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 diversity of objective function space but neglect the diversity of decision variable space. The aim of this paper is to show that explicitly managing the amount of diversity maintained in the decision variable space is useful to increase the quality of MOEAs when taking into account metrics of the objective space. Our novel Variable Space Diversity based MOEA (VSD-MOEA) explicitly considers the diversity of both decision variable and objective function space. This information is used with the aim of properly adapting the balance between exploration and intensification during the optimization process. Particularly, at the initial stages, decisions made by the approach are more biased by the information on the diversity of the variable space, whereas it gradually grants more importance to the diversity of objective function space as the evolution progresses. 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. This novel proposal yields much better results than state-of-the-art schemes when considering metrics applied on objective function space, exhibiting a more stable and robust behavior.

Keywords
Multi-objective Evolutionary Algorithms, Premature Convergence, Diversity Preservation

1 Introduction

Multi-objective Optimization Problems (MOPs) involve the simultaneous optimization of several objective functions that are usually in conflict with each other (Deb, 2001). A continuous box-constrained minimization MOP, which is the kind of problem addressed in this paper, can be defined as follows:

$$\begin{aligned}
\min \quad & \vec{f} = [f_1(\vec{x}), f_2(\vec{x}), ..., f_m(\vec{x})] \\
\text{subject to} \quad & x_i^{(L)} \le x_i \le x_i^{(U)}, \quad i = 1, 2, ..., n.
\end{aligned} \tag{1}$$

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

Given two solutions $\vec{x}, \vec{y} \in \Omega$, $\vec{x}$ dominates $\vec{y}$, which is mathematically denoted by $\vec{x} \prec \vec{y}$, iff $\forall i \in 1, 2, ..., m : f_i(\vec{x}) \leq f_i(\vec{y})$ and $\exists i \in 1, 2, ..., m : f_i(\vec{x}) < f_i(\vec{y})$. The best solutions of an MOP are those that 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 is the image (i.e., the corresponding objective function values) of the Pareto optimal set. The goal of 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 meta-heuristics 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 decision variable space to properly balance between exploration and exploitation is highly important to attain high quality solutions (Herrera and Lozano, 1996). Diversity can be taken into account in the design of several components, such as in the variation stage (Herrera and Lozano, 2003; Mitchell, 1998), the replacement phase (Segura et al., 2015) and/or the population model (Koumousis and Katsaras, 2006). The explicit consideration of diversity usually leads to improvements in terms of avoiding premature convergence, meaning that taking into account diversity in the design of EAs is especially important when dealing with long runs. Recently, some diversity management algorithms that combine the information on diversity, stopping criterion and elapsed generations have been devised. They have yielded a gradual loss of diversity that depends on the time or evaluations granted to the execution (Segura et al., 2015). Specifically, 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 highly promising results. For instance, new best-known solutions for some well-known variants of the frequency assignment problem (Segura et al., 2016), and for a two-dimensional packing problem (Segura et al., 2015) 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 (Wilson et al., 2018) and of the extended round of Google Hash Code 2020 [1] , with more than $100,000$ participants. Thus, the benefits of this type of design pattern have been shown in several different single-objective optimization problems.

One of the goals when designing Multi-objective Evolutionary Algorithms (MOEAs) is to obtain a well-spread set of solutions in objective function space. As a result, most state-of-the-art MOEAs consider the diversity of the objective space explicitly. However, this is not the case for the diversity of decision variable space. Maintaining some degree of diversity in objective space implies that full convergence is not achieved in decision variable space (Kukkonen and Lampinen, 2009). In some way, decision variable space inherits some degree of diversity due to the way in which objective space is taken into account. However, this is just an indirect way of preserving diversity of decision variable space, so in some cases the level of diversity might not be large enough to ensure a proper degree of exploration. For instance, it has been shown

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[1] https://codingcompetitions.withgoogle.com/hashcode/

that with some of the WFG test problems, in most 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 (Chacón Castillo et al., 2017). Thus, while some degree of diversity is maintained, a situation similar to premature convergence occurs, meaning that genetic operators might no longer be able to generate better trade-offs.

In light of 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), which relies on explicitly managing the amount of diversity in decision variable space. Similarly to the successful methodology applied in single-objective optimization, the stopping criterion and the number of evaluations evolved are used to vary the amount of diversity desired in decision variable space. The main difference with respect to the single-objective case is that diversity of the objective function space is simultaneously considered by using a novel objective space density estimator. Particularly, the approach grants more importance to the diversity of decision variable space in the initial stages, and it gradually grants more importance to the diversity of objective function space as the evolution progresses. In fact, in the last stage of execution, diversity of decision variable space is neglected. Thus, in the last phases, the proposed approach is quite similar to current state-of-the-art approaches. To the best of our knowledge, this is the first MOEA whose design follows this dynamic principle.

Since there currently exists quite a large number of different MOEAs (Tan et al., 2005), three popular schemes have been selected to validate our proposal, including one that promotes diversity in the variable space to deal with multi-modal multi-objective optimization. This validation was performed using several well-known benchmarks and proper quality metrics. This paper clearly shows the important benefits of properly taking into account the diversity of decision variable space. In particular, the advantages become more evident 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 (Segura et al., 2016). It is also important to clarify that, in spite of considering the variable-space diversity, our work is not a niche-based proposal for multimodal optimization (Deb and Tiwari (2005), Zhou et al. (2009), Li et al. (2016),Liang et al. (2016)). Instead, this work is oriented to show that managing explicitly the amount of diversity maintained in the decision variable space is useful to increase the quality of MOEAs when taking into account metrics of the objective space.

The rest of this paper is organized as follows. Section 2 provides a review of the previous related work. Additionally, some key components related to diversity and to the VSD-MOEA design are discussed. The VSD-MOEA proposal is detailed in Section 3. Section 4 is devoted to the experimental validation of the proposal. Finally, our conclusions and some lines of future work are given in Section 5. Note also that some supplementary materials are also provided. They include details of the experimental results with additional performance measures and some additional experiments, as well as an explanatory video.

2 Literature Review

This section is devoted to reviewing some of the most relevant works that are 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 briefly summarized.

2.1 Diversity Management in Evolutionary Algorithms

The proper balance between exploration and exploitation is one of the keys to designing successful EAs. In the single-objective domain, it is known that properly managing the diversity of decision variable space is a way to achieve this balance, and as a consequence, a large number of diversity management techniques have been devised (Pandey et al., 2014). Specifically, these methods are classified depending on the component(s) of the EA that is modified to alter the way in which diversity is maintained. A popular taxonomy identifies the following groups (Črepinšek et al., 2013): *selection-based*, *population-based*, *crossover/mutation-based*, *fitness-based*, and *replacement-based*, among others. 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 yielded very high-quality results in recent years (Segura et al., 2016), so this alternative was selected with the aim of designing a novel MOEA that explicitly incorporates a way to control the diversity of decision 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. 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 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 (Mengshoel et al., 2014). 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) proposed by Vidal et al. (2013), 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 (Segura et al., 2016) incorporates a penalty approach to gradually alter the amount of diversity maintained in the population. Specifically, the initial phases preserve a higher 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, little work related to maintaining the diversity of decision variable space has been done. The exception are those algorithms that aim to obtain diverse Pareto sets, instead of only diverse and high-quality Pareto fronts. The following section reviews some of the most important MOEAs and introduces some of the works that consider the maintenance of diversity of decision variable space.

