The Paradox of Multimodal Optimization: Concepts vs. Species in Single and Multi-objective Problems

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Abstract—It is well-known that decision-makers are often interested in searching for multiple alternative solutions. A major goal of multimodal optimization is to find such alternatives by searching for multiple peaks in the landscape. However, as claimed and demonstrated here with respect to that goal, the notion of multi-modal optimization is problematic on a fundamental level. Moreover, as discussed here, the notion of multimodal optimization is, for the most of it, restricted to single objective optimization. Following the above argumentation, this paper provides some overview on the set-base concept approach and describes how this approach can be used to produce meaningful solution alternatives for the decision-makers both for single and multi-objective problem. It is concluded that, when decision-makers are interested in finding multiple solutions, the use of the set-based concept approach is a valid alternative to multimodal optimization.

I. INTRODUCTION

Multi-Modal Optimization (MMO), which is commonly associated with single-objective optimization, primarily aims to present Decision-Makers (DMs) with multiple global and local optima. The rational is that selecting a solution may depend not just on the global performance in the optimized objective, but on other considerations.

Due to their use of a population, Evolutionary Algorithms (EAs) are a natural choice for MMO. Over several decades, special techniques have been suggested to make EAs adjusted for such a task (see reviews in [1-3]). According to [4], the techniques for MMO may be grouped into three main types. The first involves sequential (iterative/serial) approaches in which the use of the algorithm is repeated several times. A peak is expected to be found at each such run. The second is a parallel approach in which the population is divided explicitly into sub-populations and multiple peaks are expected to be found by the multi-population search. The third type concerns algorithms in which an implicit division of the population is performed by some niching/speciation technique.

Often all techniques to MMO are referred to as niching methods. Yet, to avoid confusion, here we refer to niching in the context of the third type of techniques, namely when implicit division of the population is performed. Niching can be incorporated into a standard EA to promote and maintain formation of multiple subpopulations within a single population. The formation of subpopulations supports the simultaneous search of multiple globally optimal or suboptimal solutions.

Considering reviews such as in [1-3], it is evident that the notion of MMO is commonly associated with single objective optimization problems. We note that similar to multimodal optimization, multi-objective optimization also aims at presenting DMs with multiple solutions. With this respect, two major questions should be raised. First, what is Multi-Modal Optimization for Multi-Objective Problems (MMO for MOPs), and second, why bother mixing two methods when each of them aims to provide the DMs with multiple solutions?

A secondary goal of this paper is to provide answers to the above two questions. Yet, the main goal is to highlight an apparent paradox of MMO, as related to niching/speciation, and consequently re-define what a search for alternative solutions might be.

The rest of this paper is organized as follows. In section II, Following [4], section II provides some background on the idea of a species. Next, in section III the claimed paradox is presented. In section IV, the notion of concepts, as an alternative to species, is presented. Moreover, the above two questions are also addressed in that section. This is followed, in section V, by a review on studies concerning concepts and in particular on how they can be applied to form a search for alternative solutions for MOPs. Finally, section VI concludes this paper.

II. SINGLE AND MULTI-OBJECTIVE SPECIES

In biology the term species refers to the most basic biological classification. It is comprised of individuals that are able to breed with each other but not with others. In nature, a niche can be viewed as a subspace in the environment with finite resources that must be shared among the population of that niche, while competing to survive. In EAs the term speciation (or "niching") commonly refers to an automatic technique to overcome the tendency of the population to cluster around one optimal solution in a multi-modal function optimization. Speciation techniques help maintaining diversity to prevent premature convergence, while dealing with multi-
modality. Speciation, in its original sense, could be viewed as a process that gradually divides the population into sub-populations (species). Common speciation is also a niching process as it finds the niches (optimums), while dividing the population into the niches. The sharing method, which was originally suggested by Holland, [5], is probably the most popular niching technique.

