Variation Rate: An Alternative to Maintain Diversity in Decision Space for Multi-objective Evolutionary Algorithms

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Abstract. In almost all cases the performance of a multi-objective evolutionary algorithm (MOEA) is measured in terms of its approximation quality in objective space. As a consequence, most MOEAs focus on such approximations while neglecting the distribution of the individuals in decision space. This, however, represents a potential shortcoming in certain applications as in many cases one can obtain the same or a very similar qualities (measured in objective space) in several ways (measured in decision space) which may be very valuable information for the decision maker for the realization of a project.

In this work, we propose the variable-NSGA-III (vNSGA-III) an algorithm that performs an exploration both in objective and decision space. The idea behind this algorithm is the so-called variation rate, a heuristic that can easily be integrated into other MOEAs as it is free of additional design parameters. We demonstrate the effectiveness of our approach on several benchmark problems, where we show that, compared to other methods, we significantly improve the approximation quality in decision space without any loss in the quality in objective space.

Keywords: Evolutionary computation · Multi-objective optimization · Decision space diversity

1 Introduction

In many areas such as Economy, Finance, or Industry the problem arises naturally that several conflicting objectives have to be optimized concurrently. This leads to multi-objective optimization problems (MOPs). The solution of this kind of problems is a set of vectors that are incomparable to each other in terms

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of their objective values. For some of these problems obtaining the greatest benefit from limited resources is essential. Such resources are typically represented as the variables of the problem, as the objective functions depends on them. Although by using constraints it is possible to control the value of decision variables, this would entail the loss of optimal solutions and that is not desirable for the decision-making process. For instance, in real-world problems where the value of some variables is crucial, the decision maker may prefer, among the set of optimal solutions, those that are easiest to implement as this can mean a saving in resources.

However, in almost all cases the performance of a MOEA is only measured in terms of its approximation quality in objective space. As a consequence, most MOEAs focus on such approximations while neglecting the distribution of the individuals in decision space. This represents a potential shortcoming in certain applications as in many cases one can obtain the same or a very similar quality (measured in objective space) in several ways (measured in decision space) which may be very valuable information for the decision maker for the realization of a project. In this context, there exists an additional challenge in solving a MOP, since we must find an approximation to the optimal set both in objective and decision space, in order to provide all these possible regions to the decision maker.

In this work, we propose the variable-NSGA-III (vNSGA-III) an algorithm that performs an exploration both in objective and decision space. The idea behind this algorithm is the so-called variation rate, a heuristic that can easily be integrated into other MOEAs as it is free of additional design parameters. We demonstrate the effectiveness of our approach on several benchmark problems, where we show that, compared to other methods, we significantly improve the approximation quality in decision space without any loss in the quality in objective space.

The rest of the paper is organized as follows, in Sect. 2, we present the background and the related work. In Sect. 3, a detailed description of the proposed algorithm (along with pseudo-codes) is presented. In Sect. 4, numerical results are provided. Finally, in Sect. 5, we discuss the advantages of the proposed algorithm and we discuss the possible future improvements to the algorithm.

2 Background and Related Work

Optimization refers to finding the best possible solution to a problem given a set of constraints [2]. MOP refers to the simultaneous optimization of multiple and usually conflicting objectives; as a result, a set of optimal solutions are obtained instead of having a single optimal solution. The MOP with k objectives is mathematical defined as:

$$\min_{x \in D} F(x), \tag{1}$$

where $D \subset \mathbb{R}^n$ is the domain and $F : D \subset \mathbb{R}^n \to \mathbb{R}^k$ is the objective function.

The optimality of a MOP is defined by the concept of *dominance*. Let $v, w \in \mathbb{R}^k$, the vector v is *less than* w ($v <_p w$), if $v_i < w_i$ for all $i \in \{1, \ldots, k\}$; the relation $\leq_p$ is defined analogously. A vector $y \in D$ is *dominated* by a vector $x \in D$ ($x \prec y$) with respect to (1) if $F(x) \leq_p F(y)$ and $F(x) \neq F(y)$, else y is called non-dominated by x. A point $x^* \in \mathbb{R}^n$ is Pareto optimal to (1) if there is no $y \in D$ which dominates x. The set of all the Pareto optimal points is called the Pareto set and its image is the Pareto front.