2.2 Multi-Objective Evolutionary Algorithms

In recent decades, several MOEAs have been successful in solving MOPs. Most of them are designed with the goal of providing a set of solutions with good convergence and diversity in objective space. Some representative MOEAs are the Non-Dominated Sorting Genetic Algorithm II (NSGA-II) (Deb et al., 2002), the Multi-objective Evolutionary Algorithm Based on Decomposition (MOEA/D) (Zhang and Li, 2007), the R2-Indicator-Based Evolutionary Multi-objective Algorithm (R2-EMOA) (Trautmann et al., 2013) and the S-Metric Selection Evolutionary Multi-objective Optimization Algorithm (SMS-EMOA) (Beume et al., 2007). By contrast, Evolutionary Multi-modal Multi-objective Algorithms (EMMAs) aim to identify high-quality solutions that are diverse in both the objective space and the decision variable space. Interestingly, some authors (Liu et al.,

2019) have identified that for particular problems, such as the Imbalanced Problems, EMMAs aid in the location of broader fronts in objective space, meaning that the additional exploration promoted in EMMAs yields higher-quality solutions in terms of objective space metrics.

In spite of these findings, none of the most popular MOEAs introduces special mechanisms to promote diversity in the decision variable space. It might be argued that for those particular cases where more exploration is required, EMMAs might be used. However, in the case of single-objective optimization, the recommended way of managing diversity in the decision variable space is very different in multi-modal optimization than in global optimization (Črepinšek et al., 2013). In order to illustrate that this is also the case for multi-objective optimization, the experimental validation presented in this paper takes into account both state-of-the-art MOEAs and a popular EMMA. The efforts to consider the diversity in the decision space in MOEAs and EMMAs are reviewed in the following. Note that in most cases, they are devoted to multi-modal multi-objective optimization.

One of the first approaches to promote diversity in decision variable space is based on the application of fitness sharing (Horn et al., 1994), in a way similar to single-objective optimization. Distances have been considered both in terms of the decision variable space and objective space. The main issue is that they are not taken into account simultaneously. One MOEA designed to promote diversity of both the decision variable space and objective function space is the Genetic Diversity Evolutionary Algorithm (GDEA) proposed by Toffolo and Benini (2003). In this case, each individual is assigned 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. More complex ways of integrating the information on both kinds of diversity to alter the selection mechanisms have been devised (Deb and Tiwari, 2005; Shir et al., 2009; Cuate and Schütze, 2019). Another related method involves modifying the hypervolume to integrate the decision variable space diversity into a single metric (Ulrich et al., 2010). In this approach, the proposed metric is also used to guide the selection.

Other strategies also alter the selection mechanism but following a different path. In Chan and Ray (2005), two selection operators of different nature are considered simultaneously. The first one promotes diversity and quality in the objective function space, whereas the second one promotes diversity in decision variable space. The application of mating restrictions during the selection phase has also been used to indirectly alter the amount of diversity (Ishibuchi and Shibata, 2003; Chiang and Lai, 2011).

Finally, some methods alter several components simultaneously (Shi et al., 2019; Liu et al., 2019; Zadorojniy et al., 2012). Among them, the Convergence Penalized Density EA (CPDEA) (Liu et al., 2019) is one of the most recent and effective approaches. In this case, two different variation operators are used. The first-one is devoted to exploration and is applied in the first half of the run, whereas the second one is applied in the second half and is devoted to intensification. Moreover, the replacement considers both quality and diversity in the objective space, and the density in decision variable space. Given the high-quality results reported by CPDEA, this is the EMMA used to validate our proposal.

In light of the results of the approaches described above, it is clear that considering the diversity of the decision variable space in the design phase yields benefits for decision makers, since the final solutions obtained by these methods exhibit a higher decision variable space diversity than those obtained by traditional approaches (Deb

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Algorithm 1 Main Procedure of VSD-MOEA

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

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and Tiwari, 2005; Rudolph et al., 2007). Thus, while clear improvements are obtained when metrics related to the decision variable space are taken into account, the benefits in terms of the objective function space are not as clear, and until now, they have only been attained in certain specific MOPs (Liu et al., 2019). We claim that one of the reasons for this behavior might be that the diversity of the decision variable space is considered in the whole optimization process. However, in a similar way as in the single-objective domain, reducing the importance allocated to the diversity of the decision variable space as the generations progress (Segura et al., 2015) might be truly important for obtaining better approximations of the Pareto front. Currently, no MOEA considers this idea, and this was the motivation for the design of the novel MOEA proposed in this paper.

3 Proposal

This section provides a full description of our proposal called *Variable Space Diversity based MOEA* (VSD-MOEA) [2]. 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. In this paper, our decision was to incorporate it into a dominance-based approach. Note that this category has been particularly suitable for problems with two and three 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 pseudo-code of VSD-MOEA. Parents are selected using a binary tournament selection based on dominance ranking with ties broken randomly. The variation stage is based on applying the well-known Simulated Binary Crossover (SBX) and polynomial-based mutation operators (Deb et al., 1995; Deb and Goyal, 1996). Thus, the contribution appears in the replacement phase. Note that t is used to denote the number of the current generation. The rest of this section is devoted to describe the replacement phase, including the novel objective space density estimator.

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[2]The source code in C++ of our approach is freely available at https://github.com/carlossegurag/VSD-MOEA

3.1 Replacement Phase of VSD-MOEA

The replacement phase of EAs is in charge of deciding, for each generation, which members of the previous population together with their corresponding offspring will survive. The novel replacement scheme presented here promotes a gradual movement from exploration to exploitation, which has been a highly beneficial principle in the design of single-objective optimizers (Segura et al., 2015). Specifically, the replacement phase operates as follows. First, the members of the previous population and offspring are merged in a multi-set with $2 \times p$ individuals. Then, an iterative process that selects an additional individual sequentially is used to pick the p survivors. In order to take into account the diversity of decision variable space, the Distance to Closest Survivor (DCS) of each individual is calculated at each iteration. Thus, the DCS of an individual $\vec{y} \in \Omega$ is calculated as $\min_{\vec{s} \in \mathbb{S}} Distance(\vec{y}, \vec{s})$, where $\mathbb{S}$ is the multi-set containing the currently selected survivors. Normalized Euclidean distances are considered (Barrett, 2005), so in order to calculate distances between any two individuals $\vec{a}, \vec{b} \in \Omega$, Eq. (2) is applied. Note that each variable is normalized and the sum is divided by the number of variables. Thus, this measure is expected to be less sensitive to the dimensionality of the decision variable space and to the domain of the variables (Ning et al., 2008). In the first iteration, the $\mathbb{S}$ multi-set is empty, so the DCS of each individual is infinity.

$$Distance(\vec{a}, \vec{b}) = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left(\frac{a_i - b_i}{x_i^{(U)} - x_i^{(L)}} \right)^2} \tag{2}$$

Note that individuals with larger DCS values are those that contribute more significantly to promoting exploration. In order to avoid an excessive decrease in the degree of exploration, individuals with a DCS value below a certain threshold are penalized. 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. Note that it might happen that all individuals are penalized, in which case the individual with the largest DCS is selected to survive.

In order to better understand the penalty method, it can be visualized in the following way. After selecting each survivor, a hyper-sphere centered at a candidate solution — in decision variable space — is created. Then, all the individuals that are inside the hyper-sphere are penalized, with the objective space density estimator only taking into account the survivors and the 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. The left side shows individuals in decision variable space. Current survivors are marked with a red border. Each of them is surrounded by a dashed blue circle of radius D_t. In this scenario, the penalized individuals are the ones with numbers 4, 5, and 6. In objective function space — right side — the penalized individuals are shown in gray, indicating that the objective space density estimator is not considering them.

