VSD-MOEA: A Dominance-Based Multi-Objective Evolutionary Algorithm with Explicit Variable Space Diversity Management

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***Abstract*—Most state-of-the-art Multi-objective Evolutionary Algorithms (MOEAs) promote the preservation of the diversity in the objective space, whereas the information about the diversity in the decision variables is usually neglected. In this paper, the Variable-Space-Diversity based MOEA (VSD-MOEA) is presented. VSD-MOEA is a dominance-based MOEA that considers explicitly the diversity in the decision variables and the objective space. The information gathered of both spaces is used simultaneously with the aim of properly adapting the balance between exploration and intensification during the optimization process. Particularly, at the initial stages, decisions taken by the approach are more biased by the information of the diversity in the decision variables, whereas in the last stages decisions are only based on the information of the objective space. The latter is achieved through a novel density estimator. The new method is compared with state-of-art MOEAs using several benchmarks with two and three objectives. The novel proposal attains much better results than state-of-the-art schemes, showing a more stable and robust behavior.**

I. Introduction

MULTI-OBJECTIVE Optimization Problems (MOPs) involve the simultaneous optimization of several objective functions that are usually in conflict [1]. A continuous box-constrained minimization MOP, which is the kind of problem addressed in this paper, can be defined as follows:

$$\begin{aligned} &minimize \quad \vec{F} = [f_1(\vec{\mathbf{x}}), f_2(\vec{\mathbf{x}}), ..., f_M(\vec{\mathbf{x}})] \\ &subject \quad to \quad x_i^{(L)} \leq x_i \leq x_i^{(U)}, \quad i = 1, 2, ..., n. \end{aligned} \tag{1}$$

where n corresponds to the dimension of the variable space, $\vec{\mathbf{x}}$ is a vector of n decision variables $\vec{\mathbf{x}} = (x_1, ..., x_n) \in R^n$, which are constrained by $x_i^{(L)}$ and $x_i^{(U)}$, i.e. the lower bound and upper bound, and M is the number of objective functions to optimize. The feasible space bounded by $x_i^{(L)}$ and $x_i^{(U)}$ is denoted by Ω, each solution is mapped to the objective space with the function $F : \Omega \rightarrow R^M$, which consist of M real-valued objective functions and R^M is called the *objective space*.

Given two solutions $\vec{\mathbf{x}}$, $\vec{\mathbf{y}} \in \Omega$, $\vec{\mathbf{x}}$ dominates $\vec{\mathbf{y}}$, mathematically denoted by $\vec{\mathbf{x}} \prec \vec{\mathbf{y}}$, iff $\forall m \in 1, 2, ..., M : f_m(\vec{\mathbf{x}}) \leq f_m(\vec{\mathbf{y}})$ and $\exists m \in 1, 2, ..., M : f_m(\vec{\mathbf{x}}) < f_m(\vec{\mathbf{y}})$. The best solutions of a MOP are those whose objective vectors are not dominated by any other feasible vector. These solutions are known as the Pareto optimal solutions. The Pareto set is the set of all Pareto optimal solutions, and the Pareto front are the images of the Pareto set. The goal of most multi-objective optimizers is to obtain a proper approximation of the Pareto front, i.e., a set of well distributed solutions that are close to the Pareto front.

One of the most popular metaheuristics used to deal with MOPs is the Evolutionary Algorithm (EA). In single-objective EAs, it has been shown that taking into account the diversity of the variable space to properly balance between exploration and exploitation is highly important to attain high quality solutions [2]. Diversity can be taken into account in the design of several components such as in the variation stage [3], [4], replacement phase [5] and/or population model [6]. The explicit consideration of diversity leads to improvements in terms of premature convergence avoidance, meaning that taking into account the diversity in the design of EAs is specially important when dealing with long-term executions. Recently, some diversity management algorithms that combine the information of diversity, stopping criterion and elapsed generations have been devised. They have allowed to provide a gradual loss of diversity that depends on the time or evaluations granted to the execution [5]. Particularly the aim of such a methodology is to promote exploration in the initial generations and gradually alter the behavior towards intensification. These schemes have provided really promising results. For instance, new best-known solutions for some well-known variants of the frequency assignment problem [7], and for a two-dimensional packing problem [5] have been attained using the same principles. Additionally, this principle guided the design of the winning strategy of the Second Wind Farm Layout Optimization Competition[1], which was held in the Genetic and Evolutionary Computation Conference. Thus, the benefits of such kind of design patterns have been shown in several different single-objective optimization problems.