Unlike evolutionary algorithms for single objective optimization problems (SOP), maintaining diversity in decision space is not a priority for most MOEAs; even the performance indicators are developed in order to measure the accuracy based only on the objective function (e.g., the hypervolume [15] and the DOA [7]). As an exception, we have the Δ_p indicator [12], which is the averaged Hausdorff distance, and it actually measures the distance between two general sets. For this reason, we can use it both in objective space as well as in decision space.

Although works that explicitly consider at the same time variables and objectives are scarce, one can find some related work on this topic. For instance, the NSGA (the algorithm that precedes the well-known NSGA-II [3]) uses fitness sharing in decision space. In [9], some possible techniques are proposed to spread out solutions both in objective and decision space: *pointwise expansion*, *threshold sharing*, *sequential sharing*, *simultaneous sharing multiplicative*, and *simultaneous sharing additive*. It is important to point out that the above approaches are only part of the discussion of the paper and they were not implemented; the implemented algorithm was the Niched Pareto GA, a method with phenotypic sharing. Besides, all of the described techniques depend on the normal fitness sharing method, that is, two additional parameters must be provided or approximated (the niche radius σ_{share} in each space).

The omni-optimizer algorithm [6] is proposed as a procedure that aims at solving a wide variety of optimization problems (single or multi-objective and uni- or multi-modal problems). The authors argue that to solve different kinds of problems it is necessary to know different specialized algorithms. Thus, it is desirable to have an algorithm which adapts itself for handling any number of conflicting objectives, constraints, and variables. The omni-optimizer is important in the context of this work as it uses a two-tier fitness assignment scheme based on the crowding distance of the NSGA-II. The primary fitness is computed using the phenotypes (objectives and constraint values) and the secondary fitness is computed using both phenotypes and genotypes (decision variables). The modified crowding distance computes the average crowding distance of the population both in objectives and variables. If the crowding value for some individual above average (at any space), it is assigned the larger of the two distances; else the smaller of the two distances is assigned. However, omni-optimizer has a more general purpose.

Recently, the *MOEA/D with Enhanced Variable-Space Diversity (MOEA/D-EVSD)* has been proposed in [1]. This method is an extension of the MOEA/D [14] that explicitly promotes the diversity of the decision space via an enhanced variable-space diversity control. First generations of MOEA/D-EVSD try to induce a larger diversity via promoting the mating of dissimilar individuals. Similarly to MOEA/D, a new individual is created for each subproblem. Then, instead of randomly selecting two individuals of the neighborhood, a pool of α candidate parents is randomly filled from the neighborhood with probability δ, whereas it is randomly selected from the whole population with probability $1-\delta$. Thus, the two selected parents are the ones that had the largest distance. As the δ parameter is dynamically set a gradual change between exploration and exploitation can be induced. Additionally, a final phase to further promote intensification is included, which is just a traditional MOEA/D with DE operators. For last generations of MOEA/D-EVSD the traditional mating selection of MOEA/D is conserved together with the Rand/1/bin scheme for the DE operators. Authors show that by inducing a gradual loss of diversity in the decision space, the state-of-the-art of MOEAs can be improved.

Finally, in [10], authors identify four different Pareto set and Pareto front type combinations: *Type I*, one Pareto set and one Pareto front; *Type II*, one Pareto set and multiple Pareto front parts; *Type III*, multiple Pareto subsets and one Pareto front; and *Type IV*, multiple Pareto subsets and Pareto front parts. In this work, a multi-start approach is proposed to solve problems of Type III, as authors argue that this kind of problems are rarely investigated and that standard MOEAs are not effective to preserve all Pareto subsets of equivalent quality. On the other hand, in [11], as a result of the study of multimodal problems, the authors conclude that a search in decision space is necessary to correctly solve them. In [13], a recovery technique in decision space is used to solve a problem of Type IV.

