A Visualization Technique for Accessing Solution Pool in Interactive Methods of Multiobjective Optimization

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Abstract: Interactive methods of multiobjective optimization repetitively derive Pareto optimal solutions based on decision maker’s preference information and present the obtained solutions for his/her consideration. Some interactive methods save the obtained solutions into a solution pool and, at each iteration, allow the decision maker considering any of solutions obtained earlier. This feature contributes to the flexibility of exploring the Pareto optimal set and learning about the optimization problem. However, in the case of many objective functions, the accumulation of derived solutions makes accessing the solution pool cognitively difficult for the decision maker. We propose to enhance interactive methods with visualization of the set of solution outcomes using dimensionality reduction and interactive mechanisms for exploration of the solution pool. We describe a proposed visualization technique and demonstrate its usage with an example problem solved using the interactive method NIMBUS.

Keywords: Multiobjective optimization, interactive methods, Pareto front visualization, dimensionality reduction, multidimensional scaling.

1 Introduction

Many real-world optimization problems are multiobjective in their nature. Existence of a solution optimizing all objectives simultaneously is unlikely in practice. Solving a multiobjective problem is usually understood as finding a Pareto optimal solution which is the most preferred for a decision maker (DM) [16]. Therefore most of the multiobjective optimization methods rely on preference information obtained from the DM. We concentrate on interactive methods consisting of iterations, where at each iteration the DM provides some preference information and receives solution(s) derived based on this information as feedback [3].

In many interactive methods, a solution obtained at each iteration serves as the starting point for the next iteration. The DM considers this solution and expresses preference information aiming at its improvement. It is useful to allow the DM selecting for consideration the solution obtained not only during the last iteration but any previous iteration. Few interactive methods include this possibility (see e.g. [8, 22]) and to our knowledge, none of the papers describe the selection process in detail. The issue to be addressed here is high cognitive load placed on the
DM when dealing with many-objective problem and a large number of accumulated solutions. Even though the number of iterations in an interactive solution process can be moderate [7], many interactive methods such as Tchebycheff method [33], NIMBUS [22] and others generate several Pareto optimal solutions at each iteration, which makes the solution set grow fast.

In this paper, we address the problem of assisting the DM in selecting one among many Pareto optimal solutions at each iteration of an interactive method in the case of a large number of objectives. We propose to enhance interactive methods with a technique which visualizes a set of the obtained solution outcomes and provides interactive mechanisms of its exploration. This technique is based on multidimensional scaling method [2] which maps the solution outcomes on a plane while trying to preserve distances between them. Despite significant lost of information, such dimensionality reduction creates a holistic view on the outcome set helping the DM to develop a cognitive map. This method has been successfully applied earlier for visualizing solution outcomes in multiobjective evolutionary algorithms [10], but never in interactive methods. Its integration into interactive methods requires some modification for handling inclusion of new solutions into the solution pool.

This paper is organized as follows. In Section 2 we present background information and studies underlying our research, namely basic notions of multiobjective optimization, a general structure of interactive methods and the employed approach to dimensionality reduction. In Section 3 we propose a visualization technique which can be integrated in many interactive methods. In order to demonstrate this technique in action, in Section 4 we integrate it to the interactive method NIMBUS, and use the technique for solving an example problem. Section 5 presents conclusions.

2 Background

2.1 The problem of multiobjective optimization

The multiobjective optimization problem is formulated as follows [16]:

\[
\min_{\mathbf{x} \in S} f(\mathbf{x}),
\]

where \( \mathbf{x} \) is a decision (variable) vector; \( S \subseteq \mathbb{R}^n \) is a set of feasible solutions; \( f(\mathbf{x}) = (f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_k(\mathbf{x}))^T, f_i : \mathbb{R}^n \to \mathbb{R}, i \in \{1, 2, \ldots, k\} \) are objective functions, \( k \geq 2 \).

For each decision vector \( \mathbf{x} \in S \), \( f(\mathbf{x}) \) is called its outcome.