Since using a large radius for the hyper-spheres induces a large degree of exploration, it makes sense to alter this value during the optimization process. This is precisely one of the key elements of our proposal. The sizes of the hyper-spheres are modified dynamically by taking into account the stopping criterion and elapsed generations. Specifically, the radius is decreased linearly starting from an initial distance. This means that in the initial phases, exploration is promoted. However, as the size
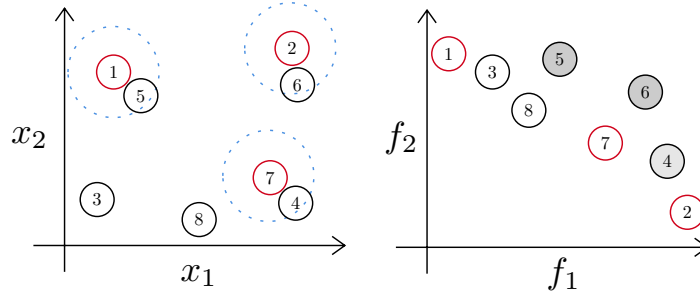
Figure 1: Penalty Method of the Replacement Phase - The left side represents the decision variable space, and the right side the objective function space.

Algorithm 2 Replacement Phase of VSD-MOEA

1: Input: P_t (Population of current generation), Q_t (Offspring of current Generation), p (Population Size) and ITV (Initial Threshold Value)
2: Output: P_{t+1}
3: $R_t \coloneqq P_t \cup Q_t$
4: $P_{t+1} \coloneqq \emptyset$
5: $Penalized \coloneqq \emptyset$
6: $D_t \coloneqq ITV - ITV \times \frac{G_{Elapsed}}{0.5 \times G_{End}}$
7: **while** $|P_{t+1}| \leq$ p **do**
8:     Compute DCS of individuals in R_t, using P_{t+1} as a reference set
9:     Move the individuals in R_t with $DCS < D_t$ to $Penalized$
10:    **if** R_t is empty **then**
11:        Compute DCS of individuals in $Penalized$, using P_{t+1} as a reference set
12:        Move the individual in $Penalized$ with the largest DCS to R_t
13:    Identify the first front (F) in $R_t \cup P_{t+1}$ with at least one individual $\vec{y} \in R_t$
14:    Use the novel density estimator (Algorithm 3) to select a new survivor from F and move it from R_t to P_{t+1}
15: **return** P_{t+1}

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of the radius decreases, only very close individuals are penalized, meaning that more exploitation is allowed. Note that this method requires a parameter that is the initial radius of the hyper-spheres or initial threshold value. This parameter is denoted by ITV. Assigning a large value to this parameter might result in many individuals being penalized, which might thus maintain non-useful diversity. However, a value that is too small might not prevent fast convergence, meaning 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 formalizes the replacement phase of VSD-MOEA. First, the population of the previous generation (P_t) and the offspring (Q_t) are merged in R_t (line 3). At each iteration, the multi-set R_t contains 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 individuals that are too close is calculated (line 6). Note that ITV denotes the initial threshold value, $G_{Elapsed}$ is the number of generations that have evolved, and G_{End} is the stopping criterion, i.e., the number of generations that are to be evolved during the execution of the VSD-MOEA. The linear decrease is calculated such that after 50% of the total number of generations, the D_t

value is below 0, meaning that no penalties are applied. This means that in the first half of the algorithm run, more exploration is induced than in traditional MOEAs. Please refer to the Supplementary Material for the sensitivity analysis of the final moment of diversity promotion. Then, an iterative process that selects an individual sequentially is executed until the survivor set contains p individuals (line 7). The iterative process works as follows. First, 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 desired. Thus, the individual with the largest DCS value is recovered, i.e., moved to the set of non-penalized individuals (lines 11 and 12), and thus survives. Finally, the objective function space is considered. Specifically, candidate non-penalized individuals and current survivors are merged. Then, the well-known non-dominated sorting procedure proposed in Deb et al. (2002) is executed on this set, stopping as soon as a front with at least one candidate individual is found, i.e., with an individual of R_t (line 13). Then, taking the identified front as an input, a novel objective space density estimator is used to select the next survivor, which is moved from R_t to P_{t+1} (line 14). The specific way in which each individual's contribution to the diversity of the objective space is measured is described in the next section.

It is important to note that the pseudo-codes presented in this paper are designed for explanatory purposes, and their corresponding implementations are not necessarily straightforward. For instance, in order to calculate the DCS values in line 11, there is no need to iterate over all solutions in P_{t+1}. Instead, when P_{t+1} is updated by including an additional individual, the distances are updated.

3.2 A Novel Density Estimator for Objective Function Space

Since the dominance definition is not related to the preservation of diversity in objective function space, dominance-based MOEAs usually incorporate objective-space density estimators to promote the survival of diverse individuals. As previously described, our density estimator selects a new survivor from the front identified in line 13 of Algorithm 2. This front (referred in Algorithm 3 as F) 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 an individual of the input front that contributes significantly in terms of the quality and diversity of the objective space.

Algorithm 3 describes the selection of the next survivor. First, the sets FP and FR are identified (lines 3 and 4). FP contains the current survivors that are in F (already selected to the next generation P_{t+1}), whereas FR contains the remaining non-penalized individuals that are in F. Then, similarly to most state-of-the-art algorithms, a step to promote the selection of extreme-points is included (Sun et al., 2018). Note that selecting the extreme-points following the criteria of the best solution for each objective might cause some drawbacks related to accepting a small improvement in one objective at the expense of significant degradation in other objectives. This issue can be solved by applying augmented functions (Deb and Abouhawwash, 2016; Sun et al., 2018), which was our design choice. Particularly, and similarly to Sun et al. (2018), the m extreme points are selected by decomposing the m-objective MOP into m single-objective problems. Specifically, the kth extreme point is the one that minimizes Eq. (3). The second term, which is multiplied by the penalization parameter ρ, is a measure of the overall quality and it is used to avoid extreme points that exhibit very poor qualities in some of the objectives. Obviously, the setting of the parameter ρ is problem-dependent, but

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Algorithm 3 Density Estimator

1: Input: P_{t+1} (Survivors), R_t (Candidates), F (Current front)
2: Output: $\vec{y} \in R_t$
3: $FP := P_{t+1} \cap F$
4: $FR := R_t \cap F$
5: $Extreme\_points := \emptyset$
6: **for** $k \in$ Number of objectives (m) **do**
7:    Select the best individual $\vec{y} \in F$ according to the k objective using Eq. 3.
8:    **if** $\vec{y} \in FR$ **then**
9:       $Extreme\_points = Extreme\_points \cup \vec{y}$
10: **if** $|Extreme\_points| > 0$ **then**
11:    $\vec{s^*} :=$ a random individual from $Extreme\_points$
12:    **return** $\vec{s^*}$
13: $MaxID := 0$
14: **for** $\vec{y} \in FR$ **do**
15:    $Improvement := \min_{\vec{s} \in FP} ID(\vec{y}, \vec{s})$ (Eq. 4)
16:    **if** $Improvement > MaxID$ **then**
17:       $MaxID := Improvement$
18:       $\vec{s^*} := \vec{y}$
19: **return** $\vec{s^*}$

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for benchmark problems where the objective functions are between 0 and some units, the suggested value is 10^{-4} (Deb and Abouhawwash, 2016), so this was the value used in our validation. Lines 6 to 9 identify, for each objective k, the candidate solutions that minimize the Augmented Function (AF). If some of the extreme points belong to the non-penalized candidates (FR), then one of them is randomly selected as a survivor and the process ends (lines 10 to 12).

$$AF_k(\vec{x}) = f_k(\vec{x}) + \rho \times \sum_{j=1}^{m} f_j(\vec{x}) \tag{3}$$

In cases where the individuals that optimize each AF are already in P_{t+1}, a contribution to objective-space diversity and quality is calculated for each individual in FR (lines 13 to 19). This contribution is calculated by taking into account the current survivors of the front (FP). Specifically, the Improvement Distance (ID) defined for the indicator IGD+ (Ishibuchi et al., 2015) is used. The ID of an individual $\vec{x}$ with respect to an individual $\vec{y}$ is calculated by taking into account only the objectives where $\vec{x}$ is better. Specifically, Eq. (4) is used.

$$ID(\vec{x}, \vec{y}) = \sqrt{\sum_{i=1}^{m} \left(\max\{0, f_i(\vec{y}) - f_i(\vec{x})\} \right)^2} \tag{4}$$

The contribution of each member $\vec{y} \in FR$ is calculated as $\min_{\vec{s} \in FP} ID(\vec{y}, \vec{s})$. Then, the individual with the highest contribution is selected as the next survivor (lines 16 to 18). Note that the process of selecting the individual with the best contribution ($\vec{s^*}$) is defined in Eq. (5).

$$\vec{s^*} = \arg\max_{\vec{y} \in FR} \min_{\vec{s} \in FP} ID(\vec{y}, \vec{s}) \tag{5}$$

Finally, note that ID has not been used earlier as a density estimator. The logic is to avoid the selection of individuals that are far from the remaining ones, just because there is a worsening in some of the objective functions. As it will be shown in the experimental validation, this novel density estimator provides important benefits when compared to more traditional density estimators.

