The Importance of the Diversity on Variable Space in the Design of Multi-objective Evolutionary Algorithms

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***Abstract*—Most current Multi-objective Evolutionary Algorithms (MOEAs) do not directly manage the population's diversity on variable space. Usually, only when the aim is to attain diverse solutions in the variable space, these kinds of mechanisms are considered. This is a remarkable difference with respect to single-objective optimizers, where even when no diverse solutions are required, the benefits of controlling diversity are well-known. The aim of this paper is to show that the quality of current MOEAs in terms of objective space metrics can be enhanced by integrating mechanisms to explicitly manage the diversity on the variable space. The key is to consider the stopping criterion and elapsed period with the aim of dynamically altering the importance granted to the diversity on the variable space and to the quality and diversity on the objective space, which is an important difference with respect to niching-based MOEAs. Particularly, more importance is given to the variable space at initial phases and the balance is moved towards the objective space as evolution progresses. A novel MOEA based on decomposition (VSD-MOEA/D) that uses these principles through a novel replacement phase is devised. Extensive experimentation shows the clear benefits provided by our design principle.**

***Index Terms*—Diversity, Decomposition, Multi-objective Optimization, Evolutionary Algorithms.**

I. Introduction

Multi-objective Evolutionary Algorithms (MOEAs) are one of the most popular approaches to deal with Multi-objective Optimization Problems (MOPs) [1], [2]. MOEAs are usually employed in complex problems where more traditional optimization techniques are not applicable [3]. A continuous box-constrained minimization MOP, which is the case addressed in this paper, involves two or more conflicting objectives as defined in (1)

$$
\begin{aligned}
min \quad & F(x) = (f_1(x), ..., f_M(x)) \\
s.t. \quad & x_i^{(L)} \leq x_i \leq x_i^{(U)}
\end{aligned} \tag{1}
$$

where $x \in \Re^D$, D is the number of variables, and each decision variable $x_i \in \Re$ is constrained by $x_i^{(L)}$ and $x_i^{(U)}$, i.e. the lower bound and the upper bound. The feasible space bounded by $x_i^{(L)}$ and $x_i^{(U)}$ is denoted by Ω. Each solution is mapped to the *objective space* Y with the function $F : \Omega \rightarrow Y \subseteq \Re^M$, which consists of M real-valued objective functions. The goal of most MOEAs is to find a proper approximation of the Pareto Front, i.e., a set of solutions whose images are well-distributed and close to the Pareto Front [4].

In recent years, the development of MOEAs has grown dramatically [5], [6], resulting in effective and broadly applicable algorithms. However, some function features provoke significant degradation on the performance of MOEAs [7], so better design principles are yet required. Regarding the design of MOEAs, several paths have been explored resulting in diverse taxonomies [4]. For instance, principles related to decomposition, dominance and quality metrics are used to design MOEAs. Current state-of-the-art MOEAs consider in some way the diversity on the objective space. In some cases, this is done explicitly through density estimators [8], whereas in other cases, this is done indirectly [9]. Since optimizing most objective space quality indicators implies attaining a well-spread set of solutions in the objective space, not considering this kind of diversity would result in quite ineffective optimizers. A quite different condition appears with respect to diversity on the variable space. Since objective space quality metrics do not consider at all the diversity on the variable space, most MOEAs designers disregard this diversity.

Differently, several state-of-the-art single-objective methods introduce mechanisms to vary the trend of the diversity on the variable space even if obtaining a diverse set of solutions is not the aim of the optimization [10]. Instead, this is done to induce a better balance between exploration and exploitation. In fact, the proper management of diversity is considered as one of the cornerstones for proper performance [11]. Thus, these differences between the design principles applied in single-objective and multi-objective evolutionary algorithms are shocking. Moreover, practitioners have shown that modern MOEAs suffer some drawbacks related to stagnation and premature convergence in subset of variables [12], [13], [14], [15]. As a result, this paper studies the hypothesis that incorporating mechanisms to manage the diversity on the decision space might bring important benefits to the field of multi-objective optimization. Note that differently to other proposals, such as niching-based MOEAs [16], [17], we are not interested in obtaining a diverse set of solutions in the decision space. Instead, we state that the quality of the results in terms of objective-space indicators can be improved further with these kinds of mechanisms.

Since controlling diversity to attain a proper balance be-

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tween exploration and intensification have been considered so important in single-objective domains [18], quite a large amount of related methods have been devised [10]. Recent research in single-objective optimization has shown that important advances are attained when the balance between exploration and intensification is managed by relating the amount of maintained population's diversity to the stopping criterion and elapsed period of execution. Particularly, these methods reduce the importance given to the preservation of diversity as the end of the optimization is approached. This principle has been used to find new best-known solutions for the Frequency Assignment Problem (FAP) [19], to improve further continuous optimizers [20] and to design the winning strategy of the extended round of Google Hash Code 2020[1], with more than $100,000$ participants. Thus, we decided to explore the incorporation of this principle in the design of MOEAs.

One of the main difficulties for incorporating the previous principle to the design of MOEAs is that meassures of the variable space and objective space must be taken into account simultaneously. The discussed design principle is based on reducing the importance of diversity on variable space as generations evolve, so we maintain this decision and indirectly increase the importance granted to diversity and quality on objective space as the execution progresses. In order to show the validity of our hypothesis, this paper proposes the *Variable Space Diversity MOEA based on Decomposition* (VSD-MOEA/D). VSD-MOEA/D simplifies MOEA/D-DE [21] by deactivating the dynamical resource allocation scheme and the notion of neighborhood, and at the same time extends it by including a novel replacement strategy that applies the discussed design principles. Validation of our proposal is carried out taking into consideration MOEA/D-DE [21], NSGA-II [22], R2-EMOA [23] and NSGA-III [24]. Remarkable benefits are attained in terms of robustness and scalability.

The rest of this paper is organized as follows. Section II provides a review of MOEAs, diversity management and some other related works. The VSD-MOEA/D proposal is detailed in section III. Section IV is devoted to an extensive experimental validation of the novel proposal and design principle. Finally, conclusions and some lines of future work are given in section V.

II. Literature Review

MOEAs that take into account the diversity on variable space are not novel. Particularly, these kinds of techniques have been applied for multimodal multi-objective optimization [25], i.e., for cases where distant solutions in terms of variable space are desired [26], [27]. Such kinds of MOEAs must maintain a large degree of diversity on variable space during the whole optimization process. In contrast, our work analyses the hyphotesis that state-of-the-art techniques can be advanced further by explicitly managing the diversity on the variable space, even if the performance is only measured in terms of metrics that only take into account the objective space. Since our aim is different, using multimodal multi-objective optimizers that maintain a large diversity for the whole optimization process is counter-productive, so more advanced ways of integrating the control of diversity are required. Thus, this section reviews some of the most important advances on diversity-aware techniques that motivated the design of VSD-MOEA/D, which are a set of methods that were adopted to single-objective optimization. Additionally, MOEAs that have considered in some way the diversity on variable space and state-of-the-art MOEAs are summarized.

