

The Importance of Diversity in the 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 in the variable space. Usually, these kinds of mechanisms are only considered when the aim is to attain diverse solutions in the variable space. This is a remarkable difference with respect to single-objective optimizers, where even when no diverse solutions are required, the benefits of diversity-aware techniques 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 in the variable space. The key is to consider the stopping criterion and elapsed period in order to dynamically alter the importance granted to the diversity in the variable space and to the quality and diversity in the objective space, which is an important difference with respect to niching-based MOEAs. Specifically, more importance is given to

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the variable space in the initial phases, a balance that is shifted towards the objective space as the evolution progresses. This paper presents a novel MOEA based on decomposition (AVSD-MOEA/D) that relies on these principles by means of a novel replacement phase. Extensive experimentation shows the clear benefits provided by our design principle.

Keywords: Diversity, Decomposition, Multi-objective Optimization, Evolutionary Algorithms.

1. Introduction

Multi-Objective Evolutionary Algorithms (MOEAs) are one of the most popular approaches for dealing 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)

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

where $x \in \mathbb{R}^D$, D is the number of variables, and each decision variable $x_i \in \mathbb{R}$ 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 $F : \Omega \rightarrow Y \subseteq \mathbb{R}^M$, 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].

15 In recent years, the development of MOEAs has grown dramatically [5, 6],
16 resulting in effective and broadly applicable algorithms. However, some func-
17 tion features provoke significant degradation of the performance of MOEAs [7],
18 meaning that better design principles are still required. Regarding the de-
19 sign of MOEAs, several paths have been explored, resulting in diverse tax-
20 onomies [4]. For instance, principles related to decomposition, dominance
21 and quality metrics are used to design MOEAs. Current state-of-the-art
22 MOEAs consider in some way the diversity in the objective space. In some
23 cases, this is done explicitly through density estimators [8], whereas in other
24 cases, this is done indirectly [9]. Since optimizing most objective space qual-
25 ity indicators implies attaining a well-spread set of solutions in the objective
26 space, not considering this kind of diversity would result in fairly ineffective
27 optimizers. A quite different condition appears with respect to diversity in
28 the variable space. Since objective space quality metrics do not consider at
29 all the diversity in the variable space, most MOEA designers disregard this
30 diversity.

31 Alternatively, several state-of-the-art single-objective methods introduce
32 mechanisms to vary the trend of the diversity in the variable space, even if
33 obtaining a diverse set of solutions is not the aim of the optimization [10].
34 Instead, this is done to induce a better balance between exploration and
35 exploitation. In fact, the proper management of diversity is considered one
36 of the cornerstones for proper performance [11]. Thus, these differences be-
37 tween the design principles applied in single-objective and multi-objective
38 evolutionary algorithms are surprising. Moreover, practitioners have shown
39 that modern MOEAs suffer some drawbacks involving stagnation and prema-

ture convergence in subsets of variables [12, 13, 14, 15]. As a result, this paper studies the hypothesis that incorporating mechanisms to manage the diversity in the variable space might yield important benefits to the field of multi-objective optimization. Note that unlike other proposals, such as niching-based MOEAs [16, 17], we are not interested in obtaining a diverse set of solutions in the variable space; rather, 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 in the variable space is so important in single-objective domains to attain a proper balance between exploration and intensification [18], a large number of related methods have been devised [10]. Recent research on single-objective optimization has shown that important advances can be achieved when the balance between exploration and intensification is managed by relating the diversity of the population to the stopping criterion and the elapsed execution time. Specifically, these methods reduce the importance given to preserving 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 in the extended round of Google Hash Code 2020¹, which featured over 100,000 participants. Thus, we decided to explore the incorporation of this principle into the design of MOEAs.

One of the main problems in incorporating the above principle into the

¹<https://codingcompetitions.withgoogle.com/hashcode/>

63 design of MOEAs is that measures of the variable and objective spaces must
 64 be considered simultaneously. This design principle is based on reducing
 65 the importance of diversity in the variable space as generations evolve, so
 66 we maintain this decision and indirectly increase the importance granted to
 67 diversity and quality in the objective space as the execution progresses. In
 68 order to show the validity of our hypothesis, this paper proposes the *Archived*
 69 *Variable Space Diversity MOEA based on Decomposition* (AVSD-MOEA/D).
 70 AVSD-MOEA/D simplifies MOEA/D-DE [21] by deactivating the dynamical re-
 71 source allocation scheme and disregarding the notion of neighborhood; at the
 72 same time, it is extended by including a novel replacement strategy that ap-
 73 plies the design principle discussed. Our proposal is validated by taking into
 74 consideration MOEA/D-DE [21], NSGA-II [22], R2-EMOA [23] and NSGA-III [24].
 75 Remarkable benefits are achieved in terms of robustness and scalability.

76 The rest of this paper is organized as follows. Section 2 provides a re-
 77 view of MOEAs, diversity management and other related works. The AVSD-
 78 MOEA/D proposal is detailed in section 3. Section 4 is devoted to an extensive
 79 experimental validation of the novel proposal and design principle. Finally,
 80 conclusions and some lines of future work are presented in section 5.

81 2. Literature Review

82 MOEAs that take into account the diversity in the variable space are not
 83 new. These kinds of techniques have been especially useful for multimodal
 84 multi-objective optimization [25], i.e., for cases where distant solutions in
 85 terms of the variable space are desired [26, 27]. These types of MOEAs must
 86 maintain a large degree of diversity in the variable space during the entire

87 optimization process. In contrast, our work analyzes the hypothesis that
 88 state-of-the-art techniques can be advanced further by explicitly managing
 89 the diversity in the variable space, even if the performance is measured in
 90 terms of metrics that only take into account the objective space. Since our
 91 aim is different, using multimodal multi-objective optimizers that maintain
 92 a large diversity for the entire optimization process is counter-productive,
 93 so more advanced ways of integrating diversity management are required.
 94 This section reviews some of the most important advances in diversity-aware
 95 techniques that motivated the design of AVSD-MOEAD, which are a set of
 96 methods that were applied in single-objective optimization. Also summarized
 97 are MOEAs that in some way consider the diversity in the variable space, as
 98 well as state-of-the-art MOEAs.

99 2.1. Diversity-aware Single-objective Optimizers

100 Striking a proper balance between exploration and exploitation is one of
 101 the keys for successful single-objective EAs [18]. Several strategies for ac-
 102 complishing this aim have been explored, and one of the most promising
 103 is to alter the trend in the diversity, whether explicitly or implicitly [10].
 104 This principle has encouraged the development of a vast quantity of diver-
 105 sity management techniques [28]. A popular classification of these methods is
 106 based on the sort of components modified in the EA. It identifies the follow-
 107 ing groups [10]: *selection-based*, *population-based*, *crossover/mutation-based*,
 108 *fitness-based*, and *replacement-based*. Additionally, it defines *uniprocess-*
 109 *driven* and *multiprocess-driven* categories, depending on the number of com-
 110 ponents that are altered.

111 *Replacement-based* methods have yielded quite promising results in re-

cent 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 been shown to be quite effective in a large variety of single-objective problems [19] is based on the principle of biasing the decisions made in the replacement phase by considering the stopping criterion and elapsed time. This design principle has been successful 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 principle. Specifically, the initial phases of the optimization explicitly preserve a greater amount of diversity than the final phases, with a gradual shift between these behaviors. Given the success of this methodology in the single-objective case, we have adopted it to design our novel MOEA.

2.2. Diversity in the Variable Space in MOEAs

In spite of the vast quantity of MOEAs proposed, none of the state-of-the-art techniques involve explicitly 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 relationship between the diversity maintained in the objective space and the diversity maintained in the variable space, so even if the diversity in the variable space is not managed explicitly, any negative effects that do appear are usually not as bad as in single-objective optimization. However, the relationship between the two different diversities depend on each MOP [32], meaning

137 that including the successful principles of single-objective optimizers might
 138 result in more robust MOEAs. Most current MOEAs that take the diversity
 139 in the variable space into account are devoted to multimodal multi-objective
 140 optimization [26, 27]. However, some attempts to apply these mechanisms
 141 in traditional multi-objective optimization have also been made.

142 The Non-Dominated Sorting Genetic Algorithm (NSGA) developed in
 143 1995 [17] was one of the first MOEAs that employed diversity in the vari-
 144 able space. Specifically, it relies on fitness sharing to discriminate between
 145 solutions in the same front. In a way, this method was designed in an opposite
 146 way to current methods: the diversity in the variable space is considered, but
 147 at the cost of disregarding the information on the diversity in the objective
 148 space. The performance of NSGA is not even close to that of current MOEAs,
 149 and one of the reasons is precisely that it does not consider the diversity in
 150 the objective space.