4 Experimental Validation

This section describes the experimental validation carried out to study the performance and gain a clear understanding of the specifics of our proposed VSD-MOEA. Our results clearly show that controlling the diversity of decision variable space provides a way to further improve the results obtained by state-of-art MOEAs. First, we discuss some technical specifications involving the benchmark problems and algorithms implemented. We then present a comparison between VSD-MOEA and state-of-the-art algorithms for long runs. Then, four additional experiments to fully validate VSD-MOEA are included. These analyses are designed to test the scalability in decision variable space, the performance with different stopping criteria, the novel diversity management mechanism in the objective space, and the implications of the initial penalty threshold.

This work takes into account some of the most popular and widely used benchmarks in the multi-objective field. These problems are the WFG (Huband et al., 2005, 2006), DTLZ (Deb et al., 2005), and UF (Zhang et al., 2008) test suites configured in a standard way. The WFG test problems were used with two and three objectives and were configured with 24 parameters, 20 of them corresponding to distance parameters and 4 to position parameters. In the DTLZ test problems, the number of variables was set to $n = m + r - 1$, where $r = \{5, 10, 20\}$ for DTLZ1, DTLZ2 to DTLZ6 and DTLZ7, respectively. The UF benchmark comprises seven problems with two objectives (UF1-7) and three problems with three objectives (UF8-10). All of them were configured with 30 variables. Note that the experiment used to analyze scalability considers different numbers of variables. The experimental validation includes three well-known state-of-the-art MOEAs and VSD-MOEA. The MOEAs that are considered are MOEA/D [3], R2-EMOA [4], and CPDEA [5]. Note that CPDEA is the only method that includes an archive, thus the final results are obtained from the archive. In the remaining methods, following the original implementations, solutions are taken from the last population. In every case, the maximum size of the solution set is equal to the population size. Note that in the Supplementary Material some results considering the incorporation of passive archives (Schütze and Hernández, 2021) in all the methods are discussed. Similar conclusions are attained, so the performance is more dependent on the selection and replacement phases, which are the main distinguishing features of each algorithm, than in the specific way of selecting the final solution set. Also note that, in the case of MOEA/D, several variants have been devised. The MOEA/D implementation considered is the one that obtained first place in the 2009 IEEE Congress on Evolutionary Computation's MOP Competition (Zhang et al., 2009).

Given that all the algorithms considered are stochastic, each execution was repeated 35 times with different seeds in all the experiments. The hypervolume indicator (HV) is used to compare results. Note that in the supplementary material, the results are also compared in terms of IGD+, with the conclusions being quite similar. The ref-

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[3] https://github.com/P-N-Suganthan/CEC2009-MOEA/blob/master/Codes-of-Accepted-Papers.rar
[4] http://inriadortmund.gforge.inria.fr/r2emoa/
[5] https://github.com/yiping0liu/CPDEA

Table 1: Crossover probability applied in each MOEA

	2 objectives	3 objectives
VSD-MOEA	0.4	0.4
CPDEA	1.0	0.6
MOEA/D	1.0	1.0
R2-EMOA	1.0	0.2

erence point used to calculate the HV is chosen to be a vector whose values are sightly larger (ten percent) than the Nadir point, as suggested in Ishibuchi et al. (2017). The normalized HV is used to facilitate the interpretation of the results (Li et al., 2014), and the value reported is computed as the ratio between the normalized HV obtained and the maximum attainable normalized HV. In this way, a value equal to one means a perfect approximation. Note that a value equal to one is not attainable because MOEAs yield a discrete approximation. In order to statistically compare the HV ratios attained by the different algorithms, the guidelines proposed in del Amo and Pelta (2013); Derrac et al. (2011) are followed. Given a set of approaches and their corresponding results, first, the Kruskal-Wallis is used as an Omnibus test to detect if there are any significant differences. In cases where there are significant differences, pair-wise statistical test are used to detect them; specifically, the Mann-Whitney post-hoc test with Hommel's correction of p-values. An algorithm X is said to beat algorithm Y when the differences between them are statistically significant, and the mean HV ratio obtained by X is higher than the mean achieved by Y. Note that in both tests, a significance level of 5% was considered.

The common configuration in all the experiments was as follows: the population size was set to 100, the stopping criterion was set to 2.5×10^6 function evaluations, and the genetic operators were Simulated Binary Crossover (SBX) and polynomial-based mutation (Deb et al., 1995; Deb and Goyal, 1996). The crossover and mutation distribution indexes were fixed to 2 and 50, respectively. The mutation probability was set to $1/n$. In order to select the crossover probabilities, five parameterizations were tested ($\{0.2, 0.4, 0.6, 0.8, 1.0\}$). These configurations were executed with all the aforementioned benchmarks in each algorithm. Then, the mean HV ratios were calculated independently for the problems with two and three objectives, and the parameterization that attained the largest mean was selected for the validation. Table 1 shows the crossover probability selected for each algorithm, whereas the specific parameterization required for each algorithm is included in Table 2. Note that for the specific parameterizations, the default values provided by the authors are maintained. In the case of VSD-MOEA, the initial threshold value (ITV) was set to 0.4, which is the recommended value for single-objective optimization (Chacón Castillo and Segura, 2020). In subsequent experiments, the implications of the ITV on the quality of the results are analyzed. Also note that scalarization functions are required in MOEA/D and R2-EMOA. In both cases, the Tchebycheff approach is used. The procedure for generating the weight vectors differs in MOEA/D and R2-EMOA. R2-EMOA was applied with 501 and 496 weight vectors for two and three objectives, respectively (Trautmann et al., 2013). In contrast, MOEA/D requires the same number of weight vectors as the population size. They were generated using the uniform design (UD) and the good lattice point (GLP) method (Ma et al., 2014; Berenguer and Coello, 2015).

Table 2: Parameterization applied in each MOEA

Algorithm	Configuration
MOEA/D	Max. updates by sub-problem (η_r) = 2, tour selection = 10, neighbor size = 10, period utility updating = 30 generations, local selection probability (δ) = 0.9
VSD-MOEA	Initial threshold value (ITV) = 0.4
R2-EMOA	Equally distributed weight vectors (ρ) = 1, offspring by iteration = 1
CPDEA	Nearest neighbors (K) = 3, weight of standard deviation (η) = 2

Table 3: Summary of the hypervolume ratio results attained for problems with two objectives. The higher the normalized hypervolume value, the better the algorithm.