According to [4], a species is defined as a set of individuals in a population that have similar characteristics and are dominated by the best individual, called the species seed. This definition is suited for single-objective optimization. Following [4], a species will depend on a parameter, called the species distance, which is denoted by \( \sigma \). The distance between two individuals \( x_i = [x_{i1}, x_{i2}, \ldots, x_{in}] \) and \( x_j = [x_{j1}, x_{j2}, \ldots, x_{jn}] \) can be defined by different distance measures, denoted by \( d(x_i, x_j) \), such as the Euclidean distance. In [4], similarity between two individuals is considered by an upper bound on the distance between them (threshold). Considering a given population \( P_N = \{x_1, x_2, \ldots, x_N\} \) of \( N \) individuals, in a single-objective problem, and a given species distance \( \sigma \), one may try to search for seeds and their associated species, within the population. According to [4], a species \( S_i \) for such a minimization problem, consists of all individuals that are within a hypersphere of a radius \( \sigma/2 \), which is centered at the seed \( x^* \), such that for every individual \( y \in S_i \), \( d(x, y) < \sigma/2 \) and \( f(y) \leq f(x^*) \). It is clear from the definition that an individual of the population may belong to more than one species. A major difficulty in using this concept of a species is the need to determine the species distance. As discussed in [4], either fixed or adaptive species distance may be used.

Referring again to [4], it is noted that its text implies that a seed dominates all neighboring solutions within the species, whereas the formulation in [4] suggests that there could be non-dominated solutions, with respect to the seed. This distinction is important when considering species for MOPs. In such a case, the way the text of [4] describes the seed is problematic, as it involves a single solution to serve as a seed. Assuming objectives are conflicting then multiple non-dominated solutions may exist within a set of similar solutions. On the other hand, the way the seed is formulated in [4] allows non-dominated solutions to be a part of a species.

In [4] two Genetic Algorithms (GAs) are described. The first, which is termed Species Conserving GA (SCGA), employs a fixed species distance. The second, which is termed Adaptive Species Conserving GA (ASCGA), applies an adaptive procedure to the size of the species distance. To highlight the way a GA can be modified for MMO, we outline the ideas of SCGA. SCGA is based on a standard GA that is amended by the following operations. At each generation a procedure is used to determine the species seeds. These are united with the offspring population at each generation to conserve the species. When the evolutionary process is terminated, the DMs are presented with a subset of the final set of the seed solutions, based on a threshold with respect to the best seed.

III. THE PARADOX OF MULTIMODAL OPTIMIZATION

Consider the two different landscapes that are shown in Fig. 1. The lower curve (thin line) has two peaks one at \( X=a \), and the other at \( X=b \). In contrast, the upper curve (thick line) has only one peak at \( X=b \). Assume that the distance between the two peaks is considered to be larger than the species distance \( \sigma \). Namely, in the context of MMO the DMs are interested in finding the two peaks. Applying a MMO technique, such as SCGA, on the problem with the landscape of the lower curve is likely to find the two peaks and present them to the DMs. Moreover, assume that the DMs have tacit knowledge, which cause them to avoid the solution \( X=b \), so they will choose \( X=a \). Now, suppose that the landscape of the same problem is actually presented by the upper curve. MMO will find the solution \( X=b \), and will not present \( X=a \) as a solution. Yet, clearly if \( X=b \) is to be avoided by the DM, there is no reason why \( X=a \), or many other solutions such as \( X=a \), should not be considered. This example illustrates the paradox of MMO. MMO claims to find alternative solutions. Does it? According to the above example, it does and it does not!

Fig. 1 Illustration of the paradox

The paradox of multi-modal optimization calls for a review on the way we define the problem of finding alternative solutions. In the niching/speciation methods alternatives are commonly investigated relative to global and local optima, by way of a distance measure. This poses a problem as seen by the case of the upper landscape of Fig. 1. Alternatives should be defined not by the landscape of the problem, or at least not just by the peaks' locations and by a distance from such a peak.

As an alternative approach to MMO, we claim that a meaningful partition of the searched set should be defined by the DMs based on their tacit knowledge. Once defined, such a partition could serve as a base to redefine the search for alternative solutions. The next section describes the idea behind a meaningful partition of the search set.

IV. CONCEPTS

The notion of a conceptual solution, or in short a design concept, as understood in engineering design, is associated with abstractive ideas, which are generated by humans, describing a generic solution to a problem. Here, however, the term concept is used to describe any meaningful subset of the searched set of all feasible solutions.

In order to define a significant search for alternative solutions to be presented to the DMs, it is insufficient to divide the searched set based only on performance. This is true

\[ \sigma \]

\[ \sigma/2 \]

\[ F(X) \]

\[ X=a \]

\[ X=b \]

\[ X \]
because when selecting a solution DMs consider their tacit knowledge about the searched space (s), along with the obtained performance in the optimization objective(s). It is claimed that, for a given problem, only the DMs are able to divide the searched set into meaningful subsets (concepts). Such a partition can serve the DMs in defining a meaningful search for alternative solutions. This claim should be viewed with respect to the idea of niching/speciation, which is done by the computer during MMO.