A. Diversity-aware Single-objective Optimizers

Attaining a proper balance between exploration and exploitation is one of the keys of sucessfull single-objective EAs [18]. Several strategies to acomplish this aim have been explored and one of the most promising is to alter the trend of diversity in an explicit or implicit way [10]. This principle has encouraged the development of a vast quantinty of diversity managment techniques [28]. A common classification of these methods is based on the sort of components modified in the EA. A popular taxonomy identifies the following groups [10]: *selection-based*, *population-based*, *crossover/mutation-based*, *fitness-based*, and *replacement-based*. Additionally it defines the categories *uniprocess-driven* and *multiprocess-driven*, depending on the number of components that are altered.

Replacement-based methods have yielded quite promising results in the last years. One of the most popular proposals belonging to this group is the *crowding* method, in which each new individual should replace similar individuals from the previous generation [29]. Several variants of this strategy have been devised, such as the *Restricted Tournament Selection* (RTS) [30]. A more recent approach that has shown to be quite effective in a wide quantity of single-objective problems [19] is based on the principle of biasing the decisions taken in the replacement phase by taking into consideration the stopping criterion and elepased period. This design principle has been successfull in continuous problems [20] and discrete problems [19], [31], including the problem proposed for Google Hash Code 2020, where the most effective optimizer was designed using this design principle. Specifically, initial phases of the optimization explicitly preserve a higher amount of diversity than final phases and the change between these behaviours is gradual. Given the success of this methodology in the single-objective case, we adopt it to design our novel MOEA.

B. Diversity on Variable Space in MOEAs

In spite of the vast quantity of proposed MOEAs, none of state-of-the-art techniques involve explictly managing the diversity in the variable space, which is a remarkable difference with respect to single-objective optimizers. One of the main reasons behind this difference is probably that there is a relation between the diversity on the objective space and the diversity on the decision variable space, so even if the diversity on decision space is not controlled explicitly, not so negative effects as in single-objective optimization usually appear. However, the relation between the two different diversities depend on each MOP [32], meaning that including

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

the successful principles of single-objective optimizers might result in more robust MOEAs. Most current MOEAs that take into account diversity on the variable space are devoted to multimodal multi-objective optimization. However, some attemps to apply these mechanisms in traditional multi-objective optimization have also been done.

The Non-Dominated Sorting Genetic Algorithm (NSGA) developed in 1995 [17] was one of the first MOEAs that employed diversity on the variable space. Particularly, fitness sharing is used to discriminate between solutions in the same front. In some way this method was designed in an opposite way than current methods: the diversity on variable space is considered but at the cost of disregarding the information of the diversity on objective space. The performance of NSGA is not even close to current MOEAs and one of the reason is precisely not considering the diversity on objective space.

In 2003, the GDEA [33] proposed by Toffolo and Benini integrated the diversity into the search as an additional objective, which modifies the ranking of the indiviuals and favors maintaining distant indidivuals during the whole optimization process. In 2005, Chan and Ray [34] proposed the application of selection operators to encorage the preservation of distant solutions both in objective and decision space. Later, Deb and Tiwari proposed the Omni-optimizer [26]. This algorithm is designed as a generic multi-objective, multi-optima optimizer. In the multi-objective case it is an extension of NSGA-II where the crowding distance considers both the objective and variable space. Since it first uses the typical rank procedure considering only the objective space, more importance is given to this space. and the diversity plays an inferior role. Unfortunately, there is no way to easily alter the importance given to each space. In 2009, Shir et al. showed that the diversity in the decision variable space can be significantly enhanced without hampering the convergence to a diverse Pareto-front approximation. Following this insight, the CMA-ES niching framework was proposed [32]. Estimation of Distribution Algorithms have also considered the information of the decision space to attain better aproximations of the Pareto set [35]. Finally, the Diversity Integrating Hypervolume-based Search Algorithm (DIVA) [36] weights the hypervolume contribution with the diversity of the decision variable space.

Note that from the discussed methods the only one that shows some improvements in terms of objective-space metrics is GDEA. However, results attained by GDEA are not as competitive as the ones attained by modern solvers so it is not currently considered as an state-of-the-art MOEA but as an easily applicable and general approach. The rest of the methods focuses on showing that solutions with a higher level of diversiy on the variable space can be obtained without a too negative effect on the approximation of the Pareto Front.

C. Multi-objective State-of-the-art Algorithms

Given the large amount of MOEAS proposed in the last decades, several taxonomies have been defined [37]. Most current techniques consider in some way at least one of the following concepts [4]: Pareto dominance, indicators and/or decomposition. Note that several MOEAS use more that one of these principles but most practitioners make the effort to classify proposals as domination-based, indicator-based or decomposition-based.

In domination-based MOEAs, the Pareto dominance relation is applied to bias the decisions of the optimizer. Although this relation stimulates convergence to the Pareto front, additional techniques to promote diversity in the objective space must be integrated. Several of the most traditional MOEAs belong to this group, and while they face some difficulties for many-objective optimization, they are considered quite effective for optimization problems with two and three objectives. Non-Dominated Sorting Genetic Algorithm-II (NSGA-II) is the most popular technique belonging to this group [22]. NSGA-III [24] extends NSGA-II by replacing the crowing selection with an strategy based on generating distributed reference points that resembles indicator-based strategies. While this method is aimed at many-objective optimization, it also provides some benefits for problems with three objectives.

Indicator-based MOEAS incorporate a measure of quality over sets of solutions to alter some components such as the selection and/or replacement [8]. Indicators take into account both the convergence and coverage, so no additional techniques to promove diversity in the objective space are required. A quite effective MOEA that belongs to this category is the R2-Indicator-Based Evolutionary Multi-objective Algorithm (R2-EMOA) [23]. SMS-EMOA [38] is also quite effective but it uses the computationally expensive hypervolume indicator, meaning that it is not so generally applicable as R2-EMOA.

Finally, decomposition-based MOEAs [39] incorporate scalarizing functions to transform the MOP into several single-objective optimization sub-problems. Those sub-problems are then solved in a simultaneously and colaborative way. The weighted Tchebycheff scalarizing approach have shown a remarkable performance. The most popular MOEA that belongs to this category is MOEA/D, which was proposed by Zhang et al. [9]. A distinctive feature of the MOEA/D is the application of neighborhoods at the level of each sub-problem. The mating selection and replacement operator takes into account this neighborhood to promote collaboration between similar subproblems. MOEA/D has gained a significant popularity in the last decade, so many extensions have been devised. Particularly, the MOEA/D-DE [40] — winner of some optimization competitions — provides important advances by incorporating DE operators, polynomial mutation, a dynamic computational resource allocation strategy, mating restrictions and a modified replacement operator to prevent the excessive replication of individuals.