	VSD-MOEA			CPDEA			MOEA/D			R2-EMOA		
	Mean	Median	Std	Mean	Median	Std	Mean	Median	Std	Mean	Median	Std
WFG1	**0.993**	0.994	0.002	0.963	0.965	0.013	0.993	0.993	0.001	0.980	0.989	0.018
WFG2	**0.996**	0.998	0.008	0.993	0.996	0.009	0.965	0.965	0.000	0.966	0.966	0.005
WFG3	**0.992**	0.992	0.000	0.973	0.973	0.002	0.992	0.992	0.000	0.991	0.991	0.000
WFG4	0.990	0.990	0.000	0.964	0.964	0.003	0.988	0.988	0.000	**0.991**	0.991	0.000
WFG5	**0.880**	0.881	0.003	0.862	0.862	0.002	0.877	0.876	0.003	**0.882**	0.882	0.002
WFG6	0.884	0.884	0.012	0.787	0.788	0.003	**0.918**	0.919	0.020	**0.914**	0.914	0.015
WFG7	0.990	0.990	0.000	0.973	0.974	0.002	0.988	0.988	0.000	**0.991**	0.991	0.000
WFG8	**0.904**	0.947	0.053	**0.875**	0.881	0.026	0.808	0.808	0.007	0.803	0.804	0.005
WFG9	**0.946**	0.961	0.027	0.791	0.791	0.002	**0.912**	0.949	0.070	0.894	0.953	0.079
DTLZ1	0.992	0.992	0.000	0.991	0.991	0.000	**0.993**	0.993	0.000	0.992	0.992	0.000
DTLZ2	0.990	0.990	0.000	0.983	0.983	0.001	0.989	0.989	0.000	**0.992**	0.992	0.000
DTLZ3	0.990	0.990	0.000	0.988	0.988	0.000	0.989	0.989	0.000	**0.992**	0.992	0.000
DTLZ4	**0.990**	0.990	0.000	0.979	0.980	0.003	0.989	0.989	0.000	0.678	0.991	0.362
DTLZ5	0.990	0.990	0.000	0.983	0.983	0.001	0.989	0.989	0.000	**0.992**	0.992	0.000
DTLZ6	**0.990**	0.990	0.000	0.807	0.820	0.088	0.989	0.989	0.000	0.685	0.667	0.088
DTLZ7	0.996	0.996	0.000	0.995	0.995	0.000	0.996	0.996	0.000	**0.997**	0.997	0.000
UF1	**0.989**	0.990	0.003	0.976	0.976	0.003	0.980	0.981	0.005	0.881	0.881	0.030
UF2	**0.987**	0.988	0.004	0.968	0.968	0.001	**0.986**	0.986	0.004	0.979	0.979	0.003
UF3	**0.876**	0.878	0.014	0.755	0.757	0.049	0.616	0.609	0.065	0.556	0.557	0.040
UF4	0.891	0.891	0.003	0.850	0.849	0.004	0.883	0.884	0.005	**0.900**	0.901	0.003
UF5	0.589	0.579	0.050	**0.676**	0.671	0.070	0.294	0.206	0.247	0.306	0.332	0.152
UF6	**0.854**	0.852	0.030	**0.839**	0.848	0.043	0.526	0.538	0.143	0.558	0.545	0.113
UF7	**0.985**	0.985	0.002	0.967	0.968	0.004	0.957	0.979	0.121	0.756	0.944	0.225
Mean	**0.943**	0.945	0.009	0.910	0.912	0.014	0.896	0.895	0.030	0.855	0.880	0.050

4.1 Comparison Against State-of-the-art MOEAs for Long Runs

Our first experiment aims to compare the performance for long runs of VSD-MOEA against state-of-the-art proposals. Long runs (2.5×10^6 function evaluations) are considered because this is the kind of execution where diversity-based EAs have been more successful. Experiments with shorter and longer runs are discussed in Section 4.3.

Table 3 shows the HV ratio obtained for the benchmark functions with two objectives. Specifically, the mean, median and standard deviation of the HV ratio is shown for each method and problem tested. The last row shows the results considering all the test problems together. For each test problem, the data for the method that yielded the largest mean is shown in **boldface**. Additionally, all the methods that were not statistically inferior than the method with the largest mean are also shown in **boldface**. From here on, the methods shown in **boldface** for a given problem are referred to as the winning methods. Based on the number of test problems where each method is in the group of the winning methods for the cases with two objectives, the best methods are VSD-MOEA and R2-EMOA with 13 and 10 wins, respectively. Thus, VSD-MOEA is the most competitive method in terms of this measure. More impressive is the fact that the mean HV ratio attained by VSD-MOEA, when all the problems are considered simultaneously, is much higher than the one attained by R2-EMOA. Note that the decision variable space diversity-aware methods (CPDEA and VSD-MOEA) reported the largest total mean. However, there is a huge difference between VSD-MOEA and CPDEA,

Table 4: Statistical Tests and Deterioration Level of the HV ratio for problems with two objectives

	↑	↓	↔	Score	Deterioration
VSD-MOEA	51	11	7	40	0.147
CPDEA	16	51	2	-35	0.911
MOEA/D	27	34	8	-7	1.290
R2-EMOA	31	29	9	2	1.643

Table 5: Summary of the hypervolume ratio results attained for problems with three objectives. The higher the normalized hypervolume value, the better the algorithm.

	VSD-MOEA			CPDEA			MOEA/D			R2-EMOA		
	Mean	Median	Std	Mean	Median	Std	Mean	Median	Std	Mean	Median	Std
WFG1	0.785	0.789	0.017	0.430	0.428	0.033	**0.968**	0.968	0.001	0.928	0.926	0.009
WFG2	**0.988**	0.989	0.001	0.923	0.924	0.006	0.967	0.976	0.034	0.905	0.962	0.070
WFG3	0.989	0.989	0.000	0.906	0.905	0.013	**0.993**	0.992	0.000	0.992	0.992	0.000
WFG4	**0.920**	0.920	0.001	0.795	0.796	0.013	0.861	0.861	0.003	0.906	0.905	0.001
WFG5	0.834	0.832	0.004	0.801	0.801	0.004	0.795	0.795	0.001	**0.842**	0.843	0.002
WFG6	0.837	0.835	0.007	0.766	0.767	0.005	0.811	0.810	0.012	**0.860**	0.860	0.007
WFG7	**0.919**	0.919	0.001	0.774	0.778	0.021	0.865	0.865	0.000	0.905	0.905	0.001
WFG8	**0.863**	0.864	0.035	0.672	0.682	0.039	0.779	0.779	0.002	0.820	0.820	0.002
WFG9	**0.822**	0.824	0.038	0.727	0.727	0.005	**0.810**	0.837	0.047	0.804	0.772	0.048
DTLZ1	**0.965**	0.965	0.001	**0.964**	0.964	0.001	0.950	0.950	0.000	0.940	0.940	0.001
DTLZ2	**0.930**	0.930	0.001	0.864	0.864	0.017	0.899	0.899	0.000	0.915	0.915	0.001
DTLZ3	**0.930**	0.930	0.001	0.830	0.916	0.239	0.899	0.899	0.000	0.912	0.915	0.004
DTLZ4	**0.930**	0.930	0.001	0.859	0.858	0.006	0.899	0.899	0.000	0.652	0.577	0.257
DTLZ5	**0.986**	0.986	0.000	0.977	0.977	0.002	0.978	0.978	0.000	**0.986**	0.986	0.000
DTLZ6	**0.986**	0.986	0.000	0.660	0.643	0.115	0.978	0.978	0.000	0.775	0.760	0.082
DTLZ7	**0.965**	0.965	0.001	0.940	0.941	0.004	0.914	0.914	0.000	0.852	0.852	0.014
UF8	**0.918**	0.920	0.011	0.699	0.711	0.045	0.778	0.777	0.006	0.853	0.905	0.104
UF9	**0.962**	0.965	0.011	0.784	0.793	0.053	0.792	0.747	0.071	0.844	0.783	0.076
UF10	**0.602**	0.581	0.095	0.122	0.121	0.060	0.309	0.270	0.150	0.268	0.209	0.132
Mean	**0.902**	0.901	0.012	0.763	0.768	0.036	0.855	0.852	0.017	0.840	0.833	0.043

showing the benefits of decreasing the importance given to the decision variable space diversity as the evolution progresses. Inspecting the data carefully, it is clear that in the cases where VSD-MOEA loses (attains lower HV), the difference with respect to the best method is not very large. For instance, the difference between the mean HV ratio attained by the best method and by VSD-MOEA was never larger than 0.1. However, all the other methods exhibited a deterioration greater than 0.1 in several cases. Specifically, it happened in 4, 3 and 6 problems for CPDEA, MOEA/D and R2-EMOA, respectively. This means that even if VSD-MOEA loses in some cases, its deterioration is always small, exhibiting a much more robust behavior than any other method.

