

Recent Results and Open Problems in Evolutionary Multiobjective Optimization

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Abstract. Evolutionary algorithms (as well as a number of other meta-heuristics) have become a popular choice for solving problems having two or more (often conflicting) objectives (the so-called multi-objective optimization problems). This area, known as EMOO (Evolutionary Multi-Objective Optimization) has had an important growth in the last 20 years, and several people (particularly newcomers) get the impression that it is now very difficult to make contributions of sufficient value to justify, for example, a PhD thesis. However, a lot of interesting research is still under way. In this paper, we will briefly review some of the research topics on evolutionary multi-objective optimization that are currently attracting a lot of interest (e.g., indicator-based selection, many-objective optimization and use of surrogates) and which represent good opportunities for doing research. Some of the challenges currently faced by this discipline will also be delineated.

Keywords: evolutionary computing, optimization

1 Introduction

The solution of problems having two or more (normally conflicting) objectives has attracted a considerable attention in the last few years. The solution of these so-called *multi-objective optimization problems* (MOPs) gives rise to a set of solutions representing the best possible trade-offs among the objectives. Such solutions, defined in decision variable space constitute the so-called *Pareto optimal set*, and their corresponding objective function values form the so-called *Pareto front*.

Although a number of mathematical programming techniques have been developed since the 1970s to solve MOPs [81], such techniques present several limitations, from which two of the most relevant are that these algorithms are normally very susceptible to the shape or continuity of the Pareto front and that they tend to generate a single element of the Pareto optimal set per run.

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Additionally, in some real-world MOPs, the objective functions are not provided in algebraic form, but are the output of a black box software (which, for example, runs a simulation to obtain an objective function value), thus limiting the applicability of mathematical programming techniques. Such limitations have motivated the development of alternative approaches from which metaheuristics¹ have been, with no doubt, the most popular and effective choice available so far (see for example [24]).

From the many metaheuristics in current use, Evolutionary Algorithms (EAs) are, clearly, the most popular in today’s specialized literature. EAs are inspired on the “survival of the fittest” principle from Darwin’s evolutionary theory [43], and simulate the evolutionary process in a computer, as a way to solve problems. EAs have become very popular as multi-objective optimizers because of their ease of use (and implementation) and generality (e.g., they are less sensitive than mathematical programming techniques to the initial points used for the search and to the specific features of a MOP). EAs have also an additional advantage: since they are population-based techniques, it is possible for them to manage a set of solutions at a time, instead of only one, as normally done by traditional mathematical programming techniques. This allows EAs to generate several elements from the Pareto optimal set in a single run.

The first Multi-Objective Evolutionary Algorithm (MOEA) was proposed in the mid-1980s by David Schaffer [103]. However, it was until the mid-1990s that MOEAs started to attract serious attention from researchers. Nowadays, it is possible to find applications of MOEAs in practically all domains.²

The remainder of this paper is organized as follows. In Section 2, we provide some basic multi-objective optimization concepts required to make this paper self-contained. Section 3 briefly describes some relevant research topics that are worth currently being explored by EMOO researchers. In Section 4, we present other challenges in the field that have been only scarcely explored. Finally, the main conclusions of this paper are provided in Section 5.

2 Basic Concepts

We are interested in solving problems of the type³:

$$\text{minimize } \mathbf{f}(\mathbf{x}) := [f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_k(\mathbf{x})] \quad (1)$$

subject to:

$$g_i(\mathbf{x}) \leq 0 \quad i = 1, 2, \dots, m \quad (2)$$

¹ A **metaheuristic** is a high level strategy for exploring search spaces by using different methods [14]. Metaheuristics have both a diversification (i.e., exploration of the search space) and an intensification (i.e., exploitation of the accumulated search experience) procedure.

² The author maintains the EMOO repository, which currently contains over 10,850 bibliographic references related to evolutionary multi-objective optimization. The EMOO repository is located at: <https://emoo.cs.cinvestav.mx>.