Since practitioners compare algorithms under different conditions, it is not easy to clearly identify the most effective ones. Given the complementary properties contributed by the different discussed methodologies, our comparisons include MOEAs belonging to each category. Particularly, NSGA-II, NSGA-III, R2-EMOA and MOEA/D-DE are the set of state-of-the-art algorithms used to validate our proposal.

III. PROPOSAL

This section is devoted to describe our proposal, the *Variable Space Diversity* MOEA *based on Decomposition* (VSD-

Algorithm 1 Main procedure of VSD-MOEA/D

```
Initialization: Generate an initial population P^0 with N individuals
Let λ = {λ_1, ..., λ_N} be a set of evenly spread weight vectors
Evaluation: Evaluate each individual in P^0 and assemble the reference vector z* with the best objective values
Assign t = 0
while (not stopping criterion) do
    for each individual P_i^t ∈ P^t do
        DE variation: Generate solution Q_i^t by applying DE/rand/1/bin using P_i^t as target vector
        Mutation: Apply polynomial mutation to Q_i^t with probability p_m
        Evaluation: Evaluate the new individual Q_i^t and update the reference vector z* with the best objective values.
    Survivor selection: Generate P^{t+1} by applying the replacement scheme described in Algorithm 2, using P^t, Q^t, λ and z* as input
    t = t + 1
```