151 In 2003, the GDEA [33] proposed by Toffolo and Benini integrated the di-
 152 versity into the search as an additional objective, which modifies the ranking
 153 of the individuals and favors maintaining distant individuals during the entire
 154 optimization process. In 2005, Chan and Ray [34] proposed the application
 155 of selection operators to encourage the preservation of distant solutions in
 156 both the objective and variable spaces. Later, Deb and Tiwari proposed the
 157 Omni-optimizer [26]. This algorithm is designed as a generic multi-objective,
 158 multi-optima optimizer. In the multi-objective case, it is an extension of
 159 NSGA-II where the crowding distance considers both the objective and vari-
 160 able spaces. Since it first uses the typical rank procedure considering only
 161 the objective space, more importance is given to this space, and the diversity

162 plays an inferior role. Unfortunately, there is no way to easily alter the im-
 163 portance given to each space. In 2009, Shir et al. showed that in many cases
 164 the diversity in the variable space can be significantly enhanced without ham-
 165 pering the convergence to a diverse Pareto front approximation. Following
 166 this insight, the CMA-ES niching framework was proposed [32]. Estimation of
 167 Distribution Algorithms have also considered the information in the variable
 168 space to attain better approximations of the Pareto set [35]. Finally, the Di-
 169 versity Integrating Hypervolume-based Search Algorithm (DIVA) [36] weighs
 170 the contribution from the hypervolume against the diversity in the variable
 171 space.

172 Note that of the methods discussed, the only one that shows any improve-
 173 ments in terms of objective-space metrics is GDEA. However, the results at-
 174 tained by GDEA are not as competitive as those attained by modern solvers,
 175 so it is not currently considered as a state-of-the-art MOEA, but rather as
 176 an easily applicable and general approach. The remaining methods focus on
 177 showing that solutions with a higher level of diversity in the variable space
 178 can be obtained without an overly negative effect on the approximation of
 179 the Pareto front.

180 *2.3. Multi-objective State-of-the-art Algorithms*

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

187 In domination-based MOEAs, the Pareto dominance relationship is applied
188 to bias the decisions of the optimizer. Although this relationship stimulates
189 convergence to the Pareto front, additional techniques to promote diversity in
190 the objective space must be integrated. Several traditional MOEAs belong to
191 this group, and while they face some difficulties for many-objective optimiza-
192 tion, they are considered quite effective for optimization problems with two
193 and three objectives. Non-Dominated Sorting Genetic Algorithm-II (NSGA-
194 II) is the most popular technique belonging to this group [22]. NSGA-III [24]
195 extends NSGA-II by replacing the crowding selection with a strategy based on
196 generating distributed reference points that implicitly decompose the objec-
197 tive space [4]. While this method is aimed at many-objective optimization,
198 it also provides some benefits for problems with three objectives.

199 Indicator-based MOEAs incorporate a measure of quality over sets of
200 solutions to alter some components, such as the selection and/or replace-
201 ment [38]. Most indicators take into account both the convergence and cov-
202 erage, so no additional techniques to promote diversity in the objective space
203 are required. A highly effective MOEA that belongs to this category is the
204 R2-Indicator-Based Evolutionary Multi-objective Algorithm (R2-EMOA) [23].
205 SMS-EMOA [8] is also quite effective but it uses the computationally expen-
206 sive hypervolume indicator, meaning that it is not as generally applicable as
207 R2-EMOA.

208 Finally, decomposition-based MOEAs [39] incorporate scalarizing func-
209 tions to transform the MOP into several single-objective optimization sub-
210 problems. Those sub-problems are then solved simultaneously and collabora-
211 tively. The weighted Tchebycheff scalarizing and its variant, the achievement

212 scalarizing function (ASF) [40, 41], have shown remarkable performance. The
 213 most popular MOEA belonging to this category is MOEA/D, which was pro-
 214 posed by Zhang et al. [9]. A distinctive feature of MOEA/D is the application
 215 of neighborhoods at the level of each sub-problem. The mating selection and
 216 replacement operator takes into account this neighborhood to promote col-
 217 laboration between similar subproblems. MOEA/D has gained a significant
 218 popularity in the last decade, and many extensions have been devised as
 219 a result. Specifically, the MOEA/D-DE [42] — winner of some optimization
 220 competitions — provides important advances by incorporating DE operators,
 221 polynomial mutation, a dynamic computational resource allocation strategy,
 222 mating restrictions and a modified replacement operator to prevent the ex-
 223 cessive replication of individuals.

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

230 3. Proposal

231 This section describes our proposal, the *Archived Variable Space Diver-*
 232 *sity MOEA based on Decomposition* (AVSD-MOEA/D)². The main novelty and
 233 motivation behind AVSD-MOEA/D is the incorporation of an explicit way to

²The source code in C++ is freely available at <https://drive.google.com/drive/folders/1JAIr0ybzyafxo2BUW99DnsUiqzZ3Wwco>

234 manage diversity in the variable space, the goal being to improve the behavior
235 in terms of objective space metrics, especially in long-term executions, which
236 is the environment where diversity-aware techniques have excelled [43]. Al-
237 though AVSD-MOEAD is inspired by MOEA/D, it has been simplified, so in
238 some ways it resembles more mature decomposition-based MOEAs, such as
239 WBGA [44]. For instance, the notion of subproblem neighborhood is not used
240 and the dynamic resource allocation usually applied in modern variants of
241 MOEA/D is deactivated. The main reason for the simplification is to show
242 that even a simple MOEA incorporating our design principles can improve
243 further more complex state-of-the-art algorithms.

244 Our proposal decomposes the MOP into several single-objective problems.
245 Notwithstanding that any scalarization approach can be employed, our strat-
246 egy applies the ASF, which has reported some of the most effective results in
247 recent years [40]. Let $\lambda_1, \dots, \lambda_N$ be a set of weight vectors and z^* a reference
248 vector. The MOP is decomposed into N scalar optimization sub-problems as
249 shown in (2).

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

250 The main novelty of AVSD-MOEAD appears in the survivor selection
251 scheme. In keeping with some of the most successful single-objective diversity-
252 aware algorithms [19], the replacement strategy relates the degree of diversity
253 in the variable space to the stopping criterion and elapsed generations. The
254 aim of this relationship is to gradually bias the search from exploration to
255 exploitation as the optimization evolves. Specifically, diversity is explicitly
256 promoted less and less until half of the total generations. Then, in the remain-

Algorithm 1 Main procedure of AVSD-MOEA/D

- 1: Input: N (Population and Archive Size), λ (a set of N weight vectors for decomposition in the population), Λ (a set of weight vectors for the R2-based archive), D_I (Initial Penalty Threshold), CR (Crossover Rate), F (Scale Factor), p_m (mutation probability)
 - 2: Output: A^t (Archive with N solutions)
 - 3: **Initialization:** Generate an initial population P^0 with N individuals
 - 4: **Evaluation:** Evaluate each individual in P^0 and assemble the reference vector z^* with the best objective values
 - 5: **Archive Initialization:** $A^0 = P^0$
 - 6: Assign $t = 0$
 - 7: **while** (not stopping criterion) **do**
 - 8: **for** each individual $P_i^t \in P^t$ **do**
 - 9: **DE variation:** Generate solution Q_i^t by applying DE/rand/1/bin with F as the mutation scale factor and CR as the crossover rate, using P_i^t as the target vector
 - 10: **Mutation:** Apply polynomial mutation to Q_i^t with probability p_m
 - 11: **Evaluation:** Evaluate the new individual Q_i^t and update the reference vector z^* with the best objective values.
 - 12: **Survivor selection:** Generate P^{t+1} by applying the replacement scheme described in Algorithm 3, using P^t , Q^t , λ , z^* and D_I as input
 - 13: **Update Archive:** Create A^{t+1} by applying Algorithm 2 using A^t , Q^t , Λ , and z^* as input.
 - 14: $t = t + 1$
 - 15: **return** A^t
-

257 ing generations, AVSD-MOEA/D behaves similarly to most popular MOEAs, i.e.
258 the diversity in the variable space is not considered explicitly.