A decision vector \( \mathbf{x}^* \) is called Pareto optimal solution of problem (1) (or Pareto optimum for short), if there does not exist another vector \( \mathbf{x} \in S \) such that \( f_i(\mathbf{x}) \leq f_i(\mathbf{x}^*) \) for all \( i \in \{1, 2, \ldots, k\} \) and \( f_j(\mathbf{x}) < f_j(\mathbf{x}^*) \) for at least one \( j \). The set of Pareto optimal solutions is called Pareto optimal set, and the set of outcomes of all Pareto optimal solutions is called Pareto front.

Solving the problem (1) is commonly understood as finding a Pareto optimum \( \mathbf{x}^* \) whose outcome \( f(\mathbf{x}^*) \) is the most preferred for the DM (see e.g. [3, 16]). Therefore, most of multiobjective optimization methods use preference information provided by the DM. In this paper, we concentrate on interactive methods for they are believed to be most promising methods of multiobjective optimization because of numerous advantages [25]. An important advantage of interactive methods is the possibility for the DM to learn about the problem during the solution process, which makes him/her more confident in the final choice [1].

2.2 Interactive methods

In interactive methods [16, 18], the DM provides preference information progressively during the solution process and obtains Pareto optima derived based on this information as feedback.
Many interactive methods have the underlying idea of exploring the Pareto optimal set by shifting DM’s attention from one solution to another. The notion of *current solution* is introduced as the Pareto optimum considered by the DM in the current iteration. The DM expresses preferences aiming (explicitly or implicitly) at improving the current solution, i.e., finding a more preferred Pareto optimum. A Pareto optimum derived based on these preferences can be considered as the current solution in the next iteration. This process of producing a sequence of Pareto optima can be viewed as moving from one Pareto optimum to another, where preference information determines the direction of movement.

In the case of a cognitively complex model underlying a multiobjective optimization problem, the DM cannot be sure that his/her preference information always leads to a more preferred solution. Besides that, sequential improvement of Pareto optimal solutions based on DM’s preferences cannot guarantee the convergence to the most preferred solution among the whole Pareto optimal set, by analogy with global optimization problems where a series of local improvements of a feasible solution does not necessarily lead to a global optimum. Therefore it is reasonable to give the DM possibility of exploring different parts of the Pareto optimal set by going back to solutions derived earlier and starting moving from them in different directions. This possibility can be implemented by saving all the obtained Pareto optima in the *solution pool* and enabling the DM in each iteration selecting any element of the pool as the current solution for the next iteration. Thus instead of a sequence of Pareto optima one can have a tree where each branch relates to such a move back.

A general structure of interactive methods including the possibility of moving back is described below step-by-step (Algorithm 1).

**Algorithm 1**

**Step 0. Initialize.** Set initial variable values and derive Pareto optimal solution(s) using an initial preference model (based on some initial DM’s preference information or a rule of thumb).

**Step 1. Update.** Add the obtained solution(s) into the pool.

**Step 2. Select.** Ask the DM to select a solution from the pool.

**Step 3. Preference expression.** If the DM regards the selected solution the most preferred, then the method stops with the selected solution as the final one. Otherwise set the selected solution as the current solution of the next iteration and ask the DM to express preferences aiming at its improvement.

**Step 4. Solution derivation.** Build the preference model based on DM’s preference information and derive new Pareto optimal solution(s) using this model. Go to Step 1.

Some authors mention the possibility of selecting the current solution from the solution pool in interactive methods (see e.g., [6, 8, 22, 30]). Many interactive methods can be easily enhanced by adding such possibility and thereby be fit into the structure described above. However to our knowledge, no papers present any details about implementing the procedure of solution selection.

As the size of the solution pool grows, it becomes cognitively more difficult for the DM to keep and operate with it in his/her mind. Indeed, comparing and choosing among a number of objects exceeding the mental capacities obviously leads to mistakes and inconsistencies as illustrated e.g., in [32]. Therefore the DM can benefit from a graphical tool visualizing the solution pool and assisting with solution selection.
2.3 Graphical representation of solution outcomes

It must be noted that most of the multiobjective optimization methods rely on the assumption that the DM compares different solutions and chooses the most preferred one only based on their outcomes. Therefore most of existing visualization techniques (see e.g. [10, 12, 13, 17]) concentrate on presenting the set of the Pareto optimal outcomes in the so-called objective space $\mathbb{R}^k$. Visualizing a set of Pareto optimal outcomes is a non-trivial task in the case $k > 3$. If the solution set is relatively small, then all components of all outcomes can be presented in a diagram such as scatter plot, bar charts, spider-web charts and others (see comprehensive surveys in [9,17]). For bigger solution sets, such representations enforce the DM to deal with abundance of information. Then dimensionality reduction methods can be helpful.