Algorithm 2 Replacement Phase of VSD-MOEA/D

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1: Input: P^t (Parent of current generation), Q^t (Offspring of current generation), λ^t (a set of weight vectors) and z* (Reference vector)
2: Output: P^{t+1}
3: R^t = P^t ∪ Q^t
4: P^{t+1} = ∅
5: Penalized = ∅
6: λ^{t+1} = ∅
7: D^t = D_I − D_I * G_Elapsed / (0.5*G_End)
8: while |P^{t+1}| ≤ N do
9:     Compute DCS in R^t using P^{t+1} as reference set
10:    Move the individuals in R^t with DCS < D^t to Penalized
11:    if R^t is empty then
12:        Compute DCS of each individual in Penalized set employing P^{t+1} as reference set
13:        Move the individual in Penalized with the largest DCS to R^t
14:    Identify the non-penalized individual R_i^t and the weight vector λ_j^t with the best scalarizing function value according to g^te(R_i^t|λ_j^t, z*)
15:    Move the non-penalized individual R_i^t to P^{t+1}
16:    Move the associated weight vector λ_j^t to λ^{t+1}
17: return P^{t+1}
```

MOEA/D). The main novelty and motivation behind VSD-MOEA/D is the incorporation of an explicit management of the diveristy on variable space with the aim of improving the behaviour in terms of objective space metrics specially in long-term executions, which is the environment where diversity-aware techniques have excelled. Although VSD-MOEA/D is inspired in MOEA/D, it was simplified so in some ways it resembles more mature decomposition-based MOEAs, such as MOGA. For instance, the notion of subproblem neighborhood is not used and the dynamic resource allocation usually applied in modern variants of MOEA/D is deactivated. The main reason for the simplification is to show that even a simple MOEA incorporating our design principles can improve further more complex state-of-the-art algorithms.

Our proposal decomposes the MOP in several single-objective problems. Notwithstanding that any scalarization approach can be employed, our strategy applies the achievement scalarizing function (ASF), which has shown some of the most effective results in recent years [24], [41]. Let $\lambda_1, ..., \lambda_N$ be a set of weight vectors and z^* a reference vector, the MOP is decomposed into N scalar optimization sub-problems as shown in (2).

$$g^{te}(x|\lambda_j, z^*) = \max_{1 \leq i \leq M} \left\{ \frac{|f_i(x) - z_i^*|}{\lambda_{j,i}} \right\} \tag{2}$$

The main novelty of VSD-MOEA/D appears in the survivor selection scheme. Following some of the most successful single-objective diversity-aware algorithms [19], the replacement strategy relates the degree of diversity on variable space to the stopping criterion and elapsed generations. The aim of this relation is to gradually bias the search from exploration to explotation as the optimization evolves. In particular, the diversity is explicitly promoted in a decreasing way until half of total generations. Then, in the remaining generations VSD-MOEA/D has a similar behavior than most popular MOEAs, i.e. the diversity on the variable space is not considered explicitly.

The main procedure of VSD-MOEA/D is shown in Algorithm 1. Its general template is quite standard. The mating and variation components are similar to those used in typical MOEAs. Particularly, in the t generation, the population P^t is used to generate the offspring Q^t with N individuals by randomly selecting at each step three indivuals to apply the $DE/rand/1/bin$ operator. Then, polynomial mutation is applied to the output of the DE operator. As in most current MOEA/D variants, the initial population is generated randomly, the number of weight vectors is equal to the population size, and the reference vector z^* used for ASF is composed by the best attained objective values. Finally, the survivor selection stage is applied. This is quite different to traditional techniques, in the sense that P^t and Q^t are merged, meaning that differently than in MOEA/D the position of each individual is not important, and a diversity-aware selection is performed. Since this is the novelty of the paper, its working operation is given in detail.

A. Novel Replacement Phase of VSD-MOEA/D

The purpose of the replacement phase (see Algorithm 2) is to select the set of survivors of the next generation. The survivor selection described in this work incorporates similar design principles to those applied in the diversity-aware single-objective optimizer DE-EDM [20]. It operates as follows. First, the parent and offspring populations are merged in a multi-set to establish the candidate set R^t (line 3). A key of the scheme is to promote the selection of individuals with a large enough contribution to diversity on variable space. Particularly, the contribution of an individual x is calculated as $\min_{p \in P^{t+1}} Distance(x, p)$, where P^{t+1} is the multi-set of the already picked survivors and the normalized Euclidean distance specified in (3) is applied. Note that in the pseudocode the tag DCS (Distance to Closest Solution) is used to denote the contribution to diversity.

$$Distance(A,B) = \left(\frac{1}{D} \sum_{i=1}^{D} \left(\frac{A_i - B_i}{x_i^{(U)} - x_i^{(L)}} \right)^2 \right)^{1/2} \quad (3)$$

In order to promote the selection of distant individuals, a threshold D^t is dynamically calculated (line 7) and individuals with a DCS value lower than the threshold are considered as undesirable individuals. Note that the calculation of D^t depends on an initial threshold value (D_I), which is a parameter of our proposal, on the number of generations that have evolved ($G_{Elapsed}$) and on the stopping criterion (G_{End}), i.e., the number of generations to evolve. Particularly, the value is decreased linearly as generations evolve. Since survivors with larger DCS values, provoke exploration steps, while survivors with short DCS values promote intensification steps, this linear decrease promotes a gradual transition from exploration to exploitation. Also note that after 50% of the total number of generations, the D^t value is below 0, meaning that no penalties are applied and a more traditional strategy focused only on the objectives values is used to perform the selection steps.

The strategy iteratively selects an individual from the candidate set (R^t) to enter the new population (P^{t+1}) until it is filled with N individuals (lines 8-16). In particular, the aim is to select a proper individual for each weight vector but at the same time fulfilling the condition imposed for the contribution to diversity on variable space. In order to fulfil this last condition, non-selected individuals with a DCS lower than D^t are moved from R^t to the $Penalized$ set (lines 9-10) and at each iteration an individual belonging to R^t is picked up to survive. The set of weight vectors considered by our strategy are initially placed in λ^t. At each iteration the individual in R^t with the best scalarizing function for any of the weight vectors in λ^t is identified (line 14). Then, such an individual is selected as a survivor (line 15) and the used weight vector is transferred to the weight vector set of the next population (line 16). Note that N individuals are selected, meaning that each weight vector is used to select a single individual. Also note that it might happen that R^t is empty prior to selecting N individuals. This means that the diversity is lower than expected so with the aim of increasing the exploration degree, the individual with the largest DCS value in the $Penalized$ set is selected to survive (lines 11 - 13).