259 The main procedure of AVSD-MOEA/D is shown in Algorithm 1. Its gen-
260 eral template is quite standard. The variation step is similar to those used
261 in typical MOEAs, meaning it is based on crossover and mutation and any
262 operators might be used. Specifically, N individuals are created in each gen-
263 eration by randomly selecting at each step three individuals to apply the
264 *DE/rand/1/bin* operator. Note that each member of the population is used
265 as the target vector once. Then, polynomial mutation is applied to the out-
266 put of the *DE* operator. As in most current MOEA/D variants, the initial
267 population is generated randomly, the number of weight vectors ($|\lambda|$) is equal
268 to the population size, and the reference vector z^* used for ASF consists of
269 the best objective values achieved. The weight vectors used in this paper are
270 based on an uniform design strategy and are specified in the experimental
271 validation section. Finally, the survivor selection stage is applied. This is
272 quite different from traditional techniques, in the sense that P^t and Q^t are
273 merged, meaning that unlike in MOEA/D, the position of each individual is
274 not important, and a diversity-aware selection is performed. Since this is the
275 novelty of the paper, its working operation is given in detail.

276 Note that AVSD-MOEA/D incorporates an external archive to store the
277 best solutions. While in MOEA/D this is considered optional, in our ap-
278 proach it is quite important because the penalty approach included to pick
279 up the survivors of the population in the replacement phase might discard
280 elite solutions for some weight vectors. Since methods based on the R2 indi-
281 cator [23] have reported quite high-quality solutions, our archive is based on

Algorithm 2 Procedure to update the R2-based archive

```
1: Input:  $A^t$  (External archive in the current generation),  $Q^t$  (Offspring of current
   generation),  $\Lambda$  (weight vectors for  $R2$ ),  $z^*$  (Reference vector)
2: Output:  $A^{t+1}$ 
3:  $R^t = A^t \cup Q^t$ 
4:  $A^{t+1} = \emptyset$ 
5: while  $|A^{t+1}| < N$  do
6:    $\forall x \in R^t : r(x) = R2(A^{t+1} \cup \{x\}; \Lambda, z^*)$ 
7:    $x^* = \operatorname{argmin}(r(x) : x \in R^t)$ 
8:    $A^{t+1} = A^{t+1} \cup \{x^*\}$ 
9:    $R^t = R^t \setminus \{x^*\}$ 
```

282 the R2 indicator applying the ASF and the weights Λ to generate the utility
283 functions. In each iteration, the archive selects N candidate solutions by
284 combining its contents with the offspring of each generation (see line 13 in
285 Algorithm 1). This is done by following a simple greedy approach (Algo-
286 rithm 2). Specifically, it iteratively selects the individual that minimizes the
287 $R2$ (lines 6-9) considering the individuals already selected with ties broken
288 randomly. Note that since $R2$ is weakly Pareto-compliant, it might happen
289 that some non-dominated individuals do not contribute to $R2$, so incorpo-
290 rating more complex archiving strategies might be helpful. However, our
291 preliminary experiments have shown that this is not overly important for
292 proper performance, so we decided to maintain its simplicity.

293 3.1. Novel Replacement Phase of AVSD-MOEA/D

294 The purpose of the replacement phase (see Algorithm 3) is to select the set
295 of survivors of the next generation. The survivor selection described in this

Algorithm 3 Replacement Phase of AVSD-MOEA/D

```

1: Input:  $P^t$  (Population of current generation),  $Q^t$  (Offspring of current gen-
   eration),  $\lambda$  (a set of weight vectors),  $z^*$  (Reference vector), and  $D_I$  (Initial
   Penalty Threshold).
2: Output:  $P^{t+1}$ 
3:  $R^t = P^t \cup Q^t$ 
4:  $P^{t+1} = \emptyset$ 
5:  $Penalized = \emptyset$ 
6:  $r\lambda = \lambda$ 
7:  $D^t = D_I - D_I * \frac{G_{Elapsed}}{0.5 * G_{End}}$ 
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 pair of non-penalized individual  $R_i^t$  and weight vector  $r\lambda_j$  with
    the best scalarizing function value according to  $g^{asf}(R_i^t | r\lambda_j, z^*)$ 
15:    Move individual  $R_i^t$  to  $P^{t+1}$ 
16:    Erase the weight vector  $r\lambda_j$  from  $r\lambda$ 
17: return  $P^{t+1}$ 

```

296 work incorporates similar design principles to those applied in the diversity-
 297 aware single-objective optimizer DE-EDM [20]. It operates as follows. First,
 298 the parent and offspring populations are merged in a multi-set to establish
 299 the candidate set R^t (line 3). A key of the scheme is to promote the se-

300 lection of individuals with a large enough contribution to diversity in the
 301 variable space. Specifically, the contribution of an individual x is calculated
 302 as $\min_{p \in P^{t+1}} \text{Distance}(x, p)$, where P^{t+1} is the multi-set of the already picked
 303 survivors and the normalized Euclidean distance specified in (3) is applied.
 304 Note that in the pseudocode, the tag DCS (Distance to Closest Solution) is
 305 used to denote the contribution to diversity.

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

306 In order to promote the selection of distant individuals, a threshold D^t
 307 is dynamically calculated (line 7) and individuals with a DCS value lower
 308 than the threshold are considered as undesirable individuals. Note that the
 309 calculation of D^t depends on an initial penalty threshold (D_I), which is a
 310 parameter of our proposal, on the number of generations that have evolved
 311 ($G_{Elapsed}$) and on the stopping criterion (G_{End}), i.e., the number of gener-
 312 ations to evolve. Specifically, the value is decreased linearly as generations
 313 evolve. Since survivors with larger DCS values provoke exploration steps,
 314 while survivors with short DCS values promote intensification steps, this lin-
 315 ear decrease promotes a gradual transition from exploration to exploitation.
 316 Also note that after 50% of the total number of generations, the D^t value
 317 is below 0, meaning that no penalties are applied and a more traditional
 318 strategy focused only on the objective values is used to perform the selection
 319 steps.

320 The strategy iteratively selects an individual from the candidate set (R^t)
 321 to enter the new population (P^{t+1}) until it is filled with N individuals (lines

322 8-16). In particular, the aim is to select a proper individual for each weight
 323 vector, while at the same time fulfilling the condition imposed for the con-
 324 tribution to diversity in the variable space. In order to satisfy this last
 325 condition, non-selected individuals with a *DCS* lower than D^t are moved
 326 from R^t to the *Penalized* set (lines 9-10), and in each iteration an individual
 327 belonging to R^t is selected to survive. The set of weight vectors considered
 328 by our strategy are initially placed in $r\lambda$. In each iteration, the individual
 329 in R^t with the best scalarizing function for any of the weight vectors in $r\lambda$
 330 is identified (line 14). Then, this individual is selected as a survivor (line
 331 15) and the weight vector used is erased from $r\lambda$ (line 16). Note that N
 332 individuals are selected, meaning that each weight vector is used to select
 333 exactly one individual. Also note that it might happen that R^t is empty
 334 prior to selecting N individuals. This means that the diversity is lower than
 335 expected, so in order to increase the amount of exploration, the individual
 336 with the largest *DCS* value in the *Penalized* set is selected to survive (lines
 337 11 - 13).

338 4. Experimental Validation

339 In this section, we provide the validation of our proposal against state-
 340 of-the-art MOEAs and explain the reasons behind the superiority of AVSD-
 341 MOEA/D. Since methods that include strategies to explicitly delay conver-
 342 gence usually require additional computational resources to excel, long-term
 343 analyses are presented. In order to draw proper conclusions, four experi-
 344 ments were carried out. First, a comparison between AVSD-MOEA/D and
 345 four state-of-the-art MOEAs is presented. This comparison focuses on show-

346 ing the benefits of AVSD-MOEA/D for benchmarks configured in standard
 347 ways. Second, an analysis to test the scalability on the number of decision
 348 variables is carried out. Third, the robustness of AVSD-MOEA/D in terms of
 349 the initial penalty threshold (D_I) is analyzed. Finally, the ability of dealing
 350 with different levels of difficulty in biased test problems is studied. Note that
 351 in order to test the quality of the approximations, the hypervolume is used.
 352 Additionally, our analyses also include some studies to better understand the
 353 implications of AVSD-MOEA/D on the diversity in the variable space. These
 354 analyses provide a better understanding of the reasons behind the proper
 355 performance of AVSD-MOEA/D and highlight the significant differences be-
 356 tween AVSD-MOEA/D and other strategies in terms of the dynamics of the
 357 population.