³ Without loss of generality, we will assume only minimization problems.

$$h_i(\mathbf{x}) = 0 \quad i = 1, 2, \dots, p \quad (3)$$

where $\mathbf{x} = [x_1, x_2, \dots, x_n]^T$ is the vector of decision variables, $f_i : \mathbb{R}^n \rightarrow \mathbb{R}$, $i = 1, \dots, k$ are the objective functions and $g_i, h_j : \mathbb{R}^n \rightarrow \mathbb{R}$, $i = 1, \dots, m$, $j = 1, \dots, p$ are the constraint functions of the problem.

To describe the concept of optimality in which we are interested, we will introduce next a few definitions.

Definition 1. Given two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^k$, we say that $\mathbf{x} \leq \mathbf{y}$ if $x_i \leq y_i$ for $i = 1, \dots, k$, and that \mathbf{x} **dominates** \mathbf{y} (denoted by $\mathbf{x} \prec \mathbf{y}$) if $\mathbf{x} \leq \mathbf{y}$ and $\mathbf{x} \neq \mathbf{y}$.

Definition 2. We say that a vector of decision variables $\mathbf{x} \in \mathcal{X} \subset \mathbb{R}^n$ is **non-dominated** with respect to \mathcal{X} , if there does not exist another $\mathbf{x}' \in \mathcal{X}$ such that $\mathbf{f}(\mathbf{x}') \prec \mathbf{f}(\mathbf{x})$.

Definition 3. We say that a vector of decision variables $\mathbf{x}^* \in \mathcal{F} \subset \mathbb{R}^n$ (\mathcal{F} is the feasible region) is **Pareto-optimal** if it is nondominated with respect to \mathcal{F} .

Definition 4. The **Pareto Optimal Set** \mathcal{P}^* is defined by:

$$\mathcal{P}^* = \{\mathbf{x} \in \mathcal{F} | \mathbf{x} \text{ is Pareto-optimal}\}$$

Definition 5. The **Pareto Front** \mathcal{PF}^* is defined by:

$$\mathcal{PF}^* = \{\mathbf{f}(\mathbf{x}) \in \mathbb{R}^k | \mathbf{x} \in \mathcal{P}^*\}$$

We thus wish to determine the Pareto optimal set from the set \mathcal{F} of all the decision variable vectors that satisfy (2) and (3). Note however that in practice, not all the Pareto optimal set is normally desirable (e.g., it may not be desirable to have different solutions that map to the same values in objective function space) or achievable.

3 Some Open Research Topics that are Worth Exploring

In spite of the significant development that MOEAs have experienced since their inception, there are still some research topics that are worth exploring in the next few years. From them, we will discuss three in this paper:

1. Algorithmic design
2. Scalability
3. Dealing with expensive objective functions

Next, we briefly discuss some of the most representative research that has been conducted on these topics.

3.1 Algorithmic design

In the early days of MOEAs, the approaches that were adopted were very simple and naive. For example, it was relatively common to use linear aggregating functions that combined all the objective functions into a single scalar value [48]. However, by the mid-1990s, several MOEAs started to adopt mechanisms such as *Pareto ranking* [43] and *nondominated sorting* [109]. In these mechanisms, the idea is to rank solutions based on Pareto optimality, such that nondominated individuals obtain the highest (best) possible rank. Since diversity is an important issue in MOEAs, in order to avoid convergence to a single solution, an additional mechanism was integrated to them: the so-called density estimator. Since the mid-1990s, a number of density estimators have been adopted, including: fitness sharing [44], clustering [129], adaptive grids [67], crowding [30], entropy [88] and parallel coordinates [54].

By the end of the 1990s, another mechanism was incorporated into MOEAs: elitism. The intuition behind the concept of *elitism* is that we need to retain the solutions that remain nondominated with respect to the new individuals that are being generated by our MOEA (otherwise, such solutions could be lost). Elitism is important not only from a practical point of view, but also for theoretical reasons, since this mechanism is required to guarantee convergence [99].