In order to better clarify these findings, pair-wise statistical tests were done among each method tested in each test problem. For the two-objective cases, Table 4 shows the number of times that each method won (column ↑), lost (column ↓) and tied (column ↔), as well as a **Score** that is calculated as the difference between the number of times that each method won and the number of times that each method lost. Additionally, for each method A, we calculated the sum of the differences between the mean HV ratio attained by the best method (the ones with the highest mean) and method A, for each problem where A was not in the group of winning methods. This value is shown in the Deterioration column. The data confirms that although VSD-MOEA loses in some cases, the overall numbers of wins and losses favors VSD-MOEA. More importantly, the total deterioration is quite lower in the case of VSD-MOEA, confirming that when VSD-MOEA loses, the deterioration is not that large.

Tables 5 and 6 show the same information for the problems with three objectives. In this case, the superiority of VSD-MOEA is even clearer. Taking into account the mean of all the test problems, VSD-MOEA again obtained a much larger mean HV ratio than

Table 6: Statistical Tests and Deterioration Level of the HV ratio for problems with three objectives

	↑	↓	↔	Score	Deterioration
VSD-MOEA	47	6	4	41	0.231
CPDEA	5	46	6	-41	2.752
MOEA/D	24	29	4	-5	1.158
R2-EMOA	27	22	8	5	1.522

the other methods. Specifically, VSD-MOEA obtained a value of 0.902, whereas the second ranked algorithm (MOEA/D) obtained a value of 0.855. In this case, the difference between the mean HV ratio obtained by the best method and by VSD-MOEA was larger than 0.1 in only one problem (WFG1). Since WFG1 is a uni-modal and biased problem, a large balance towards intensification is required, so promoting further exploration is not helpful. In contrast, all the other methods exhibited a deterioration greater than 0.1 in several cases. In particular, this happened in 3, 5 and 9 problems for MOEA/D, R2-EMOA and CPDEA, respectively. Interestingly, CPDEA attained the worst results in the three-objective case. As the number of objectives increases, more individuals are required to attain proper discrete approximations. The aim of attaining high diversity in decision variable space seems to significantly affect the quality attained in objective space, probably indicating that, as the number of objectives increases, EMMAs might be less adequate[6]. Thus, as the number of objectives increases, the dynamic balance promoted by VSD-MOEA seems more important to improve performance. VSD-MOEA is much superior to the other methods both in terms of total deterioration and of total wins and losses (see Table 6 and the data shown in **boldface** in Table 5). Particularly, VSD-MOEA was in the group of winning methods for 15 out of 19 test problems, whereas the second best-ranked algorithm (MOEA/D) was in the group of winning methods for only 4 test problems.

Regarding the kind of problem where VSD-MOEA yields the most impressive improvements, it is clear that this happens in the MOPs that exhibit some features that hinder the optimization process. VSD-MOEA excelled in problems with a strong non-separability (e.g., WFG8, WFG9, UF1-3), high multi-modality (e.g., WFG9, UF6, UF7), irregular Pareto geometries (e.g., WFG2, UF6, UF7, UF9) and complicated Pareto set shapes (e.g., UF6, UF8, UF10). Conversely, the most important decay in performance (in fact, the only one) appeared in the WFG1 problem. Promoting further intensification is normally useful in unimodal problems, and this is specially the case for biased problems, where small perturbations in decision space provoke large movements in objective function space. Thus, methods that promote the maintenance of further decision variable space diversity do not contribute positively in such kinds of problems.

4.2 Decision Variable Scalability Analysis

In order to study the scalability of VSD-MOEA in terms of the number of decision variables, all of the algorithms already described were tested with the same benchmark problems, but considering 50, 100, and 250 variables. Note that in the WFG test problems, the number of position parameters (k) and distance parameters (l) must be specified. The ratio between the number of each kind of variable was kept as in the default configuration. Thus, the number of distance parameters was set to 42, 84, and 210 when using 50, 100 and 250 variables, respectively. The rest of the decision variables were

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[6]Four additional EMMAs were tested with a similar behaviour, but some additional analyses are required to draw more general conclusions.

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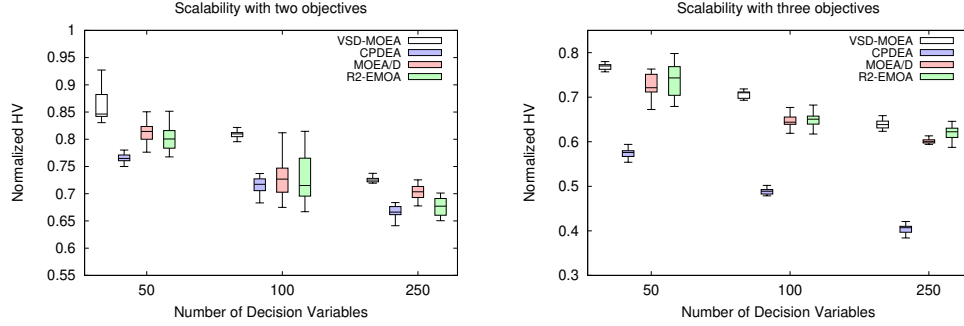

Figure 2: Box-plots of the HV ratio for 35 runs for the two-objective (left side) and three-objective (right side) problems, considering different numbers of variables

position parameters, meaning that they were 8, 16 and 40, respectively. The stopping criterion was also set to 2.5×10^6 function evaluations. Figure 2 shows the box-plots of the mean HV ratios attained with the four algorithms for the problems with two objectives and three objectives and the different dimensionalities. As expected, the HV ratio decreases as the number of variables increases in every algorithm; however, the superiority of VSD-MOEA is maintained in every case. Additionally, the variability in the case of VSD-MOEA is quite low, which is a typical feature of diversity-aware methods (Segura et al., 2016). One negative aspect regarding the performance of VSD-MOEA is that, as the number of decision variables increases, closer HV ratios are attained by other algorithms. This is especially true in the three-objective problems, where the advantages with respect to R2-EMOA are not as significant.

In order to better understand the reasons for this behavior, we selected problems WFG1 to WFG7. The WFG test problems divide the variables into two kinds of parameters (this framework uses the term parameter instead of variable): the distance parameters and the position parameters. Note that a parameter i is a distance parameter when modifying $x_i \in \vec{x}$ results in a new solution that dominates $\vec{x}$, is equivalent to $\vec{x}$, or is dominated by $\vec{x}$. However, if i is a position parameter, modifying x_i always results in a vector that is incomparable or equivalent to $\vec{x}$ (Huband et al., 2005). Additionally, note that we selected problems WFG1-WFG7 because their distance parameter values associated to all Pareto optimal solutions have exactly the same values:

$$x_{\{i=k+1:n\}} = 2i \times 0.35 \tag{6}$$

This is very important because it has been shown that for these cases, state-of-the-art MOEAs might provoke a quick convergence in the *distance parameters*, resulting in an effect that is similar to premature convergence in the single-objective case (Kukkonen and Lampinen, 2009; Chacón Castillo et al., 2017).