Different problems may require different partitions in order for the partition to be meaningful for the DMs. To clarify the above ideas, we discuss three different optimization problems. The first, concerns a single objective problem of planning the shortest path from a start point to a goal point in an environment containing obstacles. Referring to Fig. 2, one may clearly see that the feasible path plans may be divided into concepts. It is noted that the figure contains, in addition to the three obstacles, also four non-penetrable straight boundaries. One may mathematically describe a partition of the entire set of feasible solutions by considering for example the subset of paths such as P1 and P2 that are passing left to obstacle "A," and so on. There could be different partitioning which are possible.

By itself, partitioning is insufficient for the search to be meaningful. To understand the notion of meaningful concepts/meaningful partition, consider the following tacit knowledge. The DMs are concerned about the possibility that when the path is to be executed, an adversary party will try to block paths between obstacle "A" and obstacle "B." It is therefore that a meaningful partition in this case would be to divide the solutions between two concepts. The first, is a concept that contains all paths that pass between this obstacles and the second is a concept containing all other paths. On the other hand, if the DMs are concerned about the possibility that the adversary party will block any of the alternative ways to reach the goal, then they may decide to partition the set of feasible solutions into four subsets, and try to find and compare the best solution (shortest path) within each such subset. This would constitute a significant search problem as it will provide alternative solutions, which can be examined not only by their length but also in view of incoming information about the plans of the adversary party.

The second problem to be examined is that of a multi-objective design of a truss structure that should support a force at its tip. The objectives are to minimize the deflection at the tip of the truss, while minimizing its weight. These are contradicting objectives. In this case, one may claim that using the Pareto-optimality principle will result in a set of alternative solutions (the Pareto-optimal set) to choose from.

Assume that the set of feasible solutions to this problem may include truss structures of several different layouts and of different cross-sectional areas for the bars. One possible way to divide this set is to consider each possible layout as a concept, such that an individual belonging to a particular concept is defined by the cross-sectional areas of its bars. There could be different partitioning which are possible.

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propeller, it may be constructed from various materials, the number of blades should also be decided, the type of wing profile should be decided and also the geometrical parameters along the blade. Clearly there are plenty of decisions to be made. Assume that the designers define the problem as a bi-objective one. One objective is to minimize the noise, and the other one is to maximize the flight range under the available battery of the aircraft. Such objectives are conflicting, and an expert designer may end up defining thousands of concepts of interest to her. It is quite clear that in such a situation, there is a large body of relevant knowledge that is not necessarily presented in the analysis code that is used for the optimization. Applying the EA, which is presented in [7], we were able to show that the use of multiple concepts may reveal useful solutions for such a propulsion system. Without the concept partitioning, such alternatives are not exposed by the use of evolutionary multi-objective optimization.

To illustrate the significance of using concepts in such a bi-objective problem, consider the situation that is illustrated in Fig. 4. Two Pareto-fronts, which are associated each with a propeller concept, are shown in the figure. The one marked by the dashed line is clearly better than the one marked by the bold curve. The dashed front represents the performances of the Pareto-optimal solutions from a concept of a propulsion system that involves a propeller of six blades, whereas the other one corresponds to a concept with five blades. If the entire set of solutions was to be optimized using standard evolutionary multi-objective optimization, the DMs would be presented with plenty of alternatives. However, all of them would belong to the concept of six blades. With the use of concepts, the DM are presented with the additional alternatives from the concept of the five blades. Is this significant to the DM? Clearly, if the manufacturer of the propeller suggests that a propeller of six blades is much harder to manufacture as compared with five blades, then this information may result with the DM preferring solutions from the concept of five blades, even though a slight reduction in the performance is expected.

The first concept consists of all solutions satisfying \( X \leq c \). The second concept involves solutions in the interval \([c, d]\), and the third concept consists of solutions within the interval \([d, e]\). Clearly alternative solutions can be found by searching for the best solution within each concept. In this case, when considering the landscape of the bold curve the alternative solutions will be \( X = c \) for the first concept, and \( X = d \) for the second one. The solution corresponding to the right peak of the bold curve will be the third alternative as obtained from the third concept. With this approach the paradox is resolved. Alternative solutions are found regardless of the fact that the landscape presented by the bold curve has only one peak. When applying the procedure to the other curve, there are also three alternative solutions which are found. They are not the same as for the upper curve, yet this is expected given that these are two different landscapes.