358 In the first three analyzes our validation takes into account three of
 359 the most popular benchmarks in multi-objective optimization: WFG [7],
 360 DTLZ [45], and UF [46]. The remaining experiment takes into the BT prob-
 361 lems [47]. Unless otherwise stated, standard configurations were used. Specif-
 362 ically, the WFG test problems were used with two and three objectives with 24
 363 parameters³, 20 of them corresponding to distance parameters and 4 to posi-
 364 tion parameters. The DTLZ test problems were also used with two and three
 365 objectives, and the number of variables in each case was set to $D = M + r - 1$,
 366 where $r = \{5, 10, 20\}$ for DTLZ1, DTLZ2 to DTLZ6 and DTLZ7, respectively.
 367 The UF benchmark comprises seven problems with two objectives (UF1-7) and
 368 three problems with three objectives (UF8-10). Similarly, the BT benchmark

³In the WFG context, the term *parameter* is equivalent to variable.

Table 1: Parameterization of the variation phase applied in each MOEA

	2 objectives		3 objectives	
	<i>CR</i>	<i>F</i>	<i>CR</i>	<i>F</i>
AVSD-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	0.25
NSGA-III	0.75	0.25	0.5	0.75

includes eight problems with two objectives (BT1-8) and one problem with three objectives (BT9). These two last groups of problems were configured with 30 variables.

Regarding our comparisons, the set of state-of-the-art MOEAs used to validate our proposals is comprised of four popular and complementary MOEAs: NSGA-II [22], MOEA/D-DE [21], R2-EMOA [23] and NSGA-III [24]. Given that all the algorithms are stochastic, each execution was repeated 35 times in every experiment. 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 slightly larger (ten percent) than the nadir point, as suggested in [48]. The value reported is computed as the ratio between the normalized HV attained [49] and the maximum attainable normalized HV. This way, a value equal to one means a perfect approximation. Note that this value is not attainable because MOEAs yield discrete approximations. Finally, to statistically compare the HV ratios, a guideline similar to that proposed in [50] was used, which entails the use of the Shapiro-Wilk, Levene, ANOVA, Welch and Kruskal-Wallis tests. An algorithm *A1* is said to beat an algorithm *A2* when the differences between the HV ratios attained

are statistically significant, and the mean and median HV ratios obtained by *A1* are higher than the mean and median achieved by *A2*.

An important step to perform fair comparisons is the parameterization of algorithms. Note that the variation operators used in each algorithm in their original variants differ. Using the original variation operators to perform comparisons is not fair, and probably would offer more conclusions about the effectiveness of the operators than about the general framework proposed in each MOEA. However, there might also be a dependency between the general framework and the proper variation operators. We thus decided to use a common simple framework for the variation step, but to allow a different parameterization for each algorithm. Specifically, the variation phase first applies the classic DE scheme known as DE/rand/1/bin with parameters F and CR , and then it applies polynomial mutation with probability p_m and a distribution index equal to 50. Note that the use of the additional mutation in variants based on MOEA/D is quite important [21]. The additional common parameter is the population size. Since the hypervolume is highly dependent on the number of solutions used to approximate the Pareto front, all the MOEAs were configured with a common population size equal to 100 individuals.

In order to set the CR , F and p_m parameters, 40 parameterizations were tested for each algorithm. They were generated by combining four values of F (0.25, 0.5, 0.75 and 1.0), five values of CR (0.0, 0.25, 0.5, 0.75, 1.0) and two values of p_m (0.0, $\frac{1}{D}$). These configurations were executed by setting the stopping criterion to 2.5×10^6 function evaluations, with all the aforementioned benchmarks. The mean of the resulting hypervolume ratios were

412 calculated independently for the problems with two and three objectives.
 413 Then, in the experiments that followed, the parameter configuration that
 414 attained the largest mean was used. Table 1 shows the configuration of CR
 415 and F selected for each MOEA. Note that all of them yielded better results
 416 when mutation was enabled, so the benefits reported in [21] also appeared
 417 for other MOEAs. Note that in the case of AVSD-MOEA/D, CR was set to
 418 0, which reduces the strength of the perturbation performed by DE. Since
 419 AVSD-MOEA/D maintains a larger degree of diversity than other methods,
 420 low disruptive operators seem to be more helpful.

421 Note also that there are some additional parameters that are specific to
 422 some of the MOEAs. They were set to typical values used in literature. Table 2
 423 shows this additional parameterization. Note also that scalarization functions
 424 are used in MOEA/D-DE, R2-EMOA, NSGA-III and AVSD-MOEA/D. In all those
 425 cases, the ASF approach is used. However, the weight vectors employed in
 426 R2-EMOA are different from those in the remaining algorithms because in
 427 R2-EMOA, using a larger number of weight vectors than the population size
 428 is beneficial. As in the official code, R2-EMOA was applied with 501 and
 429 496 weight vectors for two and three objectives, respectively [23]. In the
 430 remaining cases — including AVSD-MOEA/D — the number of weight vectors
 431 was equal to the population size, and they were generated with the uniform
 432 design strategy described in [51]. Note that in the case of AVSD-MOEA/D,
 433 a second set of weight vectors (Λ) was considered for the external archive.
 434 Since the archive is based on $R2$, it considers the same weight vectors as
 435 R2-EMOA.

Table 2: Configuration of the specific parameters of 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
AVSD-MOEA/D	$D_I = 0.4$

4.1. Performance of MOEAs in long-term executions

One of the aims behind the design of AVSD-MOEA/D is to profit from long-term executions. Therefore, in this section we present the results attained by the different algorithms when setting the stopping criterion to 2.5×10^7 function evaluations. Table 3 shows the HV ratios obtained for the benchmark functions with two objectives. Note that the same results can be drawn with the IGD+ metric [52] and can be inspected in the supplementary material document. For each method and problem, the best, mean and standard deviation of the HV ratio values are reported. Furthermore, in order to summarize the results attained by each method, the last row shows the mean for the whole set of problems. For each test problem, the method that yielded the largest mean and those that were not statistically inferior to the best are shown in **boldface**. Similarly, the method that yielded the best HV value among all the runs is underlined. From here on, the methods shown in **boldface** for a given problem are referred to as the winning methods. AVSD-MOEA/D, R2-EMOA, MOEA/D-DE, NSGA-III and NSGA-II belonged to the winning methods in 17, 6, 2, 2 and 0 problems, respectively. The superiority of AVSD-MOEA/D is clear both in terms of this metric and

Table 3: Summary of the hypervolume ratios attained for problems with two objectives

	AVSD-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	<u>0.995</u>	0.982	0.020	0.957	0.842	0.058	0.994	0.966	0.026	0.993	0.989	0.011	0.993	0.921	0.039
WFG2	<u>0.999</u>	0.999	0.000	0.996	0.996	0.000	0.998	0.998	0.000	0.997	0.990	0.013	0.998	0.998	0.000
WFG3	<u>0.993</u>	0.993	0.000	0.992	0.992	0.000	0.980	0.978	0.001	0.992	0.992	0.000	0.992	0.991	0.000
WFG4	<u>0.991</u>	0.991	0.000	0.988	0.988	0.000	0.979	0.975	0.002	0.988	0.986	0.003	0.988	0.973	0.007
WFG5	<u>0.933</u>	0.905	0.008	0.891	0.882	0.004	0.883	0.878	0.002	0.895	0.888	0.003	0.890	0.885	0.003
WFG6	0.959	0.922	0.020	0.988	0.963	0.019	0.977	0.974	0.001	0.956	0.934	0.013	<u>0.991</u>	0.990	0.001
WFG7	<u>0.991</u>	0.991	0.000	0.988	0.988	0.000	0.980	0.977	0.001	0.988	0.988	0.000	<u>0.991</u>	0.991	0.000
WFG8	<u>0.963</u>	0.954	0.004	0.846	0.833	0.004	0.825	0.815	0.003	0.829	0.826	0.001	0.835	0.832	0.001
WFG9	<u>0.978</u>	0.976	0.002	0.974	0.954	0.039	0.941	0.873	0.071	0.798	0.796	0.001	0.975	0.939	0.051
DTLZ1	<u>0.993</u>	0.993	0.000	<u>0.993</u>	0.993	0.000	0.992	0.991	0.000	<u>0.993</u>	0.993	0.000	0.992	0.992	0.000
DTLZ2	0.991	0.991	0.000	0.989	0.989	0.000	0.987	0.986	0.001	0.989	0.989	0.000	<u>0.992</u>	0.992	0.000
DTLZ3	0.991	0.991	0.000	0.989	0.989	0.000	0.989	0.989	0.000	0.989	0.989	0.000	<u>0.992</u>	0.992	0.000
DTLZ4	0.991	0.991	0.000	0.989	0.989	0.000	0.987	0.903	0.231	0.989	0.989	0.000	<u>0.992</u>	0.803	0.320
DTLZ5	0.991	0.991	0.000	0.989	0.989	0.000	0.987	0.986	0.001	0.989	0.989	0.000	<u>0.992</u>	0.992	0.000
DTLZ6	0.991	0.991	0.000	0.989	0.986	0.014	0.989	0.989	0.000	0.989	0.989	0.000	<u>0.992</u>	0.985	0.021
DTLZ7	<u>0.997</u>	0.997	0.000	0.996	0.996	0.000	0.997	0.996	0.000	0.996	0.996	0.000	<u>0.997</u>	0.997	0.000
UF1	<u>0.995</u>	0.995	0.000	0.987	0.986	0.001	0.989	0.988	0.001	0.992	0.991	0.001	0.992	0.992	0.000
UF2	<u>0.995</u>	0.995	0.000	0.990	0.988	0.001	0.984	0.982	0.001	0.986	0.981	0.003	0.988	0.987	0.001
UF3	0.938	0.906	0.016	<u>0.991</u>	0.990	0.001	0.988	0.985	0.004	0.985	0.968	0.019	<u>0.991</u>	0.982	0.005
UF4	<u>0.979</u>	0.977	0.001	0.914	0.904	0.006	0.892	0.882	0.005	0.880	0.876	0.003	0.902	0.893	0.003
UF5	<u>0.990</u>	0.975	0.009	0.715	0.439	0.137	0.792	0.734	0.087	0.777	0.654	0.067	0.792	0.733	0.092
UF6	<u>0.962</u>	0.938	0.013	0.928	0.748	0.175	0.870	0.720	0.069	0.820	0.708	0.043	0.827	0.691	0.091
UF7	<u>0.993</u>	0.993	0.000	0.991	0.990	0.001	0.980	0.976	0.002	0.983	0.975	0.002	0.992	0.982	0.006
Mean	0.983	0.976	0.004	0.960	0.931	0.020	0.956	0.937	0.022	0.948	0.934	0.008	0.960	0.936	0.028