One of the goals in the design of Multi-objective Evolutionary Algorithms (MOEAs) is to obtain a well-spread set of solutions in the objective space. The maintenance of some degree of diversity in the objective space implies that complete convergence does not appear in the variable space [8]. In some way, the variable space inherits some degree of diversity

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[1]https://www.irit.fr/wind-competition/

due to the way in which the objective space is taken into account. However, this is just an indirect way of preserving the diversity in the variable space, so in some cases the level of diversity might not be large enough to ensure a high degree of exploration. For instance, it has been shown that with some of the WFG benchmarks, in most of the state-of-the-art MOEAs the *distance parameters* quickly converge, meaning that the approach focuses just on optimizing the *position parameters* for a long period of the optimization process [8]. Thus, while some degree of diversity is maintained, a similar situation to premature convergence is presented meaning that genetic operators might not be able to generate better trade-offs.

Attending to the differences between state-of-the-art single-objective EAs and MOEAs, this paper proposes a novel MOEA, the Variable-Space-Diversity based MOEA (VSD-MOEA), that is based on controlling the amount of diversity in the variable space in an explicit way. Similarly to the successful methodology applied in single-objective optimization, the stopping criterion and the amount of evaluations performed are used to vary the amount of desired diversity. The main difference with respect to the single-objective case is that the objective space is simultaneously considered, which is performed with a novel objective-space density estimator. Particularly, the approach grants more importance to the diversity of the variable space in the initial stages, whereas as the generations evolve, it gradually grants more importance to the diversity of the objective space. In fact, at the last period of the execution, the diversity of the variable space is neglected, so in the last phases the proposal is quite similar to current state-of-the-art approaches. To our knowledge, this is the first MOEA whose design follows this adaptive principle. Since there exist currently a quite large amount of different MOEAs [9], three popular schemes have been selected to validate our proposal. This validation has been performed with several well-known benchmarks and proper quality metrics. The important benefits of properly taking into account the diversity of the variable space is clearly shown in this paper. Particularly, the advantages are clearer in the most complex problems. Note that this is consistent with the single-objective case, where the most important benefits have been obtained in complex multi-modal cases [7].

The rest of this paper is organized as follows. Section II provides a review of related papers. Some key components related to diversity and the VSD-MOEA design are discussed. The VSD-MOEA proposal is detailed in section III. Section **??** is devoted to the experimental validation of the novel proposal. Finally, conclusions and some lines of future work are given in Section **??**. Note also that some supplementary materials are given. They include details of the experimental results with additional metrics as well as some explanatory videos.

II. Literature Review

This section is devoted to review some of the most important papers that are closely related to our proposal. First, some of the most popular ways of managing diversity in EAs are presented. Then, the state-of-the-art in MOEAs is summarized.

A. Diversity Management in Evolutionary Algorithms

The proper balance between exploration and exploitation is one of the keys to success in the design of EAs. In the single-objective domain it is known that properly managing the diversity in the variable space is a way to control such balance, and as a consequence, a large amount of diversity management techniques have been devised [10]. Particularly, these methods are classified depending on the component(s) of the EA that is modified to alter the amount of maintained diversity. A popular taxonomy identifies the following groups [11]: *selection-based*, *population-based*, *crossover/mutation-based*, *fitness-based*, and *replacement-based*. Additionally, the methods are referred to as *uniprocess-driven* when a single component is altered, whereas the term *multiprocess-driven* is used to refer to those methods that act on more than one component.