For each algorithm, the average (mean) Euclidean distance among individuals (ADI) in the population was calculated by considering only the distance parameters. Figure 3 shows how the ADI evolves for the two-objective (left side) and three-objective (right side) problems. The behavior of MOEA/D — which is not included — is similar to that of R2-EMOA in terms of how the ADI evolves. Moreover, to avoid saturating these figures, only the information for VSD-MOEA, CPDEA and R2-EMOA with 50 and 250 variables is shown. The first finding is that, as expected, the decision variable space
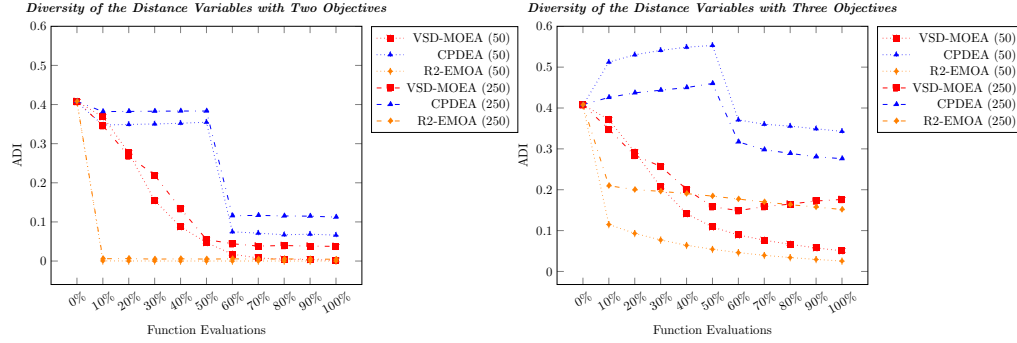
Figure 3: Evolution of ADI for problems WFG1-WFG7 with two and three objectives considering only the distance variables
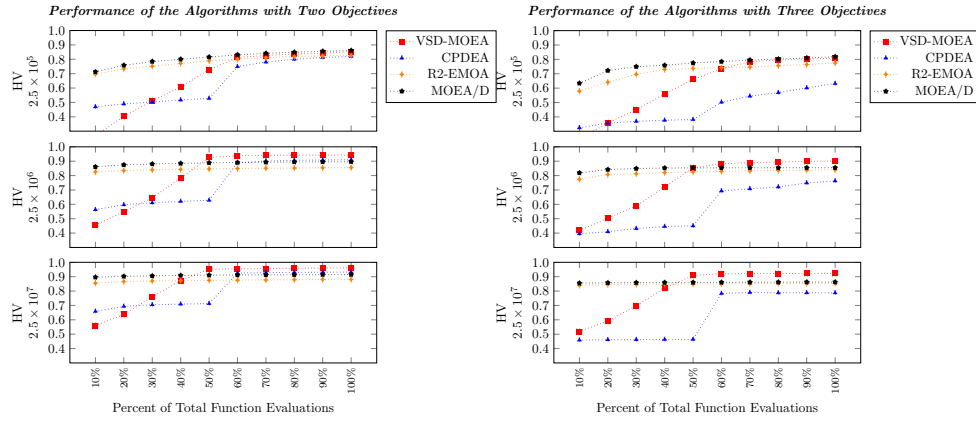

Figure 4: Performance of MOEAs for the problems with two objectives (left side) and three objectives (right side) considering three values for the stopping criterion: short-term (first row), medium-term (second row) and long-term (third row).

diversity-aware MOEAs converge much slower than the remaining algorithms. Accordingly, the difference between the diversity maintained in the first generation and that maintained after 10% of the execution, is much larger in R2-EMOA than in VSD-MOEA and CPDEA. In the case of VSD-MOEA, the decrease in ADI is quite linear until the halfway point of the execution. This is due to the way in which the threshold distance value (D_t) is calculated. Differently, in CPDEA the decrease in ADI is abrupt because it operates in two differentiated stages.

A closer inspection of the data reveals other important aspects. In the two-objective case, increasing the number of variables causes the diversity in the R2-EMOA to increase slightly. However, the amount of diversity is low even when using 250 variables, meaning that incorporating mechanisms to increase diversity might be very helpful. In the three-objective case, increasing the number of variables yields a significant increase in the resulting ADI, meaning that in this case, fast convergence is not an important issue. These results show that, as the number of objectives and variables increases, MOEAs tend to maintain a higher variable space diversity in an implicit way, meaning that explicitly controlling the variable space diversity is probably not as important.

Table 7: Final mean of HV ratio attained for the three stopping criteria reported in Figure 4.

	Two objectives				Three objectives			
	VSD-MOEA	CPDEA	MOEA/D	R2-EMOA	VSD-MOEA	CPDEA	MOEA/D	R2-EMOA
2.5×10^5	0.854	0.820	**0.861**	0.826	0.809	0.632	**0.819**	0.775
2.5×10^6	**0.943**	0.910	0.896	0.855	**0.902**	0.763	0.855	0.840
2.5×10^7	**0.962**	0.932	0.915	0.881	**0.923**	0.788	0.863	0.853

4.3 Analysis of the Stopping Criterion

Decision variable space diversity-aware methods usually excel in long runs. As a result, a large stopping criterion was used in our previous experiments. This section considers the performance of the algorithms with several stopping criteria, i.e., maximum number of function evaluations. Additionally, the trend in the HV during the execution is inspected with the aim of better understanding the optimization process.

Three different values were explored for the stopping criterion. The values considered were: 2.5×10^5, 2.5×10^6 and 2.5×10^7. These values are referred to as short-term, middle-term and long-term executions, respectively. Figure 4 plots the mean HV ratio obtained with each MOEA with two and three objectives versus the number of evaluations. Each figure is divided into three graphs corresponding to short-term, middle-term and long-term. Additionally, Table 7 shows the final mean HV attained by each model for the different stopping criteria.

The gradual shift from exploration to exploitation attained by VSD-MOEA is clear in the plots. Instead of attaining a very fast increase in HV, the increase is quite linear in the first half of the run due to the large degree of exploration promoted in this phase. In short-term executions this does not yield important benefits, so the HV ratio attained by VSD-MOEA is similar to those attained by state-of-the-art algorithms. However, as the stopping criterion is increased, the benefits of VSD-MOEA become clear. Thus, as in the single-objective case, variable space diversity-aware methods are especially useful for relatively long-term executions. However, since a faster decrease in diversity is promoted when using short-term executions, the performance is not degraded, meaning it can be used in quite different environments. Thus, the performance in the short-term is similar to current state-of-the-art algorithms, whereas in the long-term, truly significant advances are attained. Finally, note that in the case of CPDEA, there is no significant improvement in the long-term case. Thus, the lower gradual shift from exploration to exploitation promoted in CPDEA is not as helpful.