454 in terms of the mean HV. Particularly, AVSD-MOEA/D attained a value equal
 455 to 0.976, while all the remaining methods attained values between 0.931
 456 and 0.937. A careful inspection of the data shows that in those cases where
 457 AVSD-MOEA/D loses, the difference with respect to the best method is low. In
 458 fact, the difference between the mean HV ratio attained by the best method
 459 and by AVSD-MOEA/D is never greater than 0.1. However, in all the other
 460 methods, there were several problems where the distance with respect to the
 461 best approach was greater than 0.1. Specifically, it happened in 4, 4, 4 and
 462 5 problems for R2-EMOA, MOEA/D-DE, NSGA-II and NSGA-III, respectively.
 463 This means that AVSD-MOEA/D wins in most cases and that when it loses,

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

	\uparrow	\downarrow	\leftrightarrow	Score	Deterioration
AVSD-MOEA/D	78	13	1	65	0.160
MOEA/D-DE	41	50	1	-9	1.181
NSGA-II	21	66	5	-45	1.057
NSGA-III	35	52	5	-17	1.119
R2-EMOA	47	41	4	6	1.066

the difference is always small. Note also that in terms of standard deviation, AVSD-MOEA/D yields much lower values than all the other algorithms, meaning it is quite robust.

In order to better clarify these findings, pair-wise statistical tests were applied between each method tested in each test problem. For the two-objective cases, Table 4 shows the number of times that each method statistically won (column \uparrow), lost (column \downarrow) or tied (column \leftrightarrow). The **Score** column shows 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 confirm that although AVSD-MOEA/D loses in some pair-wise tests, the overall numbers of wins and losses clearly favor AVSD-MOEA/D. More importantly, the total deterioration is much lower in the case of AVSD-MOEA/D, confirming that when AVSD-MOEA/D loses, the differences are low.

Tables 5 and 6 shows the same information for the problems with three ob-

Table 5: Summary of the hypervolume ratios attained for problems with three objectives

	AVSD-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	<u>0.985</u>	0.982	0.007	0.972	0.937	0.030	0.966	0.959	0.008	0.970	0.967	0.008	0.981	0.965	0.017
WFG2	<u>0.991</u>	0.991	0.000	0.981	0.979	0.001	0.974	0.967	0.003	0.972	0.971	0.001	0.963	0.963	0.000
WFG3	<u>0.995</u>	0.994	0.000	0.990	0.990	0.000	0.986	0.975	0.006	0.966	0.954	0.007	0.992	0.992	0.000
WFG4	<u>0.943</u>	0.941	0.001	0.899	0.898	0.001	0.892	0.876	0.008	0.897	0.897	0.000	0.911	0.906	0.002
WFG5	<u>0.901</u>	0.872	0.011	0.831	0.831	0.000	0.828	0.812	0.009	0.833	0.827	0.003	0.849	0.846	0.001
WFG6	<u>0.912</u>	0.888	0.011	0.887	0.862	0.013	0.851	0.822	0.013	0.880	0.858	0.012	0.902	0.893	0.006
WFG7	<u>0.943</u>	0.942	0.001	0.899	0.898	0.001	0.892	0.865	0.010	0.897	0.897	0.000	0.906	0.904	0.001
WFG8	<u>0.910</u>	0.902	0.003	0.816	0.812	0.003	0.759	0.748	0.006	0.810	0.807	0.002	0.827	0.824	0.001
WFG9	<u>0.910</u>	0.894	0.006	0.875	0.862	0.005	0.819	0.732	0.019	0.858	0.749	0.027	0.886	0.880	0.002
DTLZ1	<u>0.967</u>	0.967	0.000	0.953	0.953	0.000	0.950	0.941	0.004	0.953	0.953	0.000	0.942	0.941	0.001
DTLZ2	<u>0.945</u>	0.944	0.000	0.914	0.914	0.000	0.905	0.892	0.008	0.913	0.913	0.000	0.916	0.915	0.001
DTLZ3	<u>0.945</u>	0.944	0.000	0.914	0.914	0.000	0.901	0.883	0.009	0.913	0.913	0.000	0.916	0.915	0.001
DTLZ4	<u>0.945</u>	0.944	0.000	0.914	0.914	0.000	0.908	0.813	0.238	0.913	0.903	0.059	0.916	0.893	0.127
DTLZ5	0.985	0.985	0.000	0.979	0.979	0.000	0.986	0.984	0.001	0.967	0.959	0.005	<u>0.986</u>	0.986	0.000
DTLZ6	0.985	0.985	0.000	0.979	0.959	0.038	0.984	0.955	0.127	0.958	0.948	0.007	<u>0.986</u>	0.985	0.008
DTLZ7	<u>0.970</u>	0.968	0.001	0.922	0.922	0.000	0.941	0.924	0.025	0.929	0.912	0.008	0.907	0.848	0.020
UF8	<u>0.922</u>	0.916	0.003	0.891	0.862	0.032	0.747	0.695	0.035	0.890	0.835	0.101	0.893	0.877	0.016
UF9	<u>0.957</u>	0.951	0.003	0.947	0.813	0.071	0.822	0.735	0.069	0.954	0.936	0.043	0.942	0.862	0.077
UF10	<u>0.831</u>	0.787	0.041	0.681	0.435	0.147	0.543	0.483	0.084	0.624	0.458	0.127	0.579	0.561	0.042
Mean	0.944	0.937	0.005	0.908	0.881	0.018	0.877	0.845	0.036	0.900	0.877	0.022	0.905	0.892	0.017

482 jectives. In this case, the number of times that each method belonged to the
 483 winning groups were 17, 2, 0, 0 and 0 for AVSD-MOEA/D, R2-EMOA, MOEA/D-
 484 DE, NSGA-III and NSGA-II, respectively. Thus, AVSD-MOEA/D yielded quite
 485 superior results. Considering the whole set of problems, AVSD-MOEA/D ob-
 486 tained a much larger mean HV ratio than the other ones. Moreover, the
 487 difference between the mean HV ratio obtained by the best method and by
 488 AVSD-MOEA/D was never greater than 0.1. However, all the other methods
 489 exhibited a deterioration in excess of 0.1 in several cases. In particular, this
 490 happened in 2, 2, 2 and 6 problems for MOEA/D-DE, R2-EMOA, NSGA-III and
 491 NSGA-II respectively. Remarkably, AVSD-MOEA/D is quite superior in both
 492 the total deterioration and in the score generated from the pair-wise statis-
 493 tical tests. In fact, its deterioration for the entire problem set is just 0.006.