In spite of the large number of MOEAs that were proposed in the 1990s, few of them were widely used. From them, clearly the **Nondominated Sorting Genetic Algorithm II** (NSGA-II) [30] was the most popular (and is still being used today).

However, a few years after NSGA-II, another interesting MOEA was proposed: the **Multi-Objective Evolutionary Algorithm based on Decomposition** (MOEA/D) [124]. The idea of using decomposition was originally proposed in mathematical programming and it consists in transforming a multi-objective problem into several single-objective optimization problems which, in the case of MOEA/D are simultaneously solved, using neighborhood search. Decomposition-based methods would eventually become very popular research trend in algorithmic design (see for example [101]) and would influence the design of the **Nondominated Sorting Genetic Algorithm III** (NSGA-III) [29] which adopts decomposition and reference points.

Nevertheless, since 2004, a different type of algorithmic design has increasingly attracted interest from researchers: indicator-based selection. The idea of this sort of MOEA was introduced in the **Indicator-Based Evolutionary Algorithm** (IBEA) [126] which consists of an algorithmic framework that allows the incorporation of any performance indicator into the selection mechanism of a MOEA. IBEA was originally tested with the hypervolume [128] and the binary ϵ indicator [127]. Indicator-based selection has attracted a lot of interest, mainly because this sort of mechanism is known to work properly in many-objective optimization (i.e., MOPs having four or more objectives).

Over the years, a number of indicator-based MOEAs have been proposed, but probably the most representative approach within this family has been the **S Metric Selection Evolutionary Multiobjective Algorithm** (SMS-

EMOA) [36]. SMS-EMOA randomly generates an initial population and then produces a single solution per iteration (i.e., it uses steady state selection) using the crossover and mutation operators from NSGA-II. Then, it applies nondominated sorting (as in NSGA-II). When the last nondominated front has more than one solution, SMS-EMOA uses hypervolume to decide which solution should be removed. Beume et al. [11] proposed a new version of SMS-EMOA in which the hypervolume contribution is not used when, in the nondominated sorting process, we obtain more than one front. In this case, they use the number of solutions that dominate to a certain individual (i.e., the solution that is dominated by the largest number of solutions is removed).

After the introduction of SMS-EMOA, most indicator-based MOEAs that have been proposed adopt a performance indicator in their density estimator,⁴ and not in their selection mechanism (see for example [59]). The actual use of a “pure” indicator-based selection mechanism has been very rare (see for example [78]).

So, at this point, one obvious question is: why is that the *hypervolume* is such an attractive choice for indicator-based selection?

The hypervolume (also known as the S metric or the Lebesgue Measure) of a set of solutions measures the size of the portion of objective space that is dominated by those solutions collectively. One of its main advantages are its mathematical properties, since it has been proved that the maximization of this performance measure is equivalent to finding the Pareto optimal set [39]. Additionally, empirical studies have shown that (for a certain number of points previously determined) the maximization of the hypervolume does indeed produce subsets of the Pareto front which are well-distributed [65, 36]. Also, the hypervolume assesses both convergence and, to a certain extent, also the spread of solutions along the Pareto front (although without enforcing uniform distribution of solutions).

However, there are several issues regarding the use of the hypervolume. First, the computation of this performance measure depends of a reference point, which can influence the results in a significant manner. Some people have proposed to use the worst objective function values in the current population, but this requires scaling of the objectives. Nevertheless, the most serious limitation of the hypervolume is its high computational cost. The best algorithms known to compute hypervolume have a polynomial complexity on the number of points used, but such complexity grows exponentially on the number of objectives [12]. This has triggered a significant amount of research regarding algorithms that can reduce the computational cost of computing the hypervolume⁵ (see for example [121, 15, 120, 57]).

⁴ In fact, the earliest use of the hypervolume into a MOEA is as a density estimator in a secondary population (see [65]).