Among the previous proposals, the replacement-based methods have attained very high-quality results in last years [7], so this alternative was selected with the aim of designing a novel MOEA incorporating an explicit way to control the diversity in the variable space. The basic principle of these methods is to bias the level of exploration in successive generations by controlling the diversity of the survivors [7]. Since premature convergence is one of the most common drawbacks in the application of EAs, modifications are usually performed with the aim of slowing down the convergence. One of the most popular proposals belonging to this group is the *crowding* method which is based on the principle that offspring should replace similar individuals from the previous generation [12]. Several replacement strategies that do not rely on crowding have also been devised. In some methods, diversity is considered as an objective. For instance, in the hybrid genetic search with adaptive diversity control (HGSADC) [13], individuals are sorted by their contribution to diversity and by their original cost. Then, the rankings of the individuals are used in the fitness assignment phase. A more recent proposal [7] incorporates a penalty approach to alter gradually the amount of diversity maintained in the population. Particularly, initial phases preserve a larger amount of diversity than the final phases of the optimization. This last method has inspired the design of the novel proposal put forth in this paper for multi-objective optimization.

It is important to remark that in the case of multi-objective optimization, few works related to the maintenance of diversity in the variable space have been developed. The following section reviews some of the most important MOEAs and introduces some of the works that consider the maintenance of diversity in the variable space.

B. Multi-objective Evolutionary Algorithms

In recent decades, several MOEAs have been proposed. While the purpose of most of them is to provide a well-spread set of solutions close to the Pareto front, several ways of facing this purpose have been devised. Therefore, several taxonomies have been proposed with the aim of better classifying the different schemes [14]. Particularly, a MOEA can be designed based on Pareto dominance, indicators and/or decomposition [15]. Since none of the groups has a remarkable superiority over the others, in this work all of them are taken into account to validate our proposal. This section introduces the three types of schemes and some of the most popular approaches belonging to each category. Then, one MOEA of each category is selected to carry out the validation of VSD-MOEA.

The dominance-based category includes those schemes where the Pareto dominance relation is used to guide the design of some of its components such as the fitness assignment, parent selection and replacement phase. The dominance relation does not inherently promotes the preservation of diversity in the objective space, therefore additional techniques such as objective-space density estimators are usually integrated with the aim of obtaining a proper spread and convergence to the Pareto front.

In order to assess the performance of MOEAs, several quality indicators have been devised. In the indicator-based MOEAs, the use of the Pareto dominance relation is substituted by some quality indicators to guide the decisions performed by the MOEA. An advantage of this kind of algorithms is that the indicators usually take into account both the quality and diversity in objective space, so incorporating additional mechanisms to promote diversity in the objective space is not required. Among the different indicators, hypervolume is a widely accepted Pareto-compliance quality indicator. The Indicator-Based Evolutionary Algorithm (IBEA) [16] was the first method belonging to this category. A more recent one is the R2-Indicator-Based Evolutionary Multi-objective Algorithm (R2-EMOA) [17], which has reported a quite promising performance in MOPs. Its most important feature is the use of the R2 indicator.

Finally, decomposition-based MOEAs [18] are based on transforming the MOP into a set of single-objective optimization problems that are tackled simultaneously. This transformation can be performed in several ways, e.g. with a linear weighted sum or with a weighted Tchebycheff function. Given a set of weights to establish different single-objective functions, the MOEA searches for a single high-quality solution for each of them. The weight vectors should be selected with the aim of obtaining a well-spread set of solutions [1]. The Multi-objective Evolutionary Algorithm Based on Decomposition (MOEA/D) [19] is the most popular decomposition-based MOEA. Its main principles include problem decomposition, weighted aggregation of objectives and mating restrictions through the use of neighborhoods.