As dimensionality reduction involves loss of information, the problem of extracting information which remains can be approached in different ways depending on the aim the visualization serves. For example, in self-organizing maps [36], artificial neural networks are trained to preserve the topological properties of the input space. Principal component analysis (PCA) [15] tries to preserve variances of data. Interactive decision maps [4,12] are based on two-dimensional projections, they are also used for the visualization of Pareto outcomes.

Multidimensional scaling method (MDS) [2, 5] aims at finding points $v_1, v_2, \ldots, v_m$ in the low-dimensional space $\mathbb{R}^s$, $s < k$, such that the distances between them are as close as possible to the distances between the original points $z_1, z_2, \ldots, z_m$ in the multidimensional space $\mathbb{R}^k$. This is achieved by minimizing the stress function

$$E_{MDS} = \sum_{i<j} \left( d(v_i, v_j) - d(z_i, z_j) \right)^2. \quad (2)$$

Here $d(\cdot, \cdot)$ is the distance between two points in the corresponding space. The procedure of finding points $v_1, v_2, \ldots, v_m$ by minimizing (2) is called mapping. We propose to use MDS for visualizing the solution pool in interactive methods because it detects the similarity between Pareto optimal outcomes, and allows the DM distinguishing areas by how much they have been explored. This helps in focusing the DM’s attention on solutions located in preferred parts of the Pareto front.

When using MDS during an interactive solution process, a problem of mapping new solution outcomes occurs. After adding them to the solution pool and recalculating low-dimensional points by minimizing (2), the points corresponding to already mapped solution outcomes will also change. In order to avoid this changing, so-called relative mapping [27] can be applied, where only coordinates of the newly added points are calculated. The stress function of relative mapping is following:

$$E_R = \sum_{i=1}^{m+n} \left( d(\hat{v}_i, \hat{v}_j) - d(\hat{z}_i, \hat{z}_j) \right)^2 + \sum_{i=m+1}^{m+n} \sum_{j=1}^{m} \left( d(\hat{v}_i, v_j) - d(\hat{z}_i, z_j) \right)^2, \quad (3)$$

where $z_1, z_2, \ldots, z_m$ are the previously mapped multidimensional points and $v_1, v_2, \ldots, v_m$ are their corresponding lower-dimensional points which are fixed, $\hat{v}$ is the number of new points, $\hat{z}_{m+1}, \hat{z}_{m+2}, \ldots, \hat{z}_{m+n}$ and $\hat{v}_{m+1}, \hat{v}_{m+2}, \ldots, \hat{v}_{m+n}$ are the new points and their corresponding lower-dimensional points, respectively.

However, after applying the relative mapping, the value of the stress function $E_{MDS}$ calculated for all the solution outcomes by formula (2) increases, which indicates deterioration of mapping quality. Therefore, after visualizing a large number of the new outcomes using relative mapping, all the mapped points must be recalculated by the MDS method again, i.e. remapping must be performed.
Our previous research was devoted to usage MDS for visualizing the Pareto front in multiobjective evolutionary algorithms [10]. A similar approach was developed in [34] for reviewing the set of obtained Pareto optimal solutions when solving the problem (1). However, the possibility of integrating MDS into interactive methods has not been studied before. In the next section, we describe the proposed visualization technique based on MDS and its integration into interactive methods.

3 Enhancement of interactive methods with visualization

The general structure of interactive methods described in Subsection 2.2 is modified and presented as a scheme in Figure 1. The visualization tool is used in Step 2 for assisting the DM in exploring the solution pool and selecting from it a Pareto optimal solution to be considered as the most preferred solution or the current solution in the next iteration. In order to enable using the visualization, a visual representation of the solution pool is constructed or updated in Step 1. We propose to allow the DM choosing, whether to use the visualization technique or select the solution in a traditional way implemented in the method. Thus, adding the visualization in the method does not imply any additional efforts from the DM. If the DM finds the visualization useless, he/she can ignore it which means that its integration into the method does not deteriorate DM’s experience.