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

	\uparrow	\downarrow	\leftrightarrow	Score	Deterioration
AVSD-MOEAD/D	74	2	0	72	0.006
MOEA/D-DE	33	38	5	-5	1.075
NSGA-II	9	64	3	-55	1.745
NSGA-III	22	50	4	-28	1.149
R2-EMOA	45	29	2	16	0.851

494 Beating all the state-of-the-art algorithms in such a large number of prob-
495 lem benchmarks is a quite significant achievement, and shows the robustness
496 of AVSD-MOEAD/D. Our results show that the superiority of AVSD-MOEAD/D
497 persists, and even increases, when problems with three objective functions
498 are considered. For a better comprehension of the strenghts and weakness
499 of the algorithms, in the Figure 1 is shown the 50% attainment surfaces for
500 WFG8 and UF5. An attainment surface approximation can be interpreted as
501 the spatial region that is statistically attained among all the runs that were
502 carried out by an algorithm [53, 54]. In other words, it can be understood as
503 *the spatial region that is achieved by the k% among all the runs by one algo-*
504 *rithm.* The most challenging characteristic of these problems are that WFG8
505 has strong dependencies among all the parameters, and UF5 is a multi-modal
506 biased problem whose Pareto optimal front is discrete and consists of 21
507 points. In both problems AVSD-MOEAD/D was the only one that converged
508 adequately to the Pareto front at least 50% among all the runs. Even more,
509 given that the standard deviation is too low it can be though that all the
510 runs converged similarly well.

511 We can better understand the reasons behind the benefits of AVSD-MOEAD/D

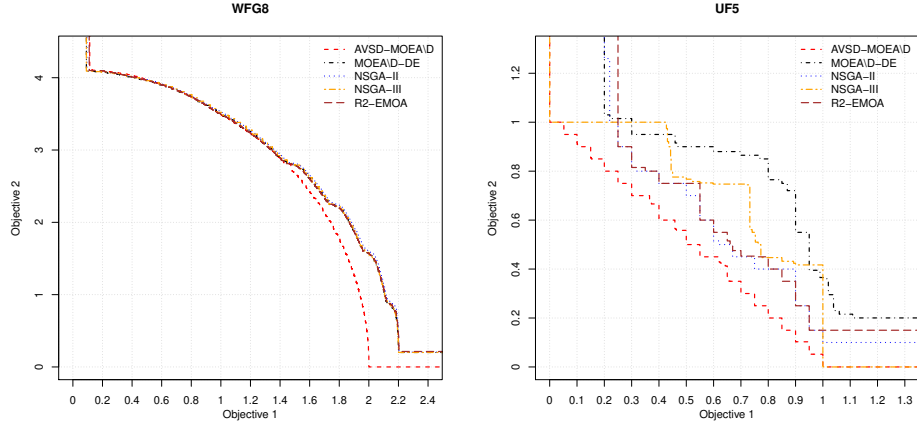


Figure 1: 50% attainment surfaces achieved for WFG8 and UF5 test problems.

512 against the state-of-the-art MOEAs by analyzing the evolution of the HV val-
 513 ues and the diversity. Note that in some MOPs, variables can be classified
 514 into two types: distance variables and position variables. A variable x_i is a
 515 distance variable when for all x , modifying x_i results in a new solution that
 516 dominates x , is equivalent to x , or is dominated by x . Differently, if x_i is a
 517 position variable, modifying x_i in x always results in a vector that is incompa-
 518 rable or equivalent to x [7]. This is important because in some cases, MOEAs
 519 do not maintain a large enough diversity in the distance variables [13], so
 520 analyzing the diversity trend for these kinds of variables provides an useful
 521 insight into the dynamics of the population.

522 In order to show the behavior of the different schemes, we selected WFG5
 523 and UF5. They are complementary in the sense that in WFG5, all the Pareto
 524 solutions exhibit constant values for the distant variables, which is not the
 525 case in UF5. Moreover, in UF5, the optimal regions are isolated in the vari-
 526 able space, meaning that more diversity is required. For each algorithm, the

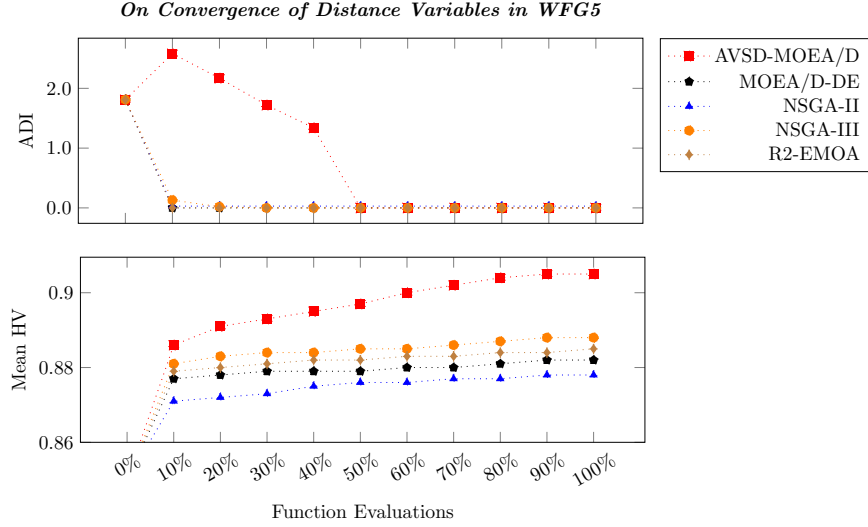


Figure 2: Diversity of distance variables (top) and mean of HV ratios (bottom) vs. elapsed time in the bi-objective WFG5 test problem. The results reported were taken from 35 runs.

diversity is calculated as the average Euclidean distance between individuals (ADI) in the population by considering only the distance variables. Figures 2 and 3 show the evolution of the ADI (top) and the mean of HV (bottom) for WFG5 and UF5, respectively. In the WFG5 problem, the distance variables quickly converged to a small region in state-of-the-art MOEAs. Thus, the differential evolution operator loses its exploring power and as a result, those MOEAs were unable to significantly improve the quality of the approximations as the evolution progresses. By contrast, in the case of AVSD-MOEA/D, the decrease in ADI is quite linear until the midpoint of the execution, and the increase in HV is gradual. The final HV attained by AVSD-MOEA/D is the largest one, which shows the important benefit of gradually decreasing the diversity.

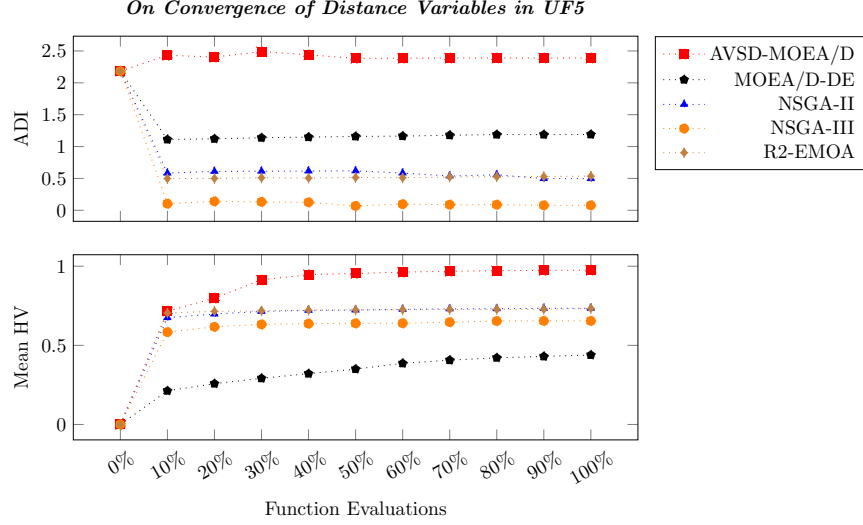


Figure 3: Diversity of distance variables (top) and mean of HV ratios (bottom) vs. elapsed time in the bi-objective UF5 test problem. The results reported were taken from 35 runs.