3 Proposed Algorithm

From the analysis of the combinations of Pareto set and front previously stated, it follows that, although most of MOEAs operate only in objective space, this is not a problem in cases like Types I, II, and IV. However, we must not lose sight of the fact that the value of the objectives depends on the variables. Thus, it is vital to maintaining the diversity of solutions in such space. In this way, when some method evaluates distribution considering only the objectives, potential search regions could be ruled out (Type III). On the other hand, if a method only takes into account the values of the variables without the objectives, then it could easily lose solutions along the Pareto front, what is highly penalized by the performance indicators. Our proposal seeks to perform an adequate grouping via a density estimator that allows obtaining a good distribution both in objective and decision space. The idea is to improve a classical density estimator, which groups the population in neighborhoods based only in the objectives. Such neighborhood structure is used to define a *variation rate* for each element in the neighborhood, according to some reference value in objective space, and certain measurement in decision space. In this way, the first grouping phase identifies promising solutions in objective space, meanwhile, the second phase favors solutions with the most different values in decision space. Thus, this variation rate represents the trade-off between these two aspects.

We consider the *variation rate* as the relation between the objective and the decision spaces. In order to properly define this rate, we need to group elements based on the value of their objectives (e.g., with the association method of the NSGA-III, the neighborhood structure of MOEA/D, the distance to a reference point, etc.). That is, we numerically assigned a reference value to the elements of each group for their ordering in objective space. Subsequently, the average distance in **decision space** of each element is computed against the rest elements in the group. Thus, the *variation rate* of each element is the quotient between its *reference value* in objective space and its *average distance* in decision space.

Let I denote a neighborhood (grouped in objective space) with v_i as the reference value for each $i \in I$, then the variation rate r_i is stated as follows:

$$r_i = \frac{v_i}{\mathtt{distP}(i, I)} \tag{2}$$

where $\mathtt{distP}(i, I)$ represents the average distance between each element $i \in I$ and the rest of elements in I, that is,

$$\mathtt{distP}(i, I) = \frac{1}{|I| - 1} \sum_{j \in I \setminus \{i\}} d(i, j). \tag{3}$$

Equation (3) depends of a function $d(i, j)$, which is the used method to measure the distance between $i, j \in I$ in the decision space. Thus, $\mathtt{distP}$ can vary according to the codification or the used norm.

As an example of how variation rate preserves the diversity, consider the following case. In Fig. 1, we can see a Type III Pareto Set/Front, that is, two lines in decision space –the Pareto set– map to the same Pareto front. Here, we have a neighborhood with three points ($\blacktriangledown$, $\blacklozenge$, and $\bigstar$) as their respective images are associated to the reference point (Z). Suppose that distance of $F(x_{\blacktriangledown})$, $F(x_{\blacklozenge})$ and $F(x_{\bigstar})$ to the reference Z is equal to one. On the other hand, $d(x_{\blacklozenge}, x_{\bigstar}) = 1$, $d(x_{\blacklozenge}, x_{\blacktriangledown}) = 2$, and $d(x_{\blacktriangledown}, x_{\bigstar}) = 2$, then,

- Variation rate of $\bigstar = \frac{1}{3/2} = \frac{2}{3}$
- Variation rate of $\blacklozenge = \frac{1}{3/2} = \frac{2}{3}$
- Variation rate of $\blacktriangledown = \frac{1}{4/2} = \frac{1}{2}$

In this way, if we select the point with the *less* variation rate, then we will conserve the most different individual in decision space with a good quality in objective space. In other words, elements with the minimum variation rate have the desired behavior.

