$.
Set P and I_s empty.
Move the first candidate from P_c to P and index 1 from I_c to I_s.
for $k = 1 : n - 1$ **do**
  $\mathbf{A} = \mathbf{D}(I_c, I_s)$ // dissimilarity from candidates to selected solutions.
  Find the nearest solution in P_c to each candidate in P according to $\mathbf{A}$ in each row.
  $d = min(\mathbf{A}, [], \mathbf{2})$.
  Find candidate i with the maximal d_i.
  Move the i-th solution from P_c to P and index i from I_c to I_s.
end for

Output: P.

B. Simulation for PD-Based Reference Set Generation

As the results in Section IV-B show, the diversity performance of the reference-based MOEAs in solving MaOPs is limited in terms of PD values. Consequently, if the reference set used in these algorithms is generated based on PD, their performance on diversity can be improved. The reference points can be selected by maximizing the PD value from a much larger initial set that is generated either randomly or using an existing method such as the one proposed in [18].

In this experiment, 100 solutions are selected from a random reference set with 3000 points and a uniform reference set with 10 000 points, respectively. Fig. 18 shows the PD values of reference sets with 2–10 objectives using the PD-based reference set generation scheme. We find that a uniformly selected reference set containing 10 000 points can achieve the same diversity level of a randomly generated reference set containing 3000 points. Fig. 19 presents the reference set after the PD-based selection for 3-objective problems. Both sets have good diversity. Thus, a reference set selected based on the PD value can enable reference-based MOEAs to achieve solutions of better diversity.

We replace the reference set generation method in NSGA-III with the PD-based method, which is termed NSGA-III-PD for convenience. We compare NSGA-III and NSGA-III-PD on DTLZ1 and DTLZ2 with 2–10 objectives. We use $g(x)$ that is a part of the DTLZ problems to show the performance of convergence as [39] and PD to assess diversity. The results are shown in Table III, which are analyzed using the Wilcoxon signed-rank test [81]. It is clear that the new reference set generated using the PD-based scheme significantly improves the

TABLE II
PD VALUES OF P (PARENT POPULATION) AND P_n (SELECTED POPULATION BY THE PD-BASED DIVERSITY MAINTENANCE SCHEME). RESULTS ARE ANALYZED USING WILCOXON SIGNED-RANK TEST

	$n = 100$		$n = 200$	
Obj #	P	P_n	P	P_n
2	1.6162e+03±2.1099e+02	1.7339e+03±2.3570e+02	1.8129e+03±2.4503e+02	**1.9489e+03±2.1205e+02**
3	1.5928e+05±1.0169e+04	**2.2184e+05±5.6274e+03**	2.1922e+05±9.8770e+03	**3.0502e+05±3.8101e+03**
4	3.2375e+06±1.5822e+05	**4.6241e+06±1.0429e+05**	5.0011e+06±1.5294e+05	**7.1498e+06±1.1297e+05**
5	3.0798e+07±9.1594e+05	**4.3179e+07±9.3915e+05**	4.9674e+07±1.4424e+06	**6.9709e+07±7.3509e+05**
6	1.8432e+08±4.8132e+06	**2.5407e+08±3.2081e+06**	3.1189e+08±6.3874e+06	**4.2528e+08±4.1760e+06**
7	8.2660e+08±2.4181e+07	**1.1120e+09±1.4090e+07**	1.4230e+09±3.1177e+07	**1.9016e+09±1.6540e+07**
8	3.0117e+09±8.1670e+07	**3.9801e+09±4.7710e+07**	5.2839e+09±1.0238e+08	**6.9010e+09±5.3581e+07**
9	9.4154e+09±1.9182e+08	**1.2056e+10±1.5229e+08**	1.6523e+10±2.3478e+08	**2.1191e+10±2.0042e+08**
10	2.5594e+10±4.2749e+08	**3.2446e+10±3.0182e+08**	4.5737e+10±7.0830e+08	**5.7618e+10±4.0182e+08**

TABLE III
PD AND $g(x)$ VALUES OF NSGA-III AND NSGA-III-PD ON DTLZ1 AND DTLZ2 WITH 2–10 OBJECTIVES. RESULTS ARE ANALYZED BY THE WILCOXON SIGNED-RANK TEST