It is important to stand out that none of the most popular algorithms in the multi-objective field introduce special mechanisms to promote diversity in variable space. However, some efforts have been dedicated to this principle. A popular approach to promote the diversity in the decision space is the application of fitness sharing [20] in a similar way than in single-objective optimization. Although, fitness sharing might be used to promote diversity both in objective and decision variable space, most popular variants consider only distances in the objective space. Another MOEA designed to promote diversity in both the decision and the objective space is the Genetic Diversity Evolutionary Algorithm (GDEA) [21]. In this case, each individual is assigned with a diversity-based objective which is calculated as the Euclidean distance in the genotype space to the remaining individuals in the population. Then, a ranking that considers both the original objectives and the diversity objective is used to sort individuals. Another somewhat popular approach is to calculate distances between candidate solutions by taking into account both the objective and variable space [22], [23] with the aim of promoting diversity in both spaces. A different proposal combines the use of two selection operators [24]. The first one promotes diversity and quality in the objective space whereas the second one promotes diversity in the decision space. A different approach was to modify the hypervolume to integrate the decision space diversity in a single metric [25]. In this approach, the proposed metric is used to guide the selection in the MOEA. Finally, some indirect mechanisms that might affect the diversity have also been taken into account. Probably, the most popular one is the use of mating restrictions [26], [18].

Attending to the results of previous described approaches, it is clear that taking into account the decision space diversity in the design phase might bring benefits to decision makers because the final solutions obtained by these methods present a larger decision space diversity than the ones obtained by traditional approaches [22], [27]. Thus, while clear improvements are obtained when taking into account metrics related to the Pareto set, the benefits in terms of the obtained Pareto front are not so clear. We claim that one of the reasons of this behavior might be that the diversity in the variable space is considered in the whole optimization process. However, in a similar way that in the single objective domain, reducing the importance granted to the diversity in the decision space as the generations progress [5] might be really important to attain better approximations of the Pareto front. Currently, no MOEA considers this idea, so this principle has guided the design of our novel MOEA.

III. Proposal

This section is devoted to fully describe our novel proposal. The novelty of VSD-MOEA appears in the replacement phase, which incorporates the use of variable space diversity and a novel objective-space density estimator. The main principle behind the design of the novel replacement is to use the stopping criterion and elapsed generations with the aim of gradually moving from exploration to exploitation during the search process. Note that this principle might be incorporated in any of the three categories of MOEAs. In this paper, our decision was to incorporate it in a dominance-based approach and apply it to problems with a low number of objectives. Thus, some of our design decisions might not be suitable for dealing with many-objective optimization problems.

The general framework of VSD-MOEA is quite standard. Algorithm 1 shows the pseudocode of VSD-MOEA. The parent selection is performed with binary tournament based on the dominance raking with ties broken randomly. The variation stage is based on applying the well-known Simulated Binary Crossover (SBX) and polynomial mutation [28], [29]. Thus, the contribution appears in the replacement phase. The rest of this section is devoted to describe the replacement phase, including the novel objective-space density estimator.

Algorithm 1 Main procedure of VSD-MOEA

Initialization: Generate an initial population P_0 with N individuals.
Evaluation: Evaluate all individuals in the population.
Assign $t = 0$
while (not stopping criterion) **do**
    Mating selection: Fill the mating pool by performing binary tournament selection on P_t, based on the non-dominated ranks (ties are broken randomly).
    Variation: Apply SBX crossover and Polynomial mutation to the mating pool to create a child population Q_t.
    Evaluation: Evaluate all individuals in Q_t.
    Survivor selecction: Generate P_{t+1} by applying the replacement scheme described in Algorithm 2, using P_t and Q_t as input.
    $t = t + 1$

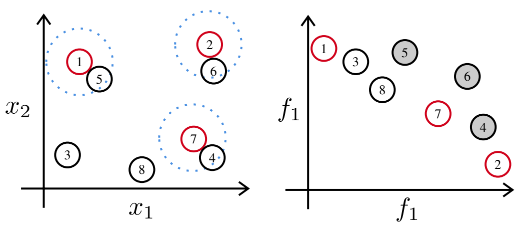

Fig. 1. Penalty Method of the Replacement Phase - The left side represents the variables space and the right side the objective space