⁵ See also:

<http://ls11-www.cs.uni-dortmund.de/rudolph/hypervolume/start>

<http://people.mpi-inf.mpg.de/~tfried/HYP/>

<http://iridia.ulb.ac.be/~manuel/hypervolume>

An alternative to deal with this problem is to approximate the actual hypervolume contributions. This is the approach adopted by the **Hypervolume Estimation Algorithm for Multi-Objective Optimization** (HyPE) [3] in which Monte Carlo simulations are used to approximate exact hypervolume values. Although this is certainly a very interesting idea, in practice HyPE does not produce results as competitive as when using exact hypervolume computations.

Another possibility is to use another performance indicator, but the fact that the hypervolume is the only unary indicator which is known to be Pareto compliant [130] has made this alternative less attractive to researchers. Nevertheless, the use of a few other performance indicators has been reported to be successful in practice. Examples of these alternative indicator that have been used within MOEAs are: $R2$ [17, 51, 33, 46, 16, 52], Δ_p [105, 98, 79] and Inverted Generational Distance plus ($IGD+$) [60, 74]. Also, the use of other mechanisms such as the maximin fitness function, which seems to be related to the ϵ indicator are very promising (see for example [77]). All of these MOEAs are computationally inexpensive and perform quite well in many-objective problems, however, their use in practice is still very limited.

It is worth indicating that while some researchers debate if decomposition-based MOEAs or indicator-based MOEAs will become the new algorithmic trend in the next few years, other alternatives to the use of Pareto-based selection have been proposed. For example, Molinet Berenguer and Coello Coello [7], proposed an approach that transforms a multi-objective optimization problem into a linear assignment problem using a set of weight vectors uniformly scattered. Uniform design is adopted to obtain the set of weights, and the Kuhn-Munkres (Hungarian) algorithm [68] is used to solve the resulting assignment problem. This approach was found to perform quite well (and at a low computational cost) in many-objective optimization problems.

3.2 Scalability

In their early days, MOEAs were mainly used to solve problems having only two or three objectives. However, once Pareto-based MOEAs became popular, the need for solving problems having more objectives was very evident. At this point, problems started to arise, since it was soon evident that Pareto-based MOEAs tend to perform poorly in many-objective optimization problems [56].

Experimental [89, 117] and analytical studies [26, 66] have identified the following limitations of Pareto-based MOEAs in many-objective problems:

1. *Deterioration of the Search Ability*: The proportion of nondominated solutions in a population increases rapidly with the number of objectives [37]. According to Bentley *et al.* [5] the number of nondominated k -dimensional vectors on a set of size n is $O(\ln^{k-1} n)$. This implies that in problems with a large number objectives, the selection of solutions is carried out almost at random or guided by diversity criteria. In fact, Mostaghim and Schmeck [85] have shown that a random search optimizer achieves better results than NSGA-II [30] in a problem with 10 objectives.

2. *Dimensionality of the Pareto front:* Due to the ‘curse of dimensionality’ the number of points required to represent accurately a Pareto front increases exponentially with the number of objectives. The number of points necessary to represent a k -dimensional Pareto front with resolution r is given by $O(kr^{k-1})$ (e.g., see [106]). This poses a challenge both to the data structures to efficiently manage that number of points and to the density estimators to achieve an even distribution of the solutions along the Pareto front.
3. *Visualization of the Pareto front:* Clearly, with more than three objectives is not possible to plot the Pareto front as usual. This is a serious problem since visualization plays a key role for a proper decision making process. In recent years, a number of visualization techniques have been proposed for many-objective problems (see for example [113]), but this is still an active research area.