		PD		$g(x)$	
	Obj #	NSGA-III	NSGA-III-PD	NSGA-III	NSGA-III-PD
DTLZ1	2	1.6727e+03±2.7442e+02	**1.8346e+03±2.1573e+02**	7.0679e-04±2.3335e-03	4.1325e-04±7.0457e-04
	3	1.3320e+05±9.4639e+03	**2.2082e+05±2.2913e+04**	1.5029e-03±3.3840e-03	2.4170e-03±3.2106e-03
	4	1.0958e+06±4.0122e+05	**4.2543e+06±5.2960e+05**	1.6038e-03±1.6340e-03	2.7882e-03±3.1630e-03
	5	1.0205e+07±1.8923e+06	**3.7418e+07±4.5229e+06**	2.3350e-03±1.8665e-03	3.7366e-03±4.8890e-03
	6	4.8452e+07±1.2605e+07	**2.1620e+08±2.0696e+07**	5.3858e-03±7.7352e-03	5.5380e-03±5.0331e-03
	7	1.5559e+08±1.1569e+08	**8.8898e+08±5.9677e+07**	5.0270e-02±2.0703e-01	8.3622e-03±4.8014e-03
	8	6.4514e+08±3.3415e+08	**2.9444e+09±5.2647e+08**	4.7582e-02±1.4214e-01	5.2672e-02±2.3234e-01
	9	2.5235e+09±2.2741e+09	**8.9356e+09±1.0713e+09**	3.8532e-01±7.1802e-01	**1.4316e-02±6.9197e-03**
	10	5.1432e+09±4.2678e+09	**2.1881e+10±3.0617e+09**	2.9395e-01±5.9308e-01	**1.5193e-02±1.4187e-02**
DTLZ2	2	1.4941e+03±1.5933e+02	**1.5904e+03±1.4061e+02**	8.3077e-06±1.7834e-05	5.4126e-06±1.6576e-05
	3	1.7236e+05±7.0653e+03	**2.3926e+05±1.1987e+04**	2.4075e-04±1.1921e-04	**1.3364e-04±1.1428e-04**
	4	1.3743e+06±2.0159e+05	**5.8579e+06±1.2859e+05**	3.3985e-04±3.0994e-04	**4.8578e-05±9.3405e-05**
	5	8.2560e+06±6.2260e+05	**6.4730e+07±7.3188e+05**	3.6085e-04±2.1909e-04	**1.2418e-04±6.5325e-05**
	6	2.5035e+07±2.8693e+06	**4.2078e+08±4.5902e+06**	7.2631e-04±5.5324e-04	**4.3826e-04±1.7594e-04**
	7	3.9486e+07±9.2457e+06	**2.0619e+09±2.3283e+07**	**8.8805e-04±4.9660e-04**	1.3534e-03±3.2693e-04
	8	9.6059e+07±1.5636e+07	**7.5109e+09±9.2085e+07**	**1.0299e-03±5.3518e-04**	2.2345e-03±3.9988e-04
	9	3.9851e+08±1.4748e+08	**2.4613e+10±2.8665e+08**	**2.3494e-03±1.3268e-03**	3.4445e-03±4.1437e-04
	10	6.0377e+08±2.0209e+08	**7.1405e+10±8.7984e+08**	**2.0842e-03±9.5192e-04**	4.6100e-03±6.2766e-04

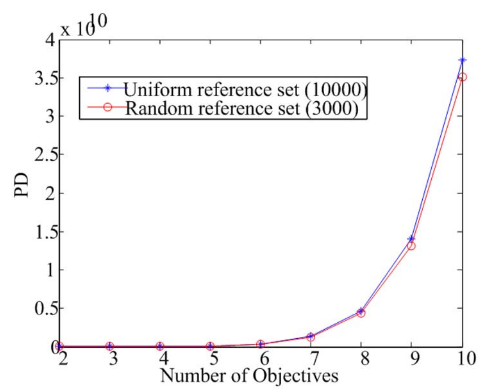

Fig. 18. PD values of reference sets with 2–10 objectives after the selection by PD guidance.

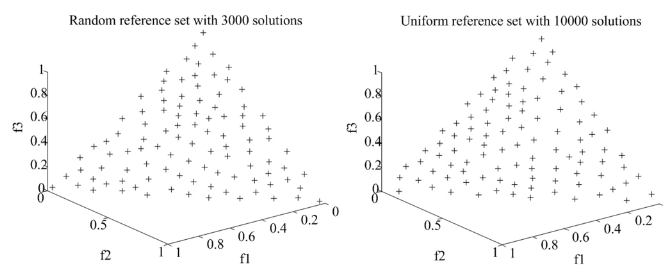

Fig. 19. Reference sets with three objectives after the selection by PD guidance from a random reference set with 3000 points and a uniform reference set with 10 000 points.

diversity performance of NSGA-III on all the test problems. Furthermore, the PD-based reference set generation has no negative effect on the convergence of DTLZ1 with 2–8 objectives, but improves the convergence of DTLZ1 with more than eight objectives and DTLZ2 with 2–6 objectives. Note that the PD-based reference set generation degrades the convergence performance of NSGA-III on DTLZ2 with more than six objectives, which remains unclear. Nevertheless, we can conclude that the PD-based reference set generation scheme can improve the diversity of reference-based MOEAs for MaOPs.

VI. CONCLUSION

A bio-inspired diversity metric, termed PD, is proposed to assess the performance of diversity of MOEAs for solving MaOPs. PD is a sum of the dissimilarity of solutions to the rest of the population in a greedy order, and the solution with the maximal dissimilarity has the highest priority to accumulate its dissimilarity. Thus, the diversity can be presented by the main dissimilarity in the population.

Through experiments on synthetic datasets, we show that PD is able to properly indicate the diversity of the population. Consequently, we used PD to assess the diversity of four MOEAs for solving MaOPs and analyze the characteristics of their diversity maintenance mechanisms. From the experimental results, we find that IBEA cannot achieve an adequately diverse solution set for MaOPs. Neither MOEA/D nor NSGA-III is able to maintain a large degree of diversity because their solution sets contain many solutions whose objective values heavily overlap. Independent of a reference set, the L_p-norm-based diversity maintenance in Two_Arch2 outperforms MOEA/D and NSGA-III in terms of PD values.

A PD-based diversity maintenance is also proposed for MOEAs, which is shown to be able to significantly improve solution diversity. Further, the PD-based diversity maintenance can be employed for the reference set generation in reference-based MOEAs, such as NSGA-III and MOEA/D, if the reference set is selected from a much larger reference set using the PD-based diversity maintenance scheme. It is shown that the diversity of NSGA-III is improved after embedding the new PD-based reference set generation method.

Although it can assess the diversity of the population of MOEAs for solving MaOPs, PD cannot be solely used to compare two solution sets for both convergence and diversity. A combination of different metrics should be adopted to completely evaluate the performance of MOEAs.

Much work remains to be done in the future. First, the complex relationship between convergence and diversity in many-objective optimization needs better understanding. Second, more experiments need to be done to verify the effectiveness of PD on MaOPs having complex PFs. Finally, the impact of p in L_p-norm based distance on the dissimilarity of MaOPs needs further investigation.

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