Notice that, for problems of type I, II, and IV, it is expected that solutions in the same neighborhood have similar reference values in objective space and average distance in decision space, then the solution with the best reference value in objective space will be preferred. On the other hand, in type III problems the elements of the neighborhood will have a similar reference value in objectives but the average distance will be bigger for the most different solution in decision space, then its quotient (variation rate) will tend to be smaller than the rest of

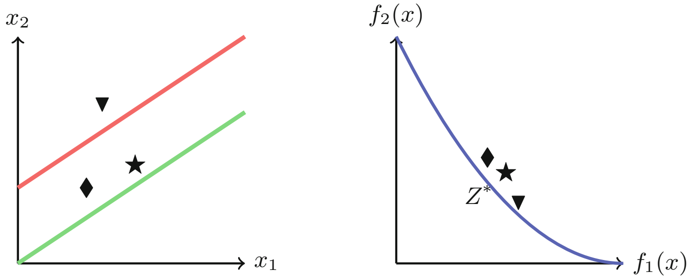


Fig. 1. Example of the computation of variation rate.

quotients. Thus, through the variation rate, we have a way to relate the objective and the decision spaces in order to choose the best element of each group.

The proposed method, called *variable-NSGA-III (vNSGA-III)*, is a modification of the NSGA-III algorithm [4] that seeks to solve the problem of diversity in the variables previously raised. Although this method is based on the NSGA-III, the *variation rate* can easily be adapted to other methods. The idea is to take advantage of the **association** method of the NSGA-III, which defines a "neighborhood". The association method assigns each element of F_j (the last front by classifying after the non-dominated sorting) to the nearest induced line by some weight $w_i \in Z$, where Z is a set of reference points. A weight can have more than one associated element, forming a neighborhood.

In the original NSGA-III, the **niching** is made by sort in ascending order the obtained groups in the association stage according to its cardinality. The element with less distance to the induced line in each group is selected, and it continues with the next group until filling the population. The proposed **niching** method does not prefer the element with the less distance value, instead it prefers the one with the smallest *variation rate*. The complete pseudocode of the vNSGA-III algorithm is shown in Algorithm 1.

4 Numerical Results

For the numerical results, we employ the following methodology. First, we compare vNSGA-III against two of the most widely used methods in the literature, NSGA-II and MOEA/D, in order to demonstrate that vNSGA-III improves the distribution in decision space without losing quality in objective space. Later, we compare our method with the MOEA/D-EVSD, that is a method with a similar purpose; (available code of MOEA/D-EVSD[1] is only for bi-objective problems, then this comparison is restricted to that kind of problems). Finally, we make a brief scalability test with the vNSGA-III and the original NSGA-III, to show how the variation rate can also improve the performance of this algorithm for many objective optimization problems (MaOPs), that is, problems with more than

[1] https://github.com/joelchaconcastillo/GECCO17_MOEA_D_MATING.

Algorithm 1. Iteration of the vNSGA-III

Require: Reference points Z, current population P_t
Ensure: Next population P_{t+1}

$S_t = \emptyset,\ i = 1$
Q_t = apply variation operators to P_t
$M_t = P_t \cup Q_t$
$(F_1, F_2 \ldots,)$ = non-dominated-sort(M_t)
while $|S_t| \leq N$ **do**
    $t = S_t \cup F_i$
    $i = i + 1$
end while
Add first fronts to P_{t+1}
F_i := last added front
Normalize F_i
Associate elements of F_i with each Z
Niching of F_i (according with the variation rate)
V_t := best niching elements
$P_{t+1} : S_t \cup V_t$

three objectives. As we test stochastic algorithms, each execution was repeated 30 times with different seeds to obtain statistical significance. The parameter settings of all the used algorithms are in Table 1.

Table 1. Parameter configuration for each algorithm. Mutation probability m_p, crossover probability c_p, neighborhood size α, first phase percent P_f, additional parameters for MOEA/D-EVSD T_{r1} and T_{r2}, and number of reference points $\#Z$.

Parameter	vNSGA-III	MOEA/D-EVSD	NSGA-II	MOEA/D
m_p	$1/n$	0.3	$1/n$	0.1
c_p	1.0	0.9	0.8	1.0
α	-	20	-	10
P_f	-	80%	-	-
T_{r1}	-	2	-	-
T_{r2}	-	25	-	-
$\#Z$	50	-	-	-

For the first comparison, we consider the problems DTLZ 1–3. We use the hypervolume indicator and Δ_p [12] to know how different is the approximation in variable and objective space. Results are shown in Table 2.