A. Replacement Phase of VSD-MOEA

The replacement phase of EAs is in charge of deciding in each generation which are the survivors among the members of the previous population and offspring. The novel replacement promotes a gradual movement from exploration to exploitation, which has been a quite beneficial principle in the design of single-objective optimizers [5]. Particularly, the replacement phase operates as follows. First, the members of the previous population and offspring are joined in a multi-set with $2 \times N$ individuals. Then, an iterative process that selects an additional individual at each iteration is used to pick up the N survivors. In order to take into account the diversity in the decision space, the Distance to Closest Survivor (DCS) of each individual is calculated at each iteration. Thus, the DCS of an individual I is calculated as $\min_{s \in S} Distance(I, s)$, where S is the multi-set containing the currently selected survivors. Normalized Euclidean distances are considered, so in order to calculate distances between any two individual A and B, Eq. (2) is applied. In the first iteration, the S multi-set is empty, so the DCS of each individual is infinity.

$$Distance(A, B) = \left(\frac{1}{n} \sum_{i=1}^{n} \left(\frac{A_i - B_i}{x_i^{(U)} - x_i^{(L)}} \right)^2 \right)^{1/2} \tag{2}$$

Note that individuals with larger DCS values are those that contribute more significantly to promote exploration. In order to avoid an excessive decrease of the exploration degree, individuals with a DCS value lower than a threshold value are penalized and they can only be selected if non-penalized individuals do not exist. Then, among the non-penalized individuals, an objective-space density estimator is used to select the additional survivor of the iteration. In our case, the novel density estimator described in the next subsection is used.

In order to better understand the penalty method, it can be visualized in the following way. After selecting each survivor, a hyper-sphere centered in such a candidate solution — in the variable space — is created. Then, all the individuals that are inside a hyper-sphere are penalized and the objective-space estimator takes into account only the survivors and non-penalized individuals. This is illustrated in Fig. 1, which represents a state where three individuals have been selected to survive and an additional survivor must be picked up. The left side shows individuals in the variable space. Current survivors are marked with a red border and each one of them is surrounded by a blue dash circle with radius D_t. In this situation, the penalized individuals are the number 4, 5, and 6. In the objective space — right side — penalized individuals are shown with gray background, indicating that the objective-space density estimator does not take them into account.

Since penalizing with a large threshold value — radius of the hyperspheres — induces a large degree of exploration, it makes sense to reduce this value during the optimization process. This is precisely one of the keys of our proposal. The sizes of the hyper-spheres are modified dynamically by taking into account the stopping criterion and elapsed generations. Particularly, the radius is decreased in a linear way starting from an initial distance. This means that in the initial phases exploration is promoted. However, as the size of the radius decreases only very close individuals are penalized, meaning that more exploitation is allowed. Note that this method requires a parameter which is the initial radius of the hyper-spheres which is denoted as D_I. Setting this parameter with a large value might provoke the penalization of a lot of individuals, thus non-useful diversity might be maintained. However, too small values might not prevent fast convergence and therefore the approach might behave as a traditional non-diversity based MOEA. The robustness of the proposal with respect to this additional parameter is studied in our experimental validation.

Algorithm 2 fully describes the replacement phase of VSD-MOEA. First, the population of the previous generation (P_t) and the offspring (Q_t) are joined in R_t (line 3). The multiset R_t contains, at each iteration, the remaining non-penalized individuals that might be selected to survive. The population of survivors (P_{t+1}) and the set containing the penalized individuals are initialized to the empty set (lines 4 and 5). Then, the threshold value (D_t) that is used to penalize too close individuals is calculated (line 6). Note that D_I denotes the initial threshold value, $G_{Elapsed}$ is the amount of generations that have been evolved, and G_{End} is the stopping criterion, i.e. the number of generations that are to be evolved in the execution of VSD-MOEA. The linear decrease is calculated so that after the 90% of the generations, the D_t value is lower than 0, meaning that no penalties are performed. This means that in the first 90% of the generations, more exploration than in traditional MOEAs is induced.