In order to properly deal with many-objective optimization problems, three main approaches have been normally adopted [72, 70, 4]:

1. As indicated before, the use of indicator-based MOEAs has been an important research trend to deal with many-objective optimization problems, in spite of the limitations of some performance indicators such as the hypervolume (see for example [62]).
2. One interesting possibility that was adopted in the early days of many-objective optimization was the use of an optimality relation that yields a solution ordering finer than that yielded by Pareto optimality. Among these alternative relations we can find average ranking [6, 40], k -optimality [37], preference order ranking [32], favour relation [110], and a method that controls the dominance area [102], among others. Besides providing a richer ordering of the solutions, these relations obtain an optimal set that it is usually a subset of the Pareto optimal set.
3. Another interesting approach which is now rarely used is to reduce the number of objectives of the problem during the search process or in an *a posteriori* manner, during the decision making process [18, 31, 71]. The main goal of this kind of reduction techniques is to identify redundant objectives (or redundant to some degree) in order to discard them. A redundant objective is one that can be removed without changing the dominance relation induced by the original objective set.

In contrast with the significant interest that many-objective optimization has attracted in recent years, scalability in decision variable space has been only recently studied in the context of multi-objective optimization (see for example [82, 125, 83, 73]). This is remarkable if we consider that large-scale multi-objective optimization problems (i.e., problems having more than 100 decision variables) are not rare in real-world applications (see for example [119]). In this area, the use of cooperative coevolutionary approaches (which have been very successful in single-objective large-scale optimization) is the most common research trend. It is worth indicating, however, that no current benchmark exists that includes large-scale multi-objective optimization problems.

A more challenging problem would consist in solving many-objective large-scale problems, but no work in this direction has been reported yet, to the best of the author's knowledge.

3.3 Dealing with expensive objective functions

In spite of the current popularity of MOEAs, one of their limitations is that, since they are stochastic search techniques, they normally require a significant number of objective function evaluations in order to generate a proper sampling that allows a reasonably good approximation of the Pareto front, even when dealing with problems of low dimensionality. This is, indeed, a serious limitation when dealing with real-world problems, because in many cases, the cost of a MOEA becomes prohibitive.

In general, MOEAs can be unaffordable for an application when:

- The evaluation of the fitness functions is computationally expensive (i.e., it takes from minutes to hours).
- The fitness functions cannot be defined in an algebraic form (e.g., when the fitness functions are generated by a simulator).
- The total number of evaluations of the fitness functions is limited by financial constraints (i.e., there is a financial cost involved in computing the fitness functions).

In recent years, a significant amount of research has been conducted to allow MOEAs to properly deal with computationally expensive problems [100]. The main approaches that have been developed in this area can be roughly divided into three main groups:

1. **Use of parallelism:** This is clearly the most obvious approach given the current access to cheap parallel architectures (e.g., GPUs [28, 8, 107]). It is worth noting, however, that in spite of the existence of interesting proposals in this area (see for example [111, 84, 1]), the basic research in this area has remained scarce, since most publications involving parallel MOEAs focus on specific applications or on parallel extensions of specific MOEAs.
2. **Surrogates:** In this case, knowledge of past evaluations of a MOEA is used to build an empirical model that approximates the fitness functions to be optimized. This approximation can then be used to predict promising new solutions at a smaller evaluation cost than that of the original problem [64, 63]. Current functional approximation models include Polynomials (response surface methodologies [92, 41]), neural networks (e.g., multi-layer perceptrons (MLPs) [55, 58, 87]), radial-basis function (RBF) networks [86, 114, 122], support vector machines (SVMs) [104, 13], Gaussian processes [115, 20], and Kriging [35, 93] models. Although frequently used in engineering applications, surrogate methods can normally be adopted only in problems of low dimensionality, which is an important limitation when dealing with real-world MOPs.