Figure 1: A general enhanced scheme of interactive methods.

The proposed visualization technique consists of mapping of solution outcomes on a plane using the MDS method and interacting with the DM for exploring the outcome set and selecting a solution. Our approach does not depend on the interactive method used, therefore the technique can be implemented for a wide range of interactive methods. We propose to visualize outcomes from the solution pool as a scatter plot of two-dimensional points mapped using the MDS method or relative mapping, that can be implemented in visualization tool (see Figure 1). The following
two operations will be used for constructing and updating this visualization:

- **map all solution outcomes** – given outcomes \( z_1, z_2, \ldots, z_m \) of all Pareto optimal solutions from the solution pool, corresponding two-dimensional points \( v_1, v_2, \ldots, v_m \) are calculated by minimizing the MDS stress function (2) as described in Subsection 2.3. Here \( m \) is the number of solution outcomes, \( z_j \in \mathbb{R}^k \) and \( v_j \in \mathbb{R}^2 \) for all \( j = 1, \ldots, m \).

- **map new solution outcomes** – given outcomes \( z_1, z_2, \ldots, z_m \) of Pareto optimal solutions from the solution pool mapped earlier, their corresponding two-dimensional points \( v_1, v_2, \ldots, v_m \), and the outcomes of newly derived Pareto optimal solutions \( \hat{z}_{m+1}, \hat{z}_{m+2}, \ldots, \hat{z}_{m+\hat{m}} \), the two-dimensional points \( \hat{v}_{m+1}, \hat{v}_{m+2}, \ldots, \hat{v}_{m+\hat{m}} \) corresponding to the new solutions are calculated by minimizing the relative mapping stress function (3) as described in Subsection 2.3.

In order to evaluate similarities between the obtained solution outcomes the MDS method requires several points. Therefore the visualization starts being constructed after a predefined number of solutions \( m \) has been collected in the solution pool. In the case of a small number of solutions, it can be easier for the DM to select one of them by straightforward comparison of the solution outcomes rather than studying the two-dimensional visualization. Therefore we propose to set initial value of \( m \) not smaller than 7.

Once new Pareto optimal solutions are derived in Step 4 (Figure 1) and added to the solution pool, the visual representation is updated in Step 1 either by mapping all solutions or only new solutions. In the first case, the locations of the previously mapped solutions will also change which may distort the cognitive map of the solution pool the DM has developed. On the other hand, mapping only new solutions may affect the accuracy of correspondence between distances in the objective space and two-dimensional space. Therefore, we propose to use a compromise strategy where new solutions are mapped during most of iterations, but the map of all solutions is recalculated on DM’s demand or after accumulation of a large number of new solutions. When the number of the added solutions \( l \) reaches the predefined threshold limit \( m_p \), the map of all Pareto optimal outcomes is recalculated by applying the MDS method again. We propose to set the limit \( m_p = 0.5m \), where \( m \) is the number of outcomes already mapped by MDS. Hence, the higher value \( m \) is, the less frequent remapping by MDS is required. The detailed procedure of constructing the map of the obtained outcomes is presented as Algorithm 2.

**Algorithm 2** Constructing the map of the solution outcomes

**Input:** The solution outcomes \( z_1, \ldots, z_m \), obtained by using an interactive method, where \( m \) is the number of outcomes.

**Output:** The 2D map (scatter plot).

**Step 1:** Set the number of solution outcomes mapped by relative MDS to \( l = 0 \).

**Step 2:** The dimensionality of the solution outcomes \( z_1, \ldots, z_m \) is reduced to 2 by the MDS method, and the two-dimensional points \( v_1, \ldots, v_m \) are displayed in a 2D scatter plot and presented to the DM. Set the value of threshold limit \( m_p = 0.5m \).

**Step 3:** When \( \hat{m} \) new solution outcomes \( \hat{z}_{m+1}, \ldots, \hat{z}_{m+\hat{m}} \) are obtained by the interactive method, two-dimensional points \( \hat{v}_{m+1}, \ldots, \hat{v}_{m+\hat{m}} \) are calculated by the relative mapping, they are added to the 2D scatter plot and we set \( m = m + \hat{m}, \ l = l + \hat{m} \). If the DM is satisfied with the obtained solution, then go to Step 5.