Then, an iterative process that selects an individual at each iteration is executed until the survivors set contains N individuals (line 7). The iterative process works as follows. First,

Algorithm 2 Replacement Phase of VSD-MOEA

1: Input: P_t (Population of current generation), Q_t (Offspring of current Generation)
2: Output: P_{t+1}
3: $R_t = P_t \cup Q_t$
4: $P_{t+1} = \emptyset$
5: $Penalized = \emptyset$
6: $D_t = D_I - D_I * \frac{G_{Elapsed}}{0.9 * G_{End}}$
7: **while** $|P_{t+1}| \leq$ N **do**
8: Compute DCS of individuals in R_t with P_{t+1} used as reference set
9: Move to $Penalized$ the individuals in R_t with $DCS < D_t$
10: **if** R_t is empty **then**
11: Compute DCS of individuals in $Penalized$ with P_{t+1} used as reference set
12: Move to R_t the individual in $Penalized$ with largest DCS
13: Identify the first front (F) in $R_t \cup P_{t+1}$ with an individual $I \in R_t$
14: Use the novel density estimator (Algorithm 2) to select a new survivor from F and move it to P_{t+1}
15: **return** P_{t+1}

the DCS value of each remaining non-penalized individual is calculated (line 8). Then, those individuals with a DCS value lower than D_t are moved to the set of penalized individuals (line 9). If all the remaining individuals are penalized (line 10), it means that the amount of exploration is lower than the desired one. Thus, the individual with the largest DCS value is recovered, i.e. moved to the non-penalized individuals set (lines 11 and 12) and consequently it survives. Finally, the objective space is taken into account. Specifically, candidate non-penalized individuals and current survivors are joined. Then, the well-known non-dominated sorting procedure [30] is executed with such a set, stopping as soon as a front with a candidate individual is found, i.e. with an individual of R_t (line 13). Then, taking the identified front as input, a novel objective-space density estimator is used to select the next survivor (line 14). The specific way in which the diversity in the objective space is measured is described in the next section.

B. A Novel Density Estimator for the Objective Space

Since the dominance definition is not related to the preservation of diversity in the objective space, dominance-based MOEAs usually incorporate objective-space density estimators to promote the survival of diverse individuals. As it was previously described, our density estimator selects a new survivor from the front identified in line 14 of Algorithm 2. This front contains at least one individual belonging to R_t and it might also contain some elements of P_{t+1}. The aim behind the selection of the next survivor is to pick up an individual of the input front that contributes significantly in terms of objective-space quality and diversity and belongs to R_t.

Algorithm **??** describes the selection of the next survivor. First, similarly to most state-of-the-art algorithms, an action to promote the selection of boundary solutions is executed. Note that selecting the best solution for each objective might provoke some drawbacks related to accepting small improvement in an objective at the cost of important worsening in other objectives [31]. To solve this issue augmented functions can be applied, which has been the alternative used in this paper. Particularly, iteratively, for each objective k the candidate solution that minimizes the Augmented Weighted Function (AWF) given in Eq. 3 is calcualated (line XXX). If such an individual belongs to R_t, i.e., it has not been selected yet as a survivor, the next survivor is such an individual and the process finalizes (line YYY). Note that, augmented functions usually take into account weight vectors with the aim of dealing with objectives that present very different scales. Since benchmarks that have similar scales in each objective have been used in this paper, there was no need to apply such weight vectors.

$$AWF_k(\vec{x}) = f_k(\vec{x}) + 10^{-4} \times \sum_{j=1}^{M} f_j(\vec{x}) \tag{3}$$

In cases where the individuals that optimize each AWF_K function are already in P_{t+1}, a contribution to objective-space diversity is calculated by taking into account the current survivors of the front (line XXX). Particularly, the "Improvement Distance" (ID) defined for the indicator IGD+ [32] is used. The ID of an individual A with respect to an individual B is calculated by taking into account only the functions where A is better. Specifically, Eq. (4) is used.

$$ID(A, B) = \left(\sum_{i=1}^{M} (max(0, B_i - A_i))^2 \right)^{1/2} \tag{4}$$

Denoting as FS the members of the input front that are already in P_{t+1}, the contribution to diversity of each member of the input front that belongs to R_t is calculated as $\min_{s \in S} ID(I, s)$. Then, the individual with a higher contribution is selected as the next survivor, with ties broken randomly (line XXX).

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