Next, we compare vNSGA-III against MOEA/D-EVSD and omni-optimizer. Test considered problems are the first four WFG tests proposed in [8] and the following bi-objective problem [6]

Table 2. Hypervolume (HV) and Δ_p (objective and decision space); best, average with standard deviation, and worst values are showed. The best value is put in bold.

Problem	Indicator	vNSGA-III	NSGA-II	MOEA/D
DTLZ1	HV	0.040700	0.076781	**0.079128**
		0.073839 (0.011847)	0.078690 (0.000675)	**0.079425** (0.000170)
		0.080123	0.079552	0.079654
	O-Δ_p	**0.015422**	0.017439	0.025133
		0.026077 (0.0683503)	0.041077 (0.016282)	**0.025495** (0.000304)
		0.056208	0.070908	**0.026016**
	D-Δ_p	**0.038723**	0.042297	0.048348
		0.075532 (0.038904)	0.080363 (0.025395)	0.054312 (0.002910)
		0.147971	0.126349	**0.058551**
DTLZ2	HV	0.379642	0.413363	**0.416942**
		0.414960 (0.008706)	0.417088 (0.001976)	**0.417757** (0.000559)
		0.420359	0.419725	0.418694
	O-Δ_p	**0.044592**	0.041514	0.044972
		0.045075 (0.012895)	0.045373 (0.001998)	0.045086 (0.000094)
		0.505410	0.049205	**0.045257**
	D-Δ_p	**0.029387**	0.074172	0.034619
		0.036727 (0.006681)	0.078942 (0.002572)	0.037074 (0.001521)
		0.051319	0.082206	**0.040618**
DTLZ3	HV	0.287586	0.365446	**0.410906**
		0.399156 (0.034941)	0.404309 (0.013330)	**0.418067** (0.002929)
		0.418205	**0.422514**	0.422293
	O-Δ_p	0.043525	0.040273	**0.040057**
		0.047231 (0.0867439)	0.071554 (0.098862)	**0.041026** (0.000499)
		0.485502	0.488509	**0.041650**
	D-Δ_p	0.041069	0.046354	**0.035459**
		0.053028 (0.023238)	0.051261 (0.004364)	**0.037630** (0.001252)
		0.083221	0.062031	**0.039935**

$$f_1(x) = \sum_{i=1}^{n} \sin(\pi x_i), \quad f_2(x) = \sum_{i=1}^{n} \cos(\pi x_i), \tag{4}$$

where $0 \leq x_i \leq 6$, and $i = 1, 2, \ldots, n$. This problem, denoted as OMNI1 in this work, is a type III combination of Pareto set/front. The used configuration for the WFG problems was the following: the stopping criterion was set to 250 generations, the population size was fixed to 200, and they were configured with two objectives and 24 parameters (20 distance parameters and 4 position parameters). On the other hand, for the OMNI1 problem the stopping criterion was set to 200 generations, the population size was fixed to 100, and $n = 5$ (number of decision variables). Numerical results are shown in Table 3.

Table 3. Hypervolume values, best, average with standard deviation, and worst values are showed. The best value is put in bold and the statistical significance is indicated, according to the Wilcoxon test with $p = 0.05$, when appropriate.