**Step 4:** Check if \( l > m_p \) or the DM wants to remap the solution outcomes. If Yes then go to Step 1, else go to Step 3.

**Step 5:** Stop.
The visualization should be accompanied with graphical tools and interactive mechanisms based on graphical user interface, allowing the DM:

- to see additional information related to the way solution were obtained, e.g. information about the extent at which solutions satisfy preferences based on which they were derived, relations between solutions related to the sequence in which they were obtained;

- to perform operations on visualized outcomes, e.g. hide selected outcomes or outcomes satisfying a given property in order to focus on the most interesting outcomes, recalculate mapping on demand;

- to get full information about the solution corresponding to any selected outcome.

The implementation of the above enhancements of the visualization might depend on the interactive method used as well as the graphical user interface of the method implementation.

4 Example implementation

In this section, we demonstrate the proposed visualization technique by solving an example problem using a popular interactive multiobjective optimization method NIMBUS [16, 19]. It is implemented in the IND-NIMBUS software platform ([28, 29]) designed for solving industrial problems, as well as in a web-based application WWW-NIMBUS available via the Internet [21]. The NIMBUS method has been applied to a number of engineering problems [11, 22, 24].

In the NIMBUS method, new Pareto optimal solutions are derived by solving scalarized problems based on preference information provided by the DM in the form of a classification. In each iteration of this method, the DM considers the current Pareto optimal solution \( x^c \in S \) and corresponding outcome and expresses preferences by classifying the objective functions \( f_i(x^c) \), \( i = 1, 2, \ldots, k \) into up to the five classes related to five types of desirable or acceptable changes of the function values [22]:

- \( I^< \) – to be improved (i.e. decreased) as much as possible;
- \( I^\leq \) – to be improved till some desirable aspiration level \( \bar{z}_i < f_i(x^c) \);
- \( I^= \) – the current function values are acceptable;
- \( I^\geq \) – may be impaired (i.e. increased) till some upper bound \( a_i > f_i(x^c) \);
- \( I^\diamond \) – the function values are allowed to change freely.

This classification must be done in such a way that at least one objective function value should be improved, and at least one is allowed to impair. The classification is used to build scalarizing functions for deriving new Pareto optimal solutions.

In synchronous NIMBUS [22], four different scalarization functions are used in order to present to the DM diverse solutions related to expressed preferences, thereby up to four different solutions can be obtained according the same preference information.

4.1 Numerical example

As an example for demonstrating the proposed visualization technique in use, we chose the five-objective river pollution problem which was implemented in IND-NIMBUS. The problem was originally presented in [26] and modified in [20], where the fifth (nonsmooth) objective function was included. The mathematical formulation of the problem is as follows:
maximize $f_1(x) = 4.07 + 2.27x_1$

maximize $f_2(x) = 2.60 + 0.03x_1 + 0.02x_2 + \frac{0.01}{1.39 - x_1^2} + \frac{0.30}{1.39 - x_2^2}$

maximize $f_3(x) = 8.21 - \frac{0.71}{1.09 - x_1^2}$

minimize $f_4(x) = -0.96 + \frac{0.96}{1.09 - x_2^2}$

minimize $f_5(x) = \max[|x_1 - 0.65|, |x_2 - 0.65|]$

subject to $0.3 \leq x_1, x_2 \leq 1.0$. (4)

It describes a (hypothetical) pollution problem of a river, where a fishery and a city are polluting water. The decision variables $x_1$ and $x_2$ represent the proportional amounts of biochemical oxygen demanding material removed from water in two treatment plants located after the fishery and after the city [23]. Here $f_1$ and $f_2$ describe the quality of water after the fishery and after the city, respectively; $f_3$ and $f_4$ show the percent return on investment at the fishery and the addition to the tax rate in the city, respectively; and $f_5$ describes the functionality of the treatment plants. Hence, the first three objective functions must be maximized, while the fourth and fifth objective functions are to be minimized.

