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A diversity indicator based on reference vectors for many-objective optimization

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ABSTRACT

Diversity estimation of Pareto front (PF) approximations is a critical issue in the field of evolutionary multiobjective optimization. However, the existing diversity indicators are usually inappropriate for PF approximations with more than three objectives. Many of them can be utilized only when compared with approximations obtained by multiple multiobjective optimizers, which makes them difficult to use online. In this paper, we propose a unary diversity indicator based on reference vectors (DIR) to estimate the diversity of PF approximations for many-objective optimization. In DIR, a set of uniform and widespread reference vectors are generated. The coverage of each solution in the objective space is evaluated by the number of representative reference vectors it is associated with. The diversity (both spread and uniformity) is determined by the standard deviation of the coverage for all the solutions. The smaller value of DIR, the better the diversity of a PF approximation is. DIR can be applied to a unary approximation without any compared approximations needed. Thus, DIR is easy to use as either an offline indicator to estimate the performance of an optimizer or an online indicator for the selection of solutions in a MOEA. In the experimental studies, both the artificial and the real PF approximations generated by seven different many-objective algorithms are used to verify DIR as an offline indicator. The effects of the number of reference vectors on DIR are also investigated. In addition, as an online indicator, DIR is integrated into a Pareto-dominance-based evolutionary multiobjective optimizer, NSGA-II. The experimental studies show it has the significant performance enhancements over the original NSGA-II on many-objective optimization problems.

1. Introduction

A multiobjective optimization problem (MOP) can be defined as follows:

$$\begin{aligned} &\text{minimize } F(x) = (f_1(x), \ldots, f_m(x))^T \\ &\text{subject to } x \in \Omega \end{aligned} \quad (1)$$

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where Ω is the *decision space*, F: $\Omega \rightarrow R^m$ consists of m real-valued objective functions. The *attainable objective set* is $\{F(x)|x \in \Omega\}$. Let $u, v \in R^m$, u is said to *dominate* v, denoted by $u \prec v$, if and only if $u_i \leq v_i$ for every $i \in \{1, \ldots, m\}$ and $u_j < v_j$ for at least one index $j \in \{1, \ldots, m\}$.[1] A solution $x^* \in \Omega$ is *Pareto-optimal* to (1) if there exists no solution $x \in \Omega$ such that $F(x)$ dominates $F(x^*)$. The set of all the Pareto-optimal points is called the *Pareto set* (*PS*) and the set of all the Pareto-optimal objective vectors is the *Pareto front* (*PF*) [37]. A PF approximation apparently can be very helpful for decision makers to understand the tradeoff relationship among different objectives and choose their preferred solutions. Over the past decades, multiobjective evolutionary algorithms (MOEAs) have been recognized as a major methodology for approximating the PFs in MOPs [9,15].

With the rapid growth of MOEAs [7,8,16,45] and other multiobjective optimizers [29] in the field of multiobjective optimization, the issue of performance assessment has become increasingly important. Various quality indicators [39,44,47] have already been proposed for performance evaluation. These indicators focus on one or several of the following aspects: 1) the convergence of the obtained PF approximation, 2) the spread (i.e., extensity) of the approximation and 3) the uniformity of the approximation. The latter two are closely related. Their combination is usually called the diversity of the approximation [32,39].

Many-objective optimization problems (MaOPs), i.e., MOPs with more than three objectives, appear widely in industrial and engineering design [18,24]. Over the recent years, the increasing amount of attention has been given to many-objective optimization in the community of MOEAs; and a wide variety of many-objective optimizers [10,13,33,43,48] have been developed and verified on problems with different characteristics [17,21,23].

However, the quality indicators to evaluate the performance of many-objective optimizers have not yet gained enough attention and concern [25]. Most indicators are infeasible or improper to evaluate PF approximations with a large number of objectives. In general, the difficulties of comparing multiple PF approximations may be summarized in the following reasons.

1. The unavailability of visual comparison for PF approximations with more than three objectives: When the number of objectives of PF approximations is more than three, visual and intuitive quality indicator can be misleading or even impossible, even though it is a prevailing comparison tool in the literature [32].
2. A compared set needed: Many indicators can only be used when compared two or more PF approximations, which makes it difficult for online investigations of a many-objective optimizer during its optimization process. In fact, the indicator that works on unary approximation not only can conduct offline estimations of the quality of an PF approximation, but also can be used to guide the selection in MOEAs in an online manner [3,5,48].
3. The lack of a reference set as a substitution of the real PF: The number of points required to accurately approximate the PF grows exponentially with more objectives. Thus, the choice of appropriate representative Pareto optimal solutions becomes an increasingly difficult task. Even worse, the true shapes and distributions of PFs are usually unknown beforehand for real-world MOPs.
4. Escalating time and space complexity: More objectives result in an exponential increase on the time and space complexity for some commonly used indicators, such as Hypervolume [49], diversity measure [14] and hyperarea difference [42]. In fact, the high space and time complexity not only limit their applicability in offline performance comparisons of high-dimensional PF approximations obtained by various many-objective optimizers, but also make it inappropriate for online evaluations of the performance of a single many-objective optimizer.

In the literature, a variety of convergence indicators have been proposed to avoid the aforementioned challenges. For this purpose, either the characteristics of the PFs in the considered test problems [26,41] or the dominance relations between the individuals [10,47] are utilized. Nevertheless, the diversity indicator seems much more difficult to design for appropriately reflecting the distribution of the approximations in many-objective optimization [39]. Over the recent years, the indicators that consider both diversity and convergence, such as Hypervolume (HV) [49] and Inverted Generational Distance (IGD) [6], are very popular in the multiobjective evolutionary optimization community [5,25,45]. IGD and HV can be defined as follows.

- Inverted Generational Distance (IGD) [6]: Let P^* be a set of points uniformly sampled over the true PF, and S be the set of solutions obtained by an EMO algorithm. The IGD value of S is computed as:

$$IGD(S, P^*) = \frac{\sum_{x \in P^*} dist(x, S)}{|P^*|} \tag{2}$$

  where $dist(x, S)$ is the Euclidean distance between a point $x \in P^*$ and its nearest neighbor in S, and $|P^*|$ is the cardinality of P^*. The lower is the IGD value, the better is the quality of S for approximating the whole PF.
- Hypervolume (HV) [49]: Let $r^* = (r_1^*, r_2^*, \ldots, r_m^*)^T$ be a reference point in the objective space that dominated by all solutions in a PF approximation S. HV metric measures the size of the objective space dominated by the solutions in S and bounded by r^*.

$$HV(S) = VOL(\bigcup_{x \in S} [f_1(x), r_1^*] \times \ldots [f_m(x), r_m^*]) \tag{3}$$

  where $VOL(\bullet)$ indicates the Lebesgue measure. Hypervolume can measure the approximation in terms of both diversity and convergency. The larger is the HV value, the better is the quality of S for approximating the whole PF.

[1] In the case of maximization, the inequality signs should be reversed.