IV. Experimental Validation

This section is devoted to carry out the validation of our proposal against state-of-the-art MOEAs. Particularly, is shown that controlling the diversity of the decision variables can be benefical to attain better approximations to the Pareto front. The latter is proven employing long-term executions with some of the most popular MOEAs. Although that this principle can be incorporated into any multi-objective paradigm, the benefits of promoting diversity are only confirmed with a decomposition-based algorithm. To have a clear insight of the performance of each selected algorithm, this section is arranged as follows. At first, the technical parameterization that governs the common comparison is presented. Then, a quite common and representative comparison between all the MOEAs in long-term executions is shown. In order, to have a better understanding of the scalability and stability, three more experiments are driven. These experiments are designed to test the scalability of the decision variables, analyze the impact of diversity among the execution, and robustness of VSD-MOEA/D with different initial penalty thresholds. The latter seeks to illustrate the effects of promoting diversity with different initial levels.

The validation of the MOEAs takes into account three of the most popular benchmarks in multi-objective optimization. These problems are the WFG [7], DTLZ [42], and UF [43], whose selected configuration is taken from the literature. Specifically, the WFG test problems were used with two and three objectives configured with 24 parameters[2], 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). This last set of problems were configured with 30 variables.

The state-of-the-art MOEAs that are taken into account are four of the most popular in multi-objective optimization. Those algorithms are NSGA-II [22], MOEA/D-DE [21], R2-EMOA [23] and NSGA-III [24]. While the former three can be classified as dominance-based, decomposition-based and indicator-based, the latter might be considered as an hybrid, since that it introduces the main framework of NSGA-II and utilizes a set of weight vectors as reference points [4]. In a similar way than some of the most popular MOEAs, MOEA/D has been taken as a representative based-decomposition algorithm, which has inspired the development a vast quantity of algorithms in its category. Particularly, in this analyses is included the MOEA/D-DE, which obtained the first place in the Congress on Evolutionary Computation 2009 (CEC-2009) [21].

Each experiment that was run in this section is configured with a population size of 100 individuals. Moreover, the variation operators integrated in all the MOEAs is the classic binomial DE scheme better known as DE/rand/1/bin. In addition, MOEA/D and VSD-MOEA/D incorporate the polynomial mutation with probability and distribuion index fixed to $1/n$ and 50, respectively. To have a fair comparison, for each MOEA the crossover probability (CR) and mutation factor (F) values were chosen by grid-search. Particularly, we have tested 20 combinations of four values of F (i.e. 0.25, 0.5, 0.75 and 1.0) and five values of CR (i.e. 0.0, 0.25, 0.5, 0.75, 1.0) with two and three objectives. The performance of each combination was measured taking into account the whole set of problems and a stopping criterion of 2.5×10^6 function evaluations. In this way each MOEA was set with the values whose performance was the best, such values are reported in Table I. Note that a detailed information can be found in the supplementary material.

The specific parameterization required by each algorithm is shown in Table II. Note that scalarization functions are required in MOEA/D-DE, R2-EMOA, NSGA-III and VSD-

[2] In the WFG context the term *parameters* is equivalent to variables.

TABLE I
DE PARAMETERIZAON APPLIED TO EACH MOEA

	2 objectives		3 objectives	
	CR	F	CR	F
VSD-MOEA/D	0.0	0.75	0.0	0.75
MOEA/D-DE	0.75	0.75	0.5	0.5
R2-EMOA	0.75	0.5	0.5	0.5
NSGA-II	0.75	0.5	0.0	0.5
NSGA-III	0.5	0.5	0.5	0.5

TABLE II
PARAMETERIZATION APPLIED TO EACH MOEA

Algorithm	Configuration
MOEA/D-DE	Max. updates by sub-problem (η_r) = 2, tour selection = 10, neighbor size = 20, period utility updating = 50 generations, local selection probability (δ) = 0.9,
R2-EMOA	$\rho = 1$, offspring by iteration = 1
VSD-MOEA/D	$D_I = 0.4$

MOEA/D. In all those cases, the ASF approach is used. Nevertheless, the weight vectors employed in R2-EMOA are distinct that in the remaining algorithms. According to the author's code, R2-EMOA was applied with 501 and 496 weight vectors for two and three objectives, respectively [23]. In contrast, to have the same quantity of weight vectors than the population size, the remaining algorithms incorporate a different distribution of weight vectors. Those weight vectors were generated with the Uniform Design (UD) and the Good Lattice Point (GLP) method [44], [45]. Given that all the algorithms are stochastic, each execution was repeated 35 times with different seeds. The hypervolume indicator (HV) is used to compare the various schemes. The reference 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 [46]. The normalized HV is used to facilitate the interpretation of the results [47], 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 such value is not attainable because MOEAs yields a discrete approximation.

Finally, to statistically compare the HV ratios, a guideline similar to that proposed in [48] was used. First a Shapiro-Wilk test was performed to check if the values of the results followed a Gaussian distribution. If so, the Levene test was used to check for the homogeneity of the variances. If the samples had equal variance, an ANOVA test was done; if not, a Welch test was performed. For non-Gaussian distributions, the non-parametric Kruskal-Wallis test was used to test whether samples are drawn from the same distribution. An algorithm X is said to beat algorithm Y when the differences between them are statistically significant, and the mean and median HV ratios obtained by X are higher than the mean and median achieved by Y.

A. *Performance of* MOEAs *in long-term executions*