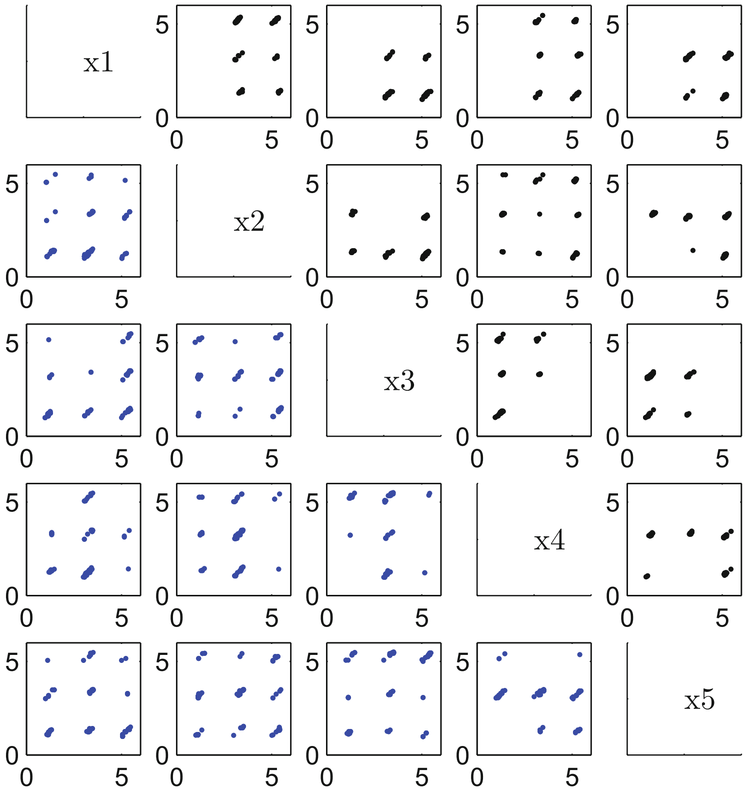
Problem	vNSGA-III	MOEA/D-EVSD	Omni-Optimizer
OMNI1$^{\downarrow}$	22.485004	22.458890	**22.530915**
	22.525381 (0.019402)	22.531425 (0.029448)	**22.567425** (0.017941)
	22.564005	22.564666	**22.592098**
WFG1$^{\uparrow}$	**4.050763**	2.816998	3.665387
	4.252966 (0.215981)	3.723304 (0.410585)	4.039288 (0.203742)
	5.042717	4.175823	4.211367
WFG2$^{\uparrow}$	**5.293999**	4.274958	4.681840
	5.428045 (0.092903)	4.810172 (0.230530)	4.763940 (0.043061)
	5.511280	5.043839	4.876360
WFG3$^{\uparrow}$	**4.877052**	3.915621	4.214724
	4.891410 (0.009166)	4.412886 (0.151054)	4.276409 (0.028887)
	4.906714	4.567030	4.331920
WFG4$^{\uparrow}$	**2.403976**	2.129897	1.959788
	2.411151 (0.003606)	2.181784 (0.029585)	1.974326 (0.011972)
	2.417486	2.228117	2.003731

It is clear that our approach requires less additional parameters than the MOEA/D-EVSD and omni-optimizer. Actually, no additional parameters than the original NSGA-III are needed.

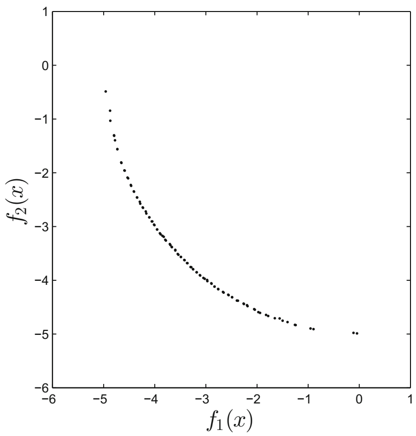
According with the values of Table 3, it is clear that our approach converges faster on the WFG problems. Although, the hypervolume value is worse for the for the OMNI1 problem, for such problem there are not significance according the Wilcoxon test. Moreover, in Fig. 2, we can see that the distribution in decision space, the main goal of this work, is better distributed with our method.

Finally, a brief scalability test is performed. We decide to compare our approach against the original NSGA-III, as this method is made to deal with MaOPs. We test on the DTLZ2 [5] problem with different number of objectives. The used parameters was the same that the used on the original paper of NSGA-III [4]. Numerical results are shown in Table 4.