As expected, explicitly promoting diversity is also beneficial for problems with disconnected optimal regions. As the data in Figure 3 show, the advantage of promoting diversity in the UF5 test problem is clear. In this case, state-of-the-art algorithms maintain some degree of diversity in the distance variables for the entire search. However, a large degree of diversity is required to obtain the 21 optimal solutions, and these MOEAs do not maintain the required amount of diversity, and as a result, they miss many of the solutions. In the case of AVSD-MOEA/D, enforcing a large degree of diversity in the initial phases promotes more exploration, which makes it possible to find additional optimal regions. Once these regions are located, they are not discarded, meaning that a larger level of diversity is maintained throughout the execution. This way, AVSD-MOEA/D not only attained better HV values for the first 10% of the total function evaluations, but it also kept looking

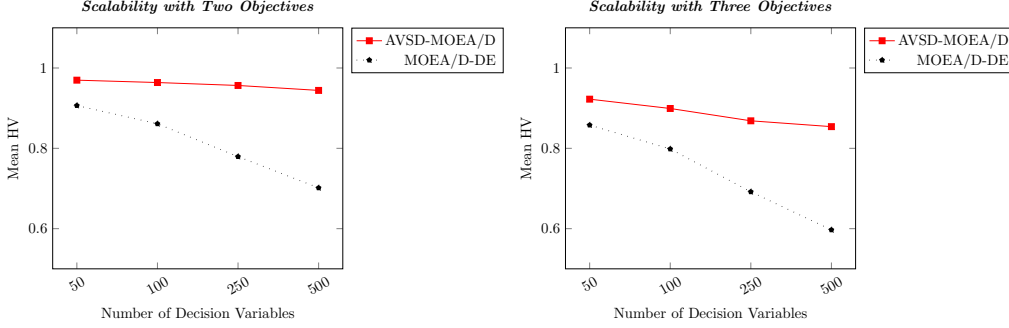


Figure 4: Mean of the HV ratio for 35 runs of the two-objective and three-objective problems for different numbers of variables

for promising regions. In fact, its HV values improved significantly until the midpoint of the execution period i.e., the final moment when diversity was explicitly promoted. Then, an additional increase was obtained due to intensification in the regions identified. This analysis shows that the dynamic of the population depends on the problem at hand. The behavior of AVSD-MOEA/D with all the problems tested was similar to those already presented. Scenarios where the optimal regions consists of constant values for the distance variables behave like WFG5, whereas the behavior in those cases where the optimal regions consist of non-constant values for the distance variables is more similar to the UF5 case. Note, however, that in these cases, different levels of diversity are required, so the behavior is not as homogeneous.

4.2. Analysis of Scalability in the Decision Variables

In order to gain a better insight into the benefits of our proposal, we present an analysis of the scalability in terms of the number of decision variables. Given the computational cost associated with this experiment, it was only performed for the decomposition-based algorithms. AVSD-MOEA/D

568 and MOEA/D-DE were applied to the same benchmark problems as in the
 569 previous experiment, but considering 50, 100, 250 and 500 variables. Note
 570 that in the WFG test problems, the number of position variables and distance
 571 variables must be specified. The number of distance variables was set to 42,
 572 84, 210 and 418 when using 50, 100, 250 and 500 variables, respectively. The
 573 remaining decision variables were position variables, meaning there were 8,
 574 16, 40 and 82 such variables, respectively. Thus, the relationship between the
 575 number of position and distance variables was kept fixed. In addition, the
 576 stopping criterion was set to 2.5×10^7 function evaluations. Figure 4 shows
 577 the mean HV ratio for the selected algorithms, considering the problems with
 578 two and three objectives, respectively. As expected, the HV ratio decreased
 579 as the number of variables increased. However, the performance of AVSD-
 580 MOEA/D is quite robust, and its decrease is less aggressive than the one in
 581 MOEA/D-DE, meaning that AVSD-MOEA/D is more helpful as the complexity
 582 increases. In fact, in our previous analyses, AVSD-MOEA/D also stood out in
 583 the most complex cases, such as WFG8 and UF5.

584 *4.3. Analysis of the Initial Penalty Threshold*

585 One of the main potential downsides of including a strategy to explicitly
 586 promote diversity is that this is usually at the cost of incorporating additional
 587 parameters. In the case of AVSD-MOEA/D, it requires setting the initial
 588 penalty threshold (D_I). Given that in single-objective cases, values close to
 589 0.4 have yielded proper performance [31, 20], $D_I = 0.4$ was used in the above
 590 experiment. This section provides a more detailed study of the implications
 591 of this parameter.

592 In order to better understand the importance of D_I , the entire set of

Mean of the HV Value with Several Initial Threshold Values

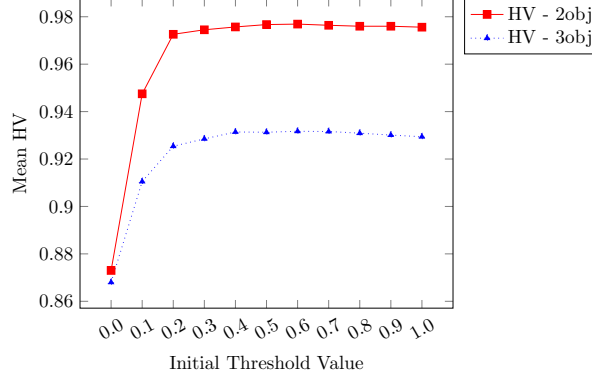


Figure 5: Mean of HV values for all the problems with several initial threshold values

benchmark problems was tested with different values of D_I . As in previous experiments, the stopping criterion was set to 2.5×10^7 function evaluations. Since normalized distances are used, the maximum attainable distance between pairs of individuals is 1.0. Also note that setting D_I to 0 implies not promoting diversity in the variable space. Thus, several values in this range were considered. 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. Figure 5 shows the mean HV ratio obtained for both the two-objective and the three-objective case with the D_I values tested. The AVSD-MOEA/D performed worst when D_I was set to 0. The HV ratio quickly increased as higher D_I values up to 0.2 were used. Larger values yielded quite similar performances. Thus, a wide range of values (from 0.2 to 1.0) exhibited very good performance, meaning that the behavior of AVSD-MOEA/D is quite robust. Thus, properly setting this parameter is not a complex task.

In order to better understand the implications of D_I on the dynamics of the population, Figure 6 shows, for AVSD-MOEA/D, the evolution of diversity in the distance variables in the WFG9 case for three different values of D_I .

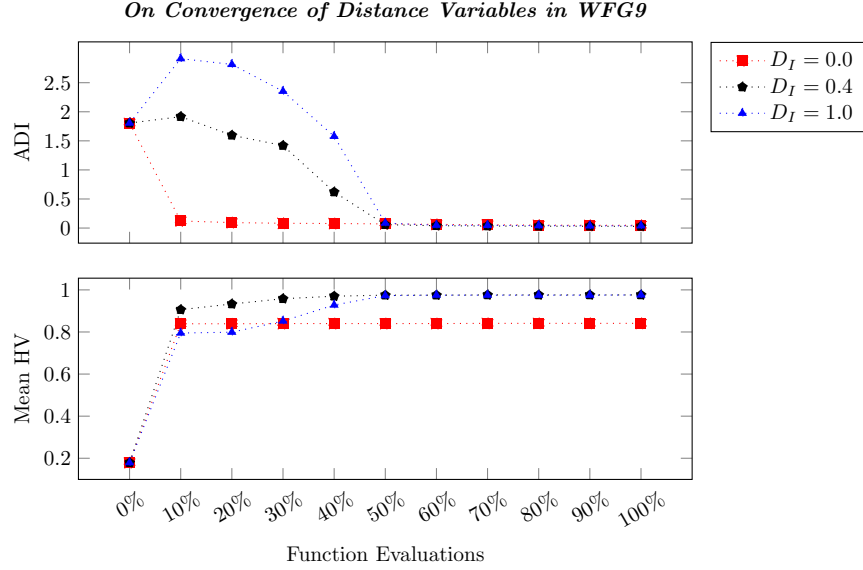


Figure 6: Diversity of distance variables (top) and mean of HV ratios (bottom) vs. elapsed time in the two-objective WFG9 test problem. The results reported were taken from 35 runs.

When setting $D_I = 0$, the diversity is reduced quite quickly, which results in premature convergence. The result is a hypervolume that is not too high. However, when $D_I = 0.4$ and $D_I = 1$ are used, the loss of diversity is slowed down, and the resulting hypervolume is quite large. Note that setting $D_I = 1$ promotes greater diversity, so the hypervolume increases slower than when $D_I = 0.4$. However, the degree of exploration in both cases is enough to yield high-quality solutions. The behavior is quite similar in every problem, which explains the stability of the algorithms for different values of D_I . Note that for shorter periods, setting a proper D_I value is probably much more important. However, for long-term executions at least, practically any value higher than 0.2 yields similar solutions, which we regard as a highly positive

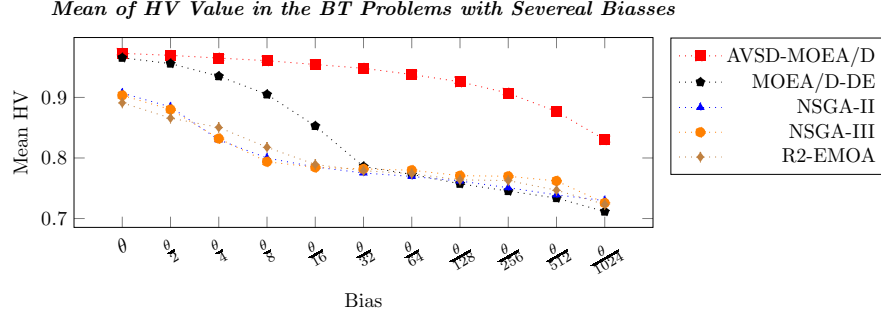


Figure 7: Mean of HV values for eight BTs problems (y-axis) against several biases ratios (x-axis). The BT2 problem is not taken into consideration due that it suffers of numerical stability.

feature.