A critical point of our proposal is to yield even better approximations extending the stopping criterion. Keeping this in mind, our comparisons are carried out with long-term executions. Therefore, in this section the stopping criterion was set at 2.5×10^7 function evaluations.

Table III shows the HV ratio obtained for the benchmark functions with two objectives. For each method and problem is reported the best, mean and standard deviation of the HV ratio values. Furthermore, to summarize each method, the last row shows the results considering the whole set of problems. For each test problem, the method that yielded the largest mean and those that were not statistically inferior than the best are shown in **boldface**. Similarly, the method that yielded the best HV values among all the runs are <u>underlined</u>. From here on, the methods shown in **boldface** for a given problem are referred to as the winning methods.

The rank of the methods based on the wins is VSD-MOEA/D, R2-EMOA, NSGA-III, MOEA/D-DE and NSGA-II, whose counts are 15, 7, 5, 5 and 2, respectively. This indicates that VSD-MOEA/D is the winner, in fact it won more than twice times than the method in second place (R2-EMOA). This superiority is confirmed with the HV ratio value considering the whole set of problems. In contrast, R2-EMOA attained the worst value of 0.897, this might occurs since some problems were not approximated properly reporting a remarkably degradation of the HV ratio. In spite that the decomposition-based MOEAs achieved the highest mean HV ratio values, the difference reported by VSD-MOEA/D (0.973) is considerably greater than MOEA/D-DE (0.931). Inspecting the data carefully, it can be seen that in the case where VSD-MOEA/D loses, 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/D 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 5, 4, 5 and 4 problems for R2-EMOA, NSGA-II, NSGA-III and MOEA/D-DE, respectively. Similar conclusions can be drawn analyzing the standard deviation. This means that even if VSD-MOEA/D loses in some cases, its deterioration and standard deviation 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 IV shows the number of times that each method statistically won (column $\uparrow$), lost (column $\downarrow$), tied (column $\leftrightarrow$) and a metric of **Score**. The latter indicates the difference between the number of times that each method won and the number of times that each method lost.

Additionally, for each method M, 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 M, for each problem where M was not in the group of winning methods. This value is shown in the Deterioration column. The data confirms that although VSD-MOEA/D loses in some cases, the overall numbers of wins and losses favors VSD-MOEA/D. More importantly, the total deterioration is quite lower in the case of VSD-MOEA/D, confirming that when VSD-MOEA/D loses, the deterioration is not that large.

Tables V and VI show the same information for the prob-

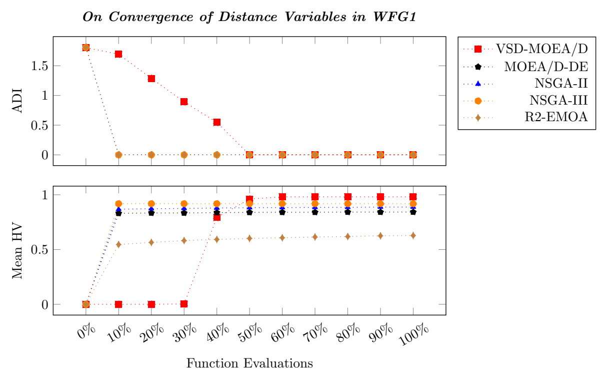

Fig. 1. Diverstiy of distance variables (first row) and mean of HV values (second row) vs. elapsed time in the bi-objective WFG1 test problem. The reported results are taken from 35 runs.

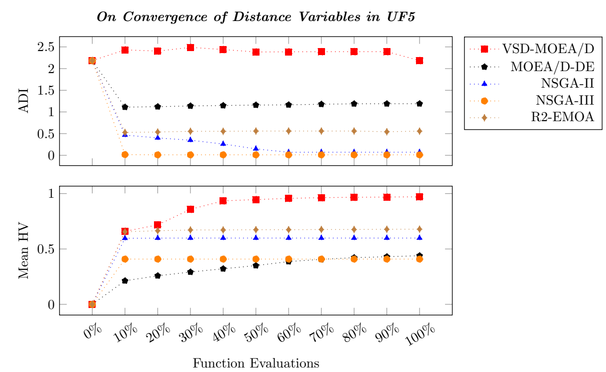

Fig. 2. Diverstiy of distance variables (first row) and mean of HV values (second row) vs. elapsed time in the bi-objective UF5 test problem. The reported results are taken from 35 runs.

lems with three objectives. In this case the rank of the methods based on the wins is VSD-MOEA/D, R2-EMOA, MOEA/D-DE, NSGA-III and NSGA-II, whose counts are 9, 9, 3, 2 and 0, respectively. Taking into account the mean of all the test problems, VSD-MOEA/D again obtained a much larger mean HV ratio than the remaining ones. Once again, the difference between the mean HV ratio obtained by the best method and by VSD-MOEA/D was never greater than 0.1. However, all the other methods exhibited a deterioration greater than 0.1 in several cases. In particular, this happened in 3, 6, 4 and 2 problems for R2-EMOA, NSGA-II, NSGA-III and MOEA/D-DE, respectively. In spite that VSD-MOEA/D is superior than the other methods in terms of total deterioration, its pair-wise statistical tests are not remarkably superior than R2-EMOA in terms of total wins and losses (see Table VI and data shown in **boldface** in Table V). This might occurs since that R2-EMOA takes into account a greater number of weight vectors, in some problems it allows the allocation of solutions in regions that contributes in a better way to HV. Nevertheless, the mean HV ratio value attained by VSD-MOEA/D is quite superior than the remaining methods. In fact the HV ratio values attained by VSD-MOEA/D in each problem is not worst than the reported by MOEA/D-DE and NSGA-III with three objectives, such methods incorporated the same number of weight vectors. To prove those arguments, in the suplementary material is shown a variant of our proposal AVSD-MOEA/D in which is incorporated an external archive based in the R2 indicator. AVSD-MOEA/D was remarkable superior than the state-of-the-art MOEAs with two and three objectives in both total deterioration (0.153 and 0.006) and term of total wins and loses (80 and 73 wins).

In order to better understand the benefits of VSD-MOEA/D against the state-of-the-art MOEAs. This section ilustrates the evolution of the HV values and the diversity of some MOPs. According to the WFG test problems, the variables can be classified into two kinds of variables: the distance variables and the position variables. Note that a variable x_i is a distance variable when for all x, modifying x_i results in a new solution that dominates x, is equivalent to x, or is dominated by x. However, if x_i is a position variable, modifying x_i in x always results in a vector that is incomparable or equivalent to x [7]. Particularly, in the WFG1 the distance variables are uni-modal and its optimal region has polynomial and flat properties, which might provoke stagnation in some MOEAs. In contrast, the UF5 is a multi-modal problem and its optimal regions are quite isolated among the decision variable space, in fact its Pareto optimal front is discretized and conformed by only 21 points. For each algorithm, the selected diversity metric is calculated as the average Euclidean distance among individuals (ADI) in the population by considering only the distance variables. Figures 1 and 2 show how the ADI (top) and the mean of HV (bottom) evolve for the WFG1 and UF5, respectively. In the WFG1 problem, the distance variables of the state-of-the-art MOEAS converged to a region approximately after the 10% of the total execution. Among the remaining function evaluations those MOEAs were not able to improve the quality of its approximations. In the case of VSD-MOEA/D, the decrease in ADI is quite linear until the halfway point of the execution. Showing that preserving diversity at different levels might improve the final approximation. Although R2-EMOA attained the best HV values in several problems, its degradation in some problems (e.g. WFG1) is quite shocking. This is not the case of VSD-MOEA/D, whose performance was always the best or almost the best.