3. **Fitness inheritance:** This technique was introduced by Smith et al. [108], and its main motivation is to reduce the total number of fitness function evaluations performed by a (single-objective) evolutionary algorithm. The mechanism works as follows: when assigning the fitness to an individual, some times we evaluate the objective function as usual, but the rest of the time, we assign fitness as an average of the fitness of the parents. This saves one fitness function evaluation, and is based on the assumption of similarity of an offspring to its parents. Fitness inheritance must not be always applied, since the algorithm needs to use the true fitness function several times, in order to obtain enough information to guide the search. The percentage of time in which fitness inheritance is applied is called *inheritance proportion*. If this inheritance proportion is 1, the algorithm is most likely to prematurely converge [23]. Extending fitness inheritance involves several issues, mainly related to its apparent limitation for dealing with non-convex Pareto fronts [34]. However, some researchers have managed to successfully adapt fitness inheritance to MOEAs [94], reporting important savings on the total number of objective function evaluations performed.

Other approaches are also possible. For example, some researchers have adopted cultural algorithms [25, 9, 10, 95], which obtain knowledge during the evolutionary process and use it to perform a more efficient search at the expense of a significantly large memory usage. Cultural algorithms were proposed by Reynolds [96, 97], as an approach that tries to add domain knowledge to an evolutionary algorithm during the search process, avoiding the need to add it *a priori*. This approach uses, in addition to the population space commonly adopted in evolutionary algorithms, a belief space, which encodes the knowledge obtained from the search points and their evaluation, in order to influence the evolutionary operators that guide the search. However, the belief space is commonly designed based on the group of problems that is to be solved. At each generation, the cultural algorithm selects some exemplar individuals from the population, in order to extract information from them that can be useful during the search. Such an information is used to update the belief space. The belief space will then influence the operators of the evolutionary algorithm, to transform them in informed operators and enhance the search process. Cultural algorithms can be an effective means of saving objective function evaluations, but since a map of decision variable space must be kept at all times, their cost will soon become prohibitive even for problems of moderate dimensionality.

4 Other Challenges

Several other topics remain scarcely explored in evolutionary multi-objective optimization. For example:

1. **Dynamic problems:** In the real world, there are problems in which the objective function values may vary over time (e.g., because of the presence

of noise), depending on certain events. The solution of such problems requires algorithms that are able to quickly “adapt” to these changes in the environment. There are relatively few MOEAs that have been designed to deal with dynamic MOPs and the current research in this area remains relatively scarce [21, 118, 27, 49, 91]. It is worth noting that dynamic problems require different types of benchmarks (see for example [38]) and performance measures (see for example [50]).

2. **Hyper-heuristics:** In spite of the fact that multi-objective memetic algorithms (i.e., MOEAs that are hybridized with a local search engine, which could be, for example, a gradient-based method [69] or a direct search method [123]) have gained popularity in recent years (see for example [42, 61, 75]), hyper-heuristics have been only scarcely explored in the context of multi-objective optimization, particularly for dealing with continuous optimization problems (see for example [45, 53]). Hyper-heuristics [22] are approaches that combine several types of heuristics, with the aim of combining their advantages in a wide class of problems. Their main motivation is to have a more general search engine that can solve a wider variety of hard optimization problems. Hyper-heuristics have been mostly developed for discrete search spaces and have been used to solve mainly single-objective optimization problems. However, their use in continuous multi-objective optimization problems, although possible, has been scarcely explored (see for example [76]). The use of other (similar) approaches that combine operators and different MOEAs into a common framework are also promising research venues (see for example [116, 47]).
3. **Automatic parameter configuration:** Although some relevant work has been conducted on parameter fine-tuning for MOEAs (see for example [19, 112, 2]), it has been only recently that researchers in evolutionary multi-objective optimization have considered the use of tools to do an automatic calibration of MOEAs (see for example [80]). One limitation for the use of such tools is that a scalar measure is required, but some researchers have relied on the use of hypervolume (see for example [90]) for that sake.

5 Conclusions

In this paper, a few research trends in evolutionary multi-objective optimization have been briefly described with the aim of encouraging more research in such areas.

The main goal of this paper is to illustrate that, in spite of its 32 years of existence, evolutionary multi-objective optimization still has several research opportunities to offer to newcomers. The contents of this paper is just a small sample of the several topics that are still available for starting a research career in this area.

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