4.4 Analysis of the Novel Density Estimator for the Objective Space

This section considers the impact on the performance of the novel density estimator for the objective space that is proposed in VSD-MOEA. For this analysis, three different density measurements are integrated in VSD-MOEA. Particularly, in addition to the Improvement Distance (ID) (Ishibuchi et al., 2015) already described, the Euclidean distance(L_2) (Kukkonen and Deb, 2006a,b) and the NSGA-II crowding distance (CD) are also taken into account. Note that in order to incorporate L_2 and CD, the only modification appears in Eq.(5), where ID is modified by the corresponding distance. VSD-MOEA was executed 35 times to solve the whole benchmark, configured as in the first experiment. Table 8 shows the mean and median of the HV ratios obtained for the whole benchmark with the three measurements. In the two-objective problems, L_2 and ID yield quite similar results, whereas CD attains lower values. Note, however, that VSD-MOEA attained a higher mean HV ratio than the remaining state-of-the-art

Table 8: Summary of the hypervolume ratio results attained with VSD-MOEA using three density estimators

	ID			L_2			CD		
	Mean	Median	Std	Mean	Median	Std	Mean	Median	Std
Two objectives	**0.943**	0.945	0.091	0.939	0.940	0.095	0.917	0.915	0.099
Three objectives	**0.902**	0.901	0.096	0.848	0.848	0.167	0.795	0.797	0.186

Table 9: Statistical Tests of the HV ratio of the state-of-the-art algorithms and VSD-MOEA with three density estimators (ID, L_2 and CD)

	Two-objectives				Three-objectives			
	↑	↓	↔	score	↑	↓	↔	score
ID	74	14	27	60	80	7	8	73
L_2	70	13	32	57	60	26	9	34
CD	20	74	21	-54	10	66	19	-56
CPDEA	21	77	17	-56	8	70	17	-62
MOEA/D	43	54	18	-11	38	38	19	0
R2-EMOA	50	46	19	4	45	34	16	11

methods with all the density estimators (see Table 3), so even with density estimators that are not as adequate, VSD-MOEA excels. The case of three-objective problems is different. In this case, the results attained with ID are quite superior to the remaining ones. This might indicate that the benefits appear in these problems only because of the application of ID; however, this is not the case. In fact, VSD-MOEA with L_2 also exhibits a very good performance in most problems. However, in the case of WFG1, it presents a huge degradation that greatly affects the overall results.

In order to better illustrate the benefits of VSD-MOEA, pair-wise statistical tests were applied by considering VSD-MOEA with the three density measurements and the state-of-the-art methods for the whole benchmark. Table 9 shows the number of wins and loses, as well as the score. The benefits of VSD-MOEA are clear when using both ID and L_2. However, the additional advantages provided by ID are remarkable, especially for the problems with three objectives.

4.5 Analysis of the Initial Threshold Value

One of the disadvantages of including a strategy for controlling diversity is that this is usually done at the expense of incorporating additional parameters in the EA designed. In the case of VSD-MOEA, the Initial Threshold Value (ITV) must be set. The higher this value is, the greater the exploration of the decision variable space. Note that in all the previous experiments, $ITV = 0.4$ was used. This is the value suggested in Chacón Castillo and Segura (2020) for a single-objective optimization strategy that was designed with principles similar to those applied in VSD-MOEA. This section is devoted to analyzing the performance of VSD-MOEA when using different ITV values. Note that, since normalized distances are used, the maximum attainable difference is 1. Additionally, when ITV is set to 0, no individual is penalized on the basis of its contribution to diversity in the decision variable space, so VSD-MOEA would behave like a more traditional MOEA, meaning that there is no explicit promotion of diversity in decision variable space. As a result, the values $ITV = \{0.0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0\}$ were tested. As in previous experiments, the whole set of benchmark problems was used and the stopping criterion was set to 2.5×10^6 function evaluations.

Figure 5 shows the box-plots of the mean HV ratios obtained for both the two-objective and the three-objective cases. In comparison to state-of-the-art algorithms,
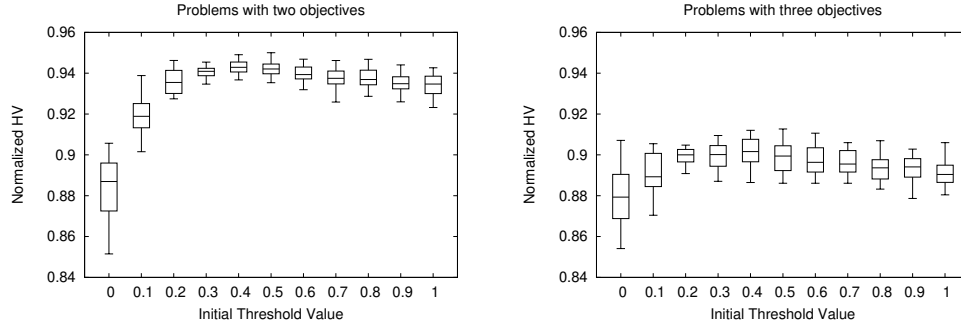
Figure 5: Box-plots of the HV ratio for 35 runs for the two-objective (left side) and three-objective (right side) problems, considering different initial threshold values

when ITV is set to 0, VSD-MOEA yielded competitive results in the two-objective case and the best results in the three-objective case (see Tables 3 and 5). Specifically, the mean values were 0.884 and 0.880 for two and three objectives, respectively. This means that the novel density estimator put forth in this paper is also helpful for methods that do not explicitly take into account the variable space diversity. However, the increase in performance when using other ITV values is clear. The HV ratio obtained quickly increases as higher ITV values up to 0.4 are used. Then, with values in the range $[0.5, 1.0]$, the performance decreases slightly. There is a large range of values where the performance is very good (e.g. $ITV \geq 0.2$), meaning that the behavior of VSD-MOEA is quite robust. Thus, properly setting this parameter is not a complex task.

5 Conclusions and Future Work

EAs have been one of the most popular approaches for dealing with complex optimization problems. Their design is a highly complex task that requires defining several components. Looking at the differences between single-objective and multi-objective optimizers, it is worth noting that several state-of-the-art single-objective optimizers explicitly consider the diversity of the variable space, particularly when dealing with long-term executions, whereas this is not the case for MOEAs. Moreover, single-objective optimizers that take diversity into account to induce a gradual shift between exploration and intensification have been particularly successful.

This paper proposes a novel MOEA, called VSD-MOEA, that takes into account the diversity of both decision variable space and objective function space. The main novelty is that the importance given to the different diversities is adapted during the optimization process. In particular, in VSD-MOEA more importance is given to the diversity of the decision variable space in the initial stages, but as the evolution progresses, it assigns more importance to the diversity of the objective function space, meaning that a gradual shift between exploration and intensification is promoted. This is performed using a penalty method that is integrated into the replacement phase. Also included is a novel density estimator based on IGD+ that is used to select from the non-penalized individuals.

The experimental validation carried out shows a remarkable improvement in VSD-MOEA when compared to state-of-the-art MOEAs both in two-objective and three-objective problems. Moreover, our proposal not only improves the state-of-the-art algo-

rithms in long-term and medium-term executions, but it also offers a competitive performance in short-term executions. The scalability analyses show that as the number of objectives and decision variables increases, the implicit variable space maintained by state-of-the-art MOEAs also increases. Thus, for a large number of objectives and decision variables, explicitly considering the diversity of decision variable space is less helpful. Additionally, the analysis of the initial threshold value, which is an additional parameter required by VSD-MOEA, shows that finding a proper value for this parameter is not a difficult task. Finally, the analysis shows that the novel density estimator has a significant impact on performance, especially in the problems with three objectives. The main conclusion is that state-of-the-art solvers can be significantly improved by explicitly taking into account the diversity of decision variable space, and by reducing the importance given to this kind of diversity as the evolution progresses.

In the future, we plan to apply the principles studied in this paper to other categories of MOEAs. For instance, including the diversity management put forth in this paper in decomposition-based and indicator-based MOEAs seems plausible. Additionally, we would like to develop an adaptive scheme to avoid setting the initial threshold value, as well as to integrate the design principles studied in this paper with multi-objective memetic algorithms. Finally, we should mention that integrating the design principles put forth in this paper with interactive approaches (Deb, 2001), where the decision maker guides the search, is complex because the stopping criterion is usually not known *a priori*. Similarly, applying the principles studied in this paper to cases where the stopping criterion is set by quality, seems complex. Thus, developing strategies to allow for the integration of the design principle studied in this research in such settings seems a worthwhile area of research.

Acknowledgments

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