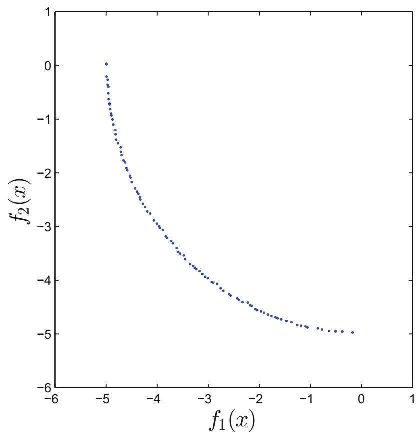
From Table 4 we can see that the large the number of objectives, the better is our approach, at least for the DTLZ2 problem. With this results, we expect that this approach could be successfully applied for MaOPs. However, an extensive analysis must be performed in order to conclude something about scalability.



(a) Decision space. Left-down vNSGA-III, right-up Omni-optimizer



(b) vNSGA-III



(c) Omni-optimizer

Fig. 2. Graphical results of the run with the median a values for the OMNI1 function.

Table 4. Δ_p values in objective space for the DTLZ2 problem with different number of objectives. The best, average with standard deviation, and worst values are showed; the best value for each case is put in bold.

k	vNSGA-III	NSGA-III
3	0.088196 0.107123 (0.013942) 0.148009	**0.081690** **0.095862** (0.012272) **0.133477**
5	0.229096 0.253322 (0.023562) 0.308298	**0.210055** **0.233658** (0.018896) **0.284361**
8	**0.293232** **0.379999** (0.046295) **0.456742**	0.366762 0.469987 (0.036129) 0.538956
10	**0.305149** **0.463134** (0.069997) **0.578061**	0.534823 0.600828 (0.035696) 0.686215

5 Conclusions and Future Work

In this work, the *variation rate*, a heuristic to explicitly handle the diversity in decision space, is proposed. This is an original proposal, in general, there are a few related work and the algorithms in the state of the art preserve diversity in decision space in distinct ways. Although two proposed techniques in [9] are kind of similar, the simultaneous sharing multiplicative and additive, they use a sum and a multiplication, respectively, instead of a quotient. Moreover, such methods depend on the σ-shared, while the variation rate if more flexible about the grouping method. We test this method via vNSGA-III, an extension of NSGA-III which uses the variation rate. The results are very promising in this field and our approach presents some advantages over others proposals.

In contrast with omi-optimizer and MOEA/D-EVSD, the implementation of the variation rate is free of additional parameters. This fact allows that this proposal can be easy include more algorithms, for instance, MOEA/D. It is only necessary to conserve certain neighborhood structure and explore the elements in each group in decision space. Moreover, the presented numerical results in the original paper, both in omi-optimizer and MOEA/D-EVSD, report a huge number of function evaluations; 500 generations for 1,000 individuals and 50,000 generations for 250 individuals, respectively.

Numerical results also show that variation rate improves the performance of the NSGA-III when the number of objectives becomes to increase. In principle, the MOEA/D-EVSD can also solve problems with any number of objectives, but it is restricted by the capabilities of the MOEA/D algorithm. On the other hand, the omni-optimizer depends on the crowding distance, and such a method is not scalable for high dimensions. Of course, variation rate by itself is not enough for the treatment of MaOPs, this depends on the operators of the NSGA-III. That is, variation rate can enhance the overall performance of a certain algorithm, but if such algorithm is not conceived to deal with MaOPs, then the addition of variation rate would be not enough to solved MaOPs.

As future work, it is necessary to develop an indicator for problems of Type III. In general, performance indicators evaluate an approximation based on the value of the objectives, but for problems as OMNI1 this is not provided enough information. Once we have such indicator, we can validate the better performance of our methods in decision space. However, it is not clear what property has to be satisfied with this approximation. We also need to test this approach in problems with different properties in decision space, in particular problems with disconnected Pareto set. Finally, the adaptation of the variation rate into a different MaOPs will allow studying the effect of this heuristic.

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