While a trivial approach for single-objective problems, the idea of using concepts for finding alternative solutions for MOPs appears to be a bit more complicated as evident from studies such as in [7].

V. SEARCHING FOR ALTERNATIVE SOLUTIONS

Our approach to searching for alternative solutions involves a-priori definition of concepts. In fact the use of concepts is not new. Originally, it was meant to support concept selection, rather than the selection of a particular solution (e.g., [8-11]). This has been termed the Set-Based Concept (SBC) approach. However, as recently noted in [7], the algorithms that were developed for concept selection can also be used for other purposes.

The SBC approach has been primarily developed in the context of multi-objective optimization. One exception can be found in [11], which deals with the use of concepts for a single-objective problem. The most studied SBC approach is known as the s-Pareto approach [9]. It involves finding which particular solutions, of which concepts, are associated with the Pareto-front that is obtained by domination comparisons among all individual solutions from all concepts. In principle,
existing multi-objective evolutionary algorithms can be easily used to find the front per each concept, and consequently a sorting procedure may be used to find the s-Pareto front and optimal set. However, such algorithms could also be tailored to simultaneously search all the concepts’ spaces to find the same information. For example, NSGA-II, [12], served as a base for finding s-Pareto in [10], and ε-MOEA [13] was tailored for that purpose in [14]. The reader is referred to [10] and [14] for discussions on why the simultaneous search approach should be preferred over independent concept searches, and why tailoring of the algorithms is needed.

In [15], it was suggested that concepts should not be selected by the s-Pareto approach. The alternative of a concept-based relaxed-Pareto approach was developed in [16], using relative (dynamic) relaxation. The work in [7] follows the above studies, but extends the application of the SBC approach from concept selection to design space exploration. Reference [7] involves three main contributions including: a. a description of a general approach to design space exploration, b. a related search algorithm, and c. a method to assess the algorithm.

In contrast to previous studies that suggest the SBC approach for concept selection, the works in [7], and [6] highlight its possible utilization for design space exploration. As in [7], also [6] employs SBC representations and the concept-based relaxed-Pareto approach, as a means to explore design spaces. The exploration algorithm in [7] is primarily based on two past studies on the SBC approach. The first is the study in [16], which combined the use of a relative SBC relaxation approach with NSGA-II, to produce Cr1-NSGA-II. The second is the study in [14], which tailored ε-MOEA to the SBC approach to produce C-ε-MOEA. However, the study in [7] substantially differs from works such as the above mainly by aiming at concept-based exploration rather than concept selection.

The main contribution of [6], as compared with [7], is the introduction of a novel method to account for run-time limitation. It involves a time control mechanism, based on the difference between the allocated run-time and the on-line estimated run-time. This difference, which changes during the search process is used to dynamically influence both the required amount of computational resources and the allocation of the available resources among the concepts. It is demonstrated in [6] that adding the suggested time control mechanism has a dramatic effect on the time required to obtain the sought information, as compared with the time it takes for the algorithm of [7].

The exploration problem that is dealt with in [6] and [7] is restated here. In fact, it can be considered as an example of the use of concepts to search for multiple alternative solutions in the context of MOPs.

Let $n_c$ be the dimension of the objective-space and $n_c$ be the number of concepts. Let $X_m \subseteq \mathbb{R}^{n_m}$ be the design-space of the $m$-th concept, and $f_m : X_m \rightarrow \mathbb{R}^{n_m}$ is the concept's objective-function. Let $n_m$ be the dimension of $X_m$. Furthermore, let $s$ be any particular design and let $m$ and $x_s$ represent the concept index and the design vector of $s$, respectively. Also, $x_{s,j}$ ($j = 1,...,n_m$) represents the $j$-th element of $x_s$, and $y_s = f_m(x_s)$ represents the performance vector of $s$, with $y_{s,j}$ ($i = 1,...,n_o$) representing the $i$-th element of $y_s$.

Without loss of generality, the complete concept-based exploration problem, which is based on a Pareto-approach, is about finding all the feasible Pareto-optimal solutions and front, for each problem of the following $n_c$ independent problems:

$$\min f_m(x) \text{ for } m = 1,...,n_c \quad (1)$$

On the other hand, the s-Pareto search problem is to find the non-dominated set of the union of solutions from all the above problems. Let $P^*$ be the set of all feasible particular designs from all concepts, then the s-Pareto set is defined as follows:

$$G^* = \{ s \in P^* \mid \nexists s' \in P^* : y_{s'} \succ y_s \} \quad (2)$$

Where $y' \succ y$ stands for $y'$ dominates $y$.