Promoting explicitly diversity among the execution is also benefical to multi-modal problems. For instance, the advantage of promoting diversity in the UF5 test problem is shown in Figure 2. Particularly, this figure shows that VSD-MOEA/D not only attained a better HV values at the first 10% of total function evaluations, it also kept looking for promising regions. In fact, its HV values improved meaningfully until a half of total execution that is the final point in which the diversity were explicitly promoted. It also shows that MOEA/D-DE finds several promising regions among the execution, such effect might be provoked by the polynomial mutation. Nevertheless, the improvements provoked by this operator does not improve two state-of-the-art MOEAS at the end of the execution. The reamining MOEAS reported the same HV and ADI values after 10% of the total function evaluations.

TABLE III
SUMMARY OF THE HYPERVOLUME RATIO RESULTS ATTAINED FOR PROBLEMS WITH TWO OBJECTIVES

	VSD-MOEA/D			MOEA/D-DE			NSGA-II			NSGA-III			R2-EMOA		
	Best	Mean	Std	Best	Mean	Std	Best	Mean	Std	Best	Mean	Std	Best	Mean	Std
WFG1	0.993	**0.981**	0.020	0.957	0.842	0.058	0.984	0.888	0.053	0.993	0.919	0.051	0.762	0.628	0.077
WFG2	0.996	0.996	0.000	0.996	0.996	0.000	0.998	**0.998**	0.000	0.997	0.996	0.000	0.998	**0.998**	0.000
WFG3	0.992	**0.992**	0.000	0.992	**0.992**	0.000	0.984	0.982	0.001	0.992	**0.992**	0.000	0.992	0.991	0.000
WFG4	0.988	**0.988**	0.000	0.988	**0.988**	0.000	0.985	0.983	0.001	0.988	**0.988**	0.000	0.991	0.987	0.006
WFG5	0.929	**0.902**	0.008	0.891	0.882	0.004	0.892	0.883	0.003	0.892	0.890	0.001	0.888	0.885	0.002
WFG6	0.955	0.918	0.020	0.988	0.963	0.019	0.980	0.978	0.001	0.980	0.959	0.010	0.991	**0.990**	0.001
WFG7	0.988	0.988	0.000	0.988	0.988	0.000	0.984	0.982	0.001	0.988	0.988	0.000	0.991	**0.990**	0.000
WFG8	0.959	**0.950**	0.004	0.846	0.833	0.004	0.821	0.815	0.003	0.832	0.829	0.001	0.837	0.834	0.001
WFG9	0.975	**0.973**	0.002	0.974	0.954	0.039	0.941	0.853	0.071	0.799	0.798	0.001	0.975	0.936	0.063
DTLZ1	0.993	**0.993**	0.000	0.993	**0.993**	0.000	0.992	0.991	0.000	0.993	**0.993**	0.000	0.992	0.992	0.000
DTLZ2	0.989	0.989	0.000	0.989	0.989	0.000	0.989	0.988	0.001	0.989	0.989	0.000	0.992	**0.992**	0.000
DTLZ3	0.989	0.989	0.000	0.989	0.989	0.000	0.989	0.932	0.229	0.989	0.989	0.000	0.992	**0.992**	0.000
DTLZ4	0.989	**0.989**	0.000	0.989	**0.989**	0.000	0.990	0.926	0.204	0.989	**0.989**	0.000	0.992	0.740	0.348
DTLZ5	0.989	0.989	0.000	0.989	0.989	0.000	0.989	0.988	0.001	0.989	0.989	0.000	0.992	**0.992**	0.000
DTLZ6	0.989	**0.989**	0.000	0.989	0.986	0.014	0.989	0.984	0.024	0.989	**0.989**	0.000	0.992	0.456	0.366
DTLZ7	0.996	0.996	0.000	0.996	0.996	0.000	0.997	**0.997**	0.000	0.996	0.996	0.000	0.997	**0.997**	0.000
UF1	0.994	**0.994**	0.000	0.987	0.986	0.001	0.990	0.989	0.001	0.992	0.989	0.002	0.993	0.992	0.000
UF2	0.994	**0.993**	0.000	0.990	0.988	0.001	0.984	0.982	0.001	0.989	0.985	0.002	0.988	0.987	0.001
UF3	0.934	0.904	0.016	0.991	**0.990**	0.001	0.975	0.967	0.008	0.935	0.781	0.097	0.984	0.974	0.006
UF4	0.974	**0.971**	0.002	0.914	0.904	0.006	0.898	0.888	0.006	0.889	0.885	0.002	0.908	0.898	0.005
UF5	0.988	**0.971**	0.011	0.715	0.439	0.137	0.785	0.598	0.173	0.690	0.409	0.144	0.803	0.679	0.160
UF6	0.961	**0.936**	0.014	0.928	0.748	0.175	0.819	0.752	0.030	0.743	0.526	0.177	0.897	0.732	0.049
UF7	0.993	**0.992**	0.000	0.991	0.990	0.001	0.981	0.978	0.002	0.968	0.956	0.023	0.988	0.977	0.004
Mean	0.980	**0.973**	0.004	0.960	**0.931**	0.020	0.954	**0.927**	0.035	0.939	**0.905**	0.022	0.954	**0.897**	0.047

TABLE IV
STATISTICAL TESTS AND DETERIORATION LEVEL OF THE HV RATIO FOR PROBLEMS WITH TWO OBJECTIVES

	↑	↓	↔	Score	Deterioration
VSD-MOEA/D	64	27	1	37	0.170
MOEA/D-DE	41	45	6	-4	1.140
NSGA-II	24	64	4	-40	1.235
NSGA-III	41	47	4	-6	1.730
R2-EMOA	51	38	3	13	1.916

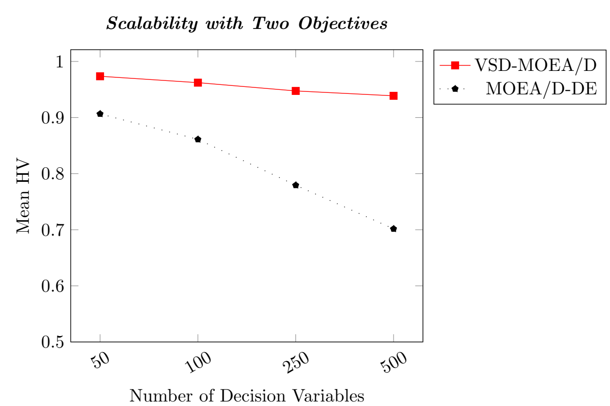

Fig. 3. Mean of the HV ratio for 35 runs for the two-objective problems considering different numbers of variables

B. Decision Variable Scalability Analysis

In order, to have a better insight of the benefits of our proposal, the scalability in term of the number of decision variables is tested. In particular, this experiment was carried out with the decomposition-based algorithms. Such MOEAs were applied with the same benchmark problems, but considering 50, 100, 250 and 500 variables. Note that in the WFG test problems, the number of position variables and distance variables must be specified. Specifically, the number of distance variables was set to 42, 84, 210 and 418 when using 50, 100, 250 and 500 variables, respectively. The rest of the decision variables were position variables, meaning that they were 8, 16, 40 and 82, respectively. In addition, the stopping criterion was set to 2.5×10^7 function evaluations. Figures 3 and 4 show the mean HV ratio for the selected algorithms, considering the problems with two and three objectives, respectively. In spite that the HV ratio decreases as the number of variables increases, with two and three objectives the performance of VSD-MOEA/D is quite robust, in fact its deterioration is much lower than MOEA/D-DE.

C. Analysis of the Initial Threshold Value

Possibly, the main downside of including a strategy to explicitly promoting the diversity is the need of incorporating an additional parameter. For instance, VSD-MOEA/D requires to set an initial threshold value (D_I). Given the evidence of several findings in the literature, in the previous experiments a value of $D_I = 0.4$ was used. However, in this section a more detailed study of this parameter is driven.

In this section is analized the overall performance of VSD-MOEA/D using different D_I values. Thereafter, in a more specifically way, the effect of this parameter is analized in WFG9 and UF10 test problems, in two and three objectives, respectively. Note that, since normalized distances are used, the maximum difference that can appear is 1.0, which belongs to the main diagonal of the box-constrained minimization MOP. Additionally, note that when D_I is set to

TABLE V
SUMMARY OF THE HYPERVOLUME RATIO RESULTS ATTAINED FOR PROBLEMS WITH THREE OBJECTIVES

	VSD-MOEA/D			MOEA/D-DE			NSGA-II			NSGA-III			R2-EMOA		
	Best	Mean	Std	Best	Mean	Std	Best	Mean	Std	Best	Mean	Std	Best	Mean	Std
WFG1	0.971	**0.968**	0.007	0.972	0.937	0.030	0.960	0.899	0.042	0.971	0.966	0.011	0.976	0.939	0.028
WFG2	0.980	**0.979**	0.001	0.981	**0.979**	0.001	0.951	0.922	0.027	0.973	0.970	0.002	0.963	0.962	0.000