4.4. On the Convergence of MOEAs in Test Problems with Bias Features

As pointed out in [47, 55, 7], the bias feature is one of the most challenging difficulties that MOEAs might face. Recently, the BTs test problems were proposed to facilitate the study of the ability of MOEAs for dealing with biases. In this context bias means that small variations in the decision space around the Pareto set cause significant changes in vicinities of some Pareto front solutions [7]. Particularly, those problems are built with transformations that induce position-related bias and distance-related bias. While the former means that a small change on the position-related variables of one solution in the Pareto set projects a significant change along the Pareto front. The later imposes that a small variation on the distance-related variables of one solution in the Pareto set causes a significant deterioration on the convergence towards the Pareto front.

In order, to analyze the capability of the MOEAs to deal with bias features

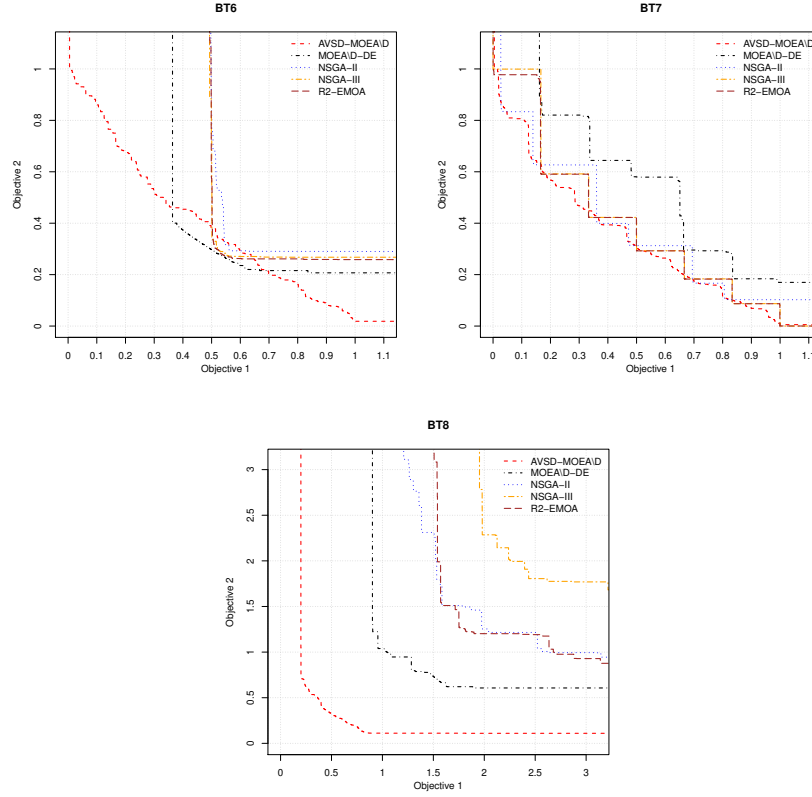


Figure 8: 50% attainment surfaces achieved for BT6 and BT8 test problems with a bias of $\frac{\theta}{32}$

the BTs problems are taken into account. Specifically, this section analyses the sensitivity of the algorithms imposing several levels of bias in the distance-related variables. Initially, for each problem the position-related bias and distance-related bias (θ) are kept exactly as the one proposed in the original work [47]. Then, for each problem its initial distance-related bias value (θ) is iteratively decreased by a factor of two. Specifically, the distance-related bias taken into account are $\{\theta, \frac{\theta}{2}, \frac{\theta}{4}, \frac{\theta}{8}, \frac{\theta}{16}, \frac{\theta}{32}, \frac{\theta}{64}, \frac{\theta}{128}, \frac{\theta}{256}, \frac{\theta}{512}, \frac{\theta}{1028}\}$. Figure 7 shows the mean HV ratio obtained with several distance-related biases. Also note

643 that the BT2 problem is not taken into consideration due that increasing
 644 its bias values provokes numerical instability since that it incorporates a
 645 different bias transformation, nevertheless all the results can be consulted
 646 in the supplementary document. Taking exactly the original configuration
 647 (bias of θ) [47] AVSD-MOEA/D is slightly better than MOEA/D-DE, but as
 648 soon as the bias is decreased to $\frac{\theta}{32}$ the performance of MOEA/D-DE decays
 649 aggressively. Furthermore, the performance of AVSD-MOEA/D is superior
 650 than 0.9 with biases values upper or equal to $\frac{\theta}{256}$ which is quite superior
 651 than the state-of-the-art MOEAs whose values at that point are approximately
 652 of 0.75. Figure 8 shows the 50% of attainment surface of BT6, BT7 and
 653 BT8 with a bias of $\frac{\theta}{32}$. BT6 and BT8 have simple nonlinear Pareto set while
 654 BT7 has a complicated nonlinear Pareto set. BT8 is multimodal. Although
 655 that MOEA/D-DE converged to a region of the Pareto front with BT6 AVSD-
 656 MOEA/D covered a huge region of the Pareto front, in fact this shows that
 657 for this problem promoting diversity in the decision space results in diversity
 658 in the objective space. In addition, AVSD-MOEA/D converges quite well in
 659 complicates nonlinear Pareto sets shown in the 50% attained surface of BT7
 660 (Figure 8). Finally but not less important AVSD-MOEA/D shows a superior
 661 behaviour with biased and multimodal problems as is the case of BT8 whose
 662 attainment surfaces have converged much better to the Pareto front.

663 5. Conclusion

664 Premature convergence is one of the most typical drawbacks of EAs.
 665 MOEAs indirectly promote the preservation of diversity in the variable space
 666 because of the implicit relationship between the diversity maintained in the

667 objective space and the one maintained in the variable space. However, for
 668 many problems the degree of diversity maintained is not sufficient to ensure
 669 the exploratory power of genetic operators and locate the optimal regions.
 670 In single-objective optimization, many of the state-of-the-art algorithms ex-
 671 plicitly manage diversity. Specifically, those schemes that relate the degree
 672 of diversity to the elapsed period of execution and to the stopping criterion
 673 have excelled. This paper shows that this design principle is also helpful in
 674 the area of multi-objective optimization, where the optimization of many of
 675 the most complex popular benchmark problems can be improved further by
 676 applying this design principle.

677 In order to prove this hypothesis, a novel replacement operator based on
 678 the aforementioned design principle is applied to generate a decomposition-
 679 based MOEA that takes into account the diversity in both the variable and ob-
 680 jective spaces. This is done using a dynamic penalty method. Note that since
 681 the aim of the approach is to improve the results when considering metrics
 682 in the objective space, the importance given to the diversity in the variable
 683 space is reduced as the evolution progresses, meaning that in the later phases,
 684 our proposal behaves more similarly to traditional MOEAs. Additionally, tak-
 685 ing into account recent advances, and to ensure that our proposal maintains
 686 high-quality solutions despite the penalty scheme, an external archive based
 687 on the R2-indicator is incorporated. Because of this, we refer to our pro-
 688 posal as *Archived Variable Space Diversity MOEA based on Decomposition*
 689 (*AVSD-MOEA/D*).

690 The experimental validation carried out shows the remarkable improve-
 691 ment provided by AVSD-MOEA/D in comparison to state-of-the-art MOEAs

with both two-objective and three-objective problems. The scalability analyses show that as the number of decision variables increases, the benefits of including proper diversity management are even more important, so the differences in performance increase. In fact, the most remarkable benefits emerge for the most complex cases. Moreover, the analysis of the initial penalty threshold, which is an additional parameter required by AVSD-MOEA/D, shows that the method is quite robust, which makes finding a proper parameter value an easy task. Finally, in order to better understand the reasons behind the huge superiority of our proposal, some analyses involving the dynamics of the populations are provided. In comparison to state-of-the-art algorithms, our proposal clearly slows down convergence.

In the future, we plan to apply the principles studied in this paper to other categories of MOEAs. For instance, including the diversity management method presented in this paper in indicator-based MOEAs seems plausible. Additionally, in order to obtain even better results, these strategies are going to be incorporated with continuation and/or individual improvement methods.

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