Let $F^*$ be the union of all the solutions of the complete concept-based exploration problem (see eq. 1). Then the first exploration problem type, as described in [7], is to find the concept-based relaxed Pareto-optimal set, which is defined without loss of generality, for a minimization problem, as follows:

$$R^* = \{ s \in F^* \mid \exists s' \in G^* : y_s \succ y_{s'} + r \} \quad (3)$$

where vector $r = (r_1,...,r_{n_o}) \in \mathbb{R}_{+}^{n_o}$ is a vector of relaxation, which is defined by the users prior to the search. It is noted that the difficulty is that the relaxation zone, which contains the sought information, is relative to the s-Pareto front, which in itself is unknown prior to the search. Searching for $R^*$ results with solution alternatives that are neither from one concept, nor from the s-Pareto front. The obtained alternatives are meaningful, as they come from alternative concepts. Moreover, the solution alternatives, which are contained in $R^*$ may be dominated by others. Yet, they performance reduction is within an agreed relaxation, and the dominate solutions are from a different concept as compared with the dominating solutions.

The interested reader may find two alternative EAs to search for the concept-based relaxed Pareto-optimal set, $R^*$, one in [7], and the other in [6].

VI. DISCUSSION AND CONCLUSIONS

This paper raises and discusses a paradox concerning niching/speciation and multimodal optimization. The paradox concerns a major aim of multimodal optimization, which is to find alternative solutions to be presented to the decision-makers. With this respect, it is suggested and demonstrated that concepts, which are meaningful subsets of the set of the
feasible solutions, could be used as an alternative notion to that of species. Using set-based concepts, a search for alternative solutions can be defined. One such possibility, for the case of multi-objective problems, is described. It concerns finding the concept-based relaxed Pareto-optimal set. Such an approach provides decision-makers with plenty of meaningful solutions to choose from, which do not only account for preferences of objectives, but also for preferences of concepts.

In the following, we refer to the use of the set-based concept approach for finding alternative solutions, as multi-concept optimization. To allow using multi-concept optimization by the industry, reliable and efficient algorithms should be developed. This is true for both single and multi-objective problems. Similar to the case of multimodal and multiobjective optimization, population-based algorithms are a natural choice for the case of multi-concept optimization. As already observed from references such as [7], [10], and [14], the development of tailored algorithms for multi-concept optimization can benefit from existing evolutionary algorithms. Yet, it will also depend on devising a systematic approach and tools to test such algorithms, as recently attempted in [7]. Future development of such tailored algorithms is likely to be focused on parallelism and interactivity.

Spreading the application of multi-concept optimization will depend not only on its development and on its recognition by the research community. It will require exposing its applicability to the industry. With this respect, some real-life demonstrations are available on the s-Pareto approach. In collaboration with a researcher from the Israel Aerospace Industry, the author's research group has recently demonstrated the applicability of the concept-based relaxed-Pareto approach to a real-life problem. A report on this work should be expected in the near future.

An important aspect of developing such demonstrations is the need to define the concepts of interest to the decision-makers. Users of optimization tools in the industry are not accustomed to defining concepts. Yet, they implicitly define one concept, when defining the searched space in any optimization problem that they face. It seems to be a matter of educating the potential users of multi-concept-optimization to become accustomed to splitting the searched set into meaningful concepts. With this respect, note that concepts seem to be related to discrete variables in some sense; yet, they do not have to be strictly defined by such variables (e.g., [17]). The key element to their definition for a particular problem is that partitioning of the set of feasible solutions should be done with a cognitive understanding of their meaning to the decision-makers. This should come with the ability to label such subsets (concepts) with linguistic terms, which are implicitly related to the significance of the concepts to the decision-makers.

Finally, the reader should realize that we are not suggesting to drop the use of multi-modal optimization. Clearly, there are several reasons for the use of speciation and multi-modal optimization, which goes beyond what multi-concept optimization aims at. Nevertheless, when it comes to providing decision-makers with alternative solutions, both in single and multi-objective optimization problems, we suggest that the declared paradox cannot be ignored.

REFERENCES