A Systematic Way of Structuring Real-World Multiobjective Optimization Problems

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Abstract. In recent decades, the benefits of applying multiobjective optimization (MOO) methods in real-world applications have rapidly increased. The MOO literature mostly focuses on problem-solving, typically assuming the problem has already been correctly formulated. The necessity of verifying the MOO problem and the potential impacts of having an incorrect problem formulation on the optimization results are not emphasized enough in the literature. However, verification is crucial since the optimization results will not be meaningful without an accurate problem formulation, not to mention the resources spent in the optimization process being wasted.

In this paper, we focus on the MOO problem structuring, which we believe deserves more attention. The novel contribution is the proposed systematic way of structuring MOO problems that leverages problem structuring approaches from the literature on multiple criteria decision analysis (MCDA). They are not directly applicable to the formulation of MOO problems since the objective functions in the MOO problem depend on decision variables and constraint functions, whereas MCDA problems have a given set of solution alternatives characterized by criterion values. Therefore, we propose to