WFG3	0.990	0.990	0.000	0.990	0.990	0.000	0.983	0.974	0.005	0.929	0.915	0.008	0.992	**0.992**	0.000
WFG4	0.899	0.897	0.000	0.899	0.898	0.001	0.898	0.879	0.008	0.885	0.881	0.002	0.915	**0.909**	0.002
WFG5	0.860	0.837	0.009	0.831	0.831	0.000	0.832	0.812	0.012	0.830	0.828	0.001	0.848	**0.846**	0.001
WFG6	0.866	0.842	0.011	0.887	0.862	0.013	0.861	0.838	0.013	0.897	0.880	0.030	0.904	**0.893**	0.005
WFG7	0.900	0.898	0.001	0.899	0.898	0.001	0.892	0.874	0.009	0.897	0.897	0.000	0.912	**0.904**	0.002
WFG8	0.890	**0.881**	0.004	0.816	0.812	0.003	0.765	0.752	0.007	0.807	0.806	0.001	0.826	0.824	0.001
WFG9	0.885	0.871	0.004	0.875	0.862	0.005	0.822	0.721	0.027	0.747	0.741	0.002	0.884	**0.881**	0.003
DTLZ1	0.953	**0.953**	0.000	0.953	**0.953**	0.000	0.953	0.795	0.312	0.953	**0.953**	0.000	0.942	0.941	0.001
DTLZ2	0.914	0.914	0.000	0.914	0.914	0.000	0.894	0.879	0.009	0.913	0.913	0.000	0.916	**0.915**	0.001
DTLZ3	0.914	0.914	0.000	0.914	0.914	0.000	0.892	0.395	0.432	0.913	0.913	0.000	0.916	**0.915**	0.001
DTLZ4	0.915	**0.914**	0.000	0.914	**0.914**	0.000	0.900	0.731	0.269	0.913	0.913	0.000	0.916	0.850	0.214
DTLZ5	0.979	0.979	0.000	0.979	0.979	0.000	0.981	0.979	0.001	0.978	0.971	0.003	0.986	**0.986**	0.000
DTLZ6	0.979	**0.979**	0.000	0.979	0.959	0.038	0.982	0.932	0.177	0.974	0.968	0.003	0.986	0.551	0.355
DTLZ7	0.922	0.922	0.000	0.922	0.922	0.000	0.946	0.926	0.029	0.950	**0.939**	0.006	0.889	0.850	0.019
UF8	0.897	**0.890**	0.004	0.891	0.862	0.032	0.861	0.832	0.057	0.553	0.550	0.001	0.903	0.885	0.007
UF9	0.953	**0.950**	0.001	0.947	0.813	0.071	0.937	0.879	0.066	0.871	0.815	0.041	0.953	0.846	0.080
UF10	0.789	**0.746**	0.042	0.681	0.435	0.147	0.629	0.295	0.171	0.553	0.539	0.066	0.579	0.566	0.056
Mean	0.919	**0.912**	0.004	0.908	**0.881**	0.018	0.891	**0.806**	0.088	0.869	**0.861**	0.009	0.906	**0.866**	0.041

TABLE VI
STATISTICAL TESTS AND DETERIORATION LEVEL OF THE HV RATIO FOR PROBLEMS WITH THREE OBJECTIVES

	↑	↓	↔	Score	Deterioration
VSD-MOEA/D	53	19	4	34	0.117
MOEA/D-DE	40	31	5	9	0.710
NSGA-II	8	63	5	-55	2.126
NSGA-III	29	44	3	-15	1.081
R2-EMOA	50	23	3	27	0.985

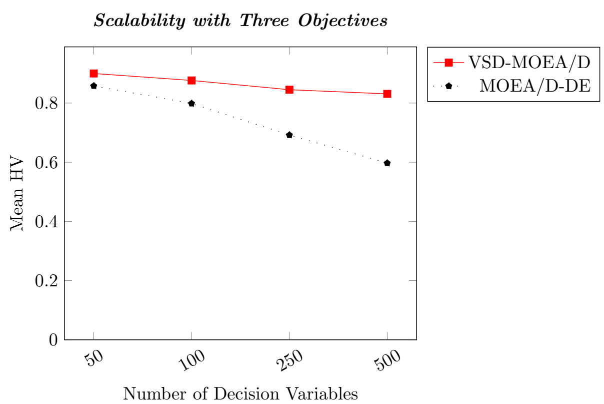

Fig. 4. Mean of the HV ratio for 35 runs for the three-objective problems considering different numbers of variables

0.0, no individual is penalized on the basis of its decision variable space diversity contribution, so VSD-MOEA would behave like a more traditional MOEA. Specifically, the values $D_I = \{0.0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0\}$ were tested. As in previous experiments, the whole set of benchmark problems was used and the stopping criterion was set to 2.5×10^7 function evaluations.

Figure 5 shows the mean HV ratio obtained for both the two-objective and the three-objective case.

The worst performance of the VSD-MOEA/D is when it is set to $D_I = 0.0$. The HV ratio obtained quickly increases as higher D_I values up to 0.2 are used. Larger values provide a quite similar performance. In fact, there is a wide range of values (from 0.2 to 1.0) where the performance is very good, meaning that the behavior of VSD-MOEA is quite robust. Thus, properly setting this parameter is not a complex task.

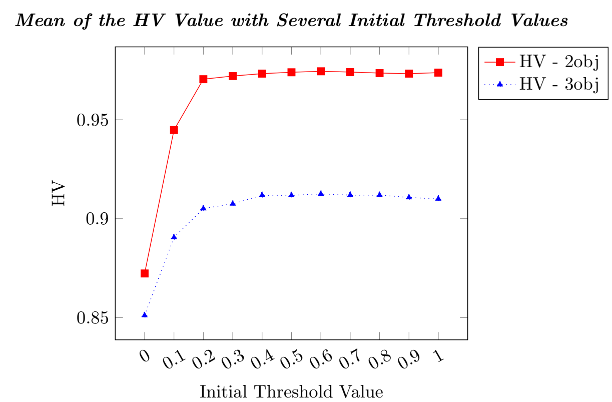

Fig. 5. Mean of HV values taking into account all the problems with several initial threshold values

In the same way than in the previous experiments, the Figures 6 and 7 show the evolution of diversity (top side) and HV ratio (bottom side) among the execution. The WFG9 test problem is multi-modal and deceptive. In addition, the UF10 test problem is highly multi-frontal and can be considered as one of the most challenging problems. Such diagrams belong to VSD-MOEA/D with the values $D_I = \{0.0, 0.4, 1.0\}$. Interestingly, the behavior of VSD-MOEA/D with $D_I = 0.0$ is quite similar than the state-of-the-art MOEAs, which confirms or previous claim. The motivation behind those diagrams is to ilustrate that to achieve a better balance between exploration and exploitation can be the explicit promotion of diversity among the execution. Therefore, those figures show that in multi-objective optimization –depending in each MOP– there

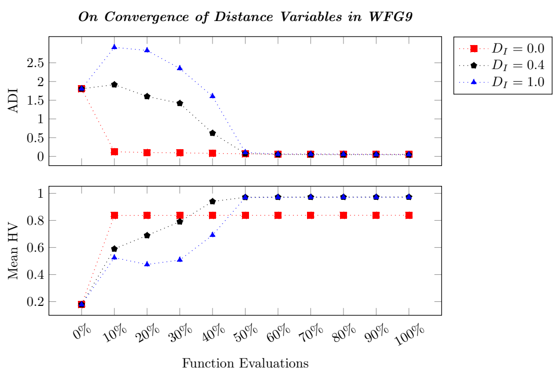

Fig. 6. Diverstiy of distance variables (first row) and mean of HV values (second row) vs. elapsed time in the two-objective WFG9 test problem. The reported results are taken from 35 runs.

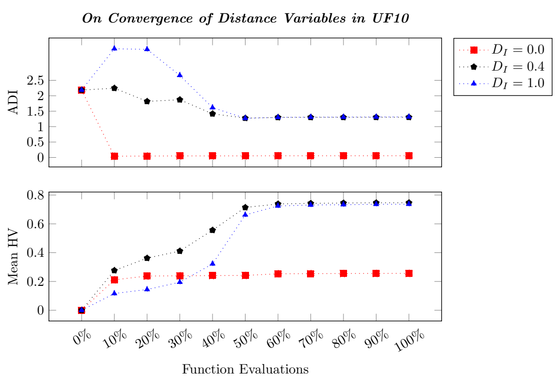

Fig. 7. Diverstiy of distance variables (first row) and mean of HV values (second row) vs. elapsed time in the three-objective UF10 test problem. The reported results are taken from 35 runs.

is a relation between the diversity and the quality solutions, in fact visually the shapes of the ADI and HV ratio complement each other. Even more the HV ratio values are constantly improving as the execution time elapses.

V. Conclusion

Multi-objective Evolutionary Algorithms are one popular strategy to deal with complex optimization problems. However, one of the most critical drawbacks of EAs is quite present in long-term executions where a fast and uncontrolled convergence might comes up, resulting in a waste of computational resources. A quite popular strategy to manage the convergence of a EA is to explicitly control de diversity in the population. This strategy relies in the incorporation of a replacement operator. In this way, the most complex problems can be approximated quite good.

This paper proposes a decomposition-based MOEA, that take sinto account the diversity of both decision varaible space and objective function space. The main novelty is that the convergence is managed to different levels through several diversities which are adapted during the optimization process. In particular, in VSD-MOEA more importance is given to the diversity of decision variable space at the initial stages, but at later stages of the evolutionary process, it gradually grants more importance to the diversity of objective function space. This is performed using a penalty method that is integrated into the replacement phase.

The experimental validation carried out shows a remarkable improvement in VSD-MOEA when it is compared to state-of-the-art MOEAs both in two-objective and three-objective problems. The scalability analyses shows that as the number of objectives and decision variables increases, the implicit variable space maintained by state-of-the-art MOEAs also increases. Finally, the analysis of the initial threshold distance, which is an additional parameter required by VSD-MOEA, shows that finding a proper value for this parameter is not a difficult task.

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. Finally, in order to obtain even better results, these strategies are going to be incorporated into a multi-objective memetic algorithm.

Acknowledgments

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