The DM’s strategy and solution process when solving the original four-objective river pollution problem [26] using NIMBUS method was described in [14]. Below we describe the process of solving the problem (4) using synchronous NIMBUS implemented in IND-NIMBUS, where the DM gets additional support from our visualization technique. When addressing multiobjective optimization problems the DM can have different priorities across objectives in mind. Further we assume that the DM has higher priority to improving the quality of the water after the fishery and the city. The solution process described below is divided into several stages according to the DM’s actions related to the usage of the visualization technique:

**Stage 1.** When starting solving the problem by using the IND-NIMBUS, at first a so-called neutral compromise solution is obtained using an initial preference model and presented to the DM. Naturally the DM is not satisfied with the obtained solution, therefore he/she tries to improve it by making several different classifications of the objective functions. During the solution process the DM selects the most preferred solution from the obtained four solutions as the current solution and tries to improve it in the next iteration. This process is repetitive, and the solution pool is constantly updated with the new derived solutions.

**Stage 2.** After a predefined number of the solutions is collected in the solution pool, the visualization technique is started to be used by the DM (see Figure 2a). Here the points of the map correspond to the obtained solution outcomes. We omit drawing axes of the two-dimensional coordinate system due to the fact that the coordinates do not have individual meaning, as the only important aspect of mapping is preserving distance between points. The points of the scatter plot are coloured using RdYlGn colour scheme, where colour of each mapped point represents its distance to the reference point that express the current DM’s preferences (red colour corresponds to large distance, green – to small distance). The numbers near the points mean the order in which the corresponding solutions were obtained. The presented map of obtained outcomes is constructed by using the MDS method, when the 8th solution has been selected as the current one. Now the DM can explore the map, see the relations between the outcomes and think about the further directions of the solution process. It can be noticed from the map that the 10th solution is located furthest from the area of the objective space where the DM started the solution process. As the DM wants to explore the objective space in direction further away from first solution, he decides to select the 10th solution as the current one.
Stage 3. The DM tries to improve the 10th solution by using a different classification of objective functions. Then the solution pool is updated by new outcomes and they are added to the map by using the relative mapping (see Figure 2b). The points mapped using MDS have circular shape while the new points are presented as squares. Here the graph of the solution process is also displayed (the arrows are drawn between the points corresponding to obtained outcomes which once served as current solutions). The location of new points confirms that the selection of 10th solution as the current solution and provision of the preference information allowed the DM to advance in exploring the objective space, e.g. obtain Pareto optimal solutions which demonstrate bigger differences from earlier obtained solutions. Afterwards, the DM wants to remap all the obtained outcomes by MDS in order to see relations between them more precisely, and the updated map is presented (see Figure 2c). After remapping, the places of the points on the map have been changed slightly comparing with the previous ones, which does not affect the cognitive map developed in the DM’s mind. However, after remapping the furthest location of 15th solution outcome from earlier solutions is more expressed. Here the arrows are drawn between all the solutions from the solution pool in sequence order in which the solutions were obtained (see Figure 2c). Next, the DM can select other solution from the solution pool as the current solution for further improvement, change the solution strategy by giving higher priority to other objectives, and search for more preferable solutions in unexplored parts of the decision space with the support of the MDS-based visualization technique, or using only the original IND-NIMBUS user interface. Hence, the obtained map helps the DM to keep in mind a holistic image of the current state of the solution pool, as well as the history of the solution process.

It must be pointed out that the purpose of this example is not to describe the whole solution process of the problem, but to demonstrate the performance and flexibility of the proposed visualization technique. Hence, the three presented stages cover the main aspects of its usage during the solution process.

5 Conclusions

The core idea of interactive methods is using a Pareto optimum derived during each iteration (so-called current solution) as the starting point for the next iteration. The possibility of selecting Pareto optima derived in any of previous iterations as the current solution contributes to the flexibility and freedom of Pareto optimal set exploration. This aspect of implementing interactive methods has not received any attention in the literature.
In this paper we have proposed to enhance interactive methods with a technique visualizing the outcomes from the solution pool and assisting the DM in its exploration and solution selection. The resulting visualization is presented in the form of an interactive 2D scatter plot obtained using MDS method, which helps the DM to detect similarity between outcomes and focus on more preferred parts of the Pareto front. This visualization facilitates the DM in developing a cognitive map of the set of solution outcomes. We have described an general approach of creating and integrating the visualization into interactive methods, and also illustrated it with a simple example. However the visualization should be implemented using a graphical user interface and, depending on the method, enhanced with graphical and interactive elements improving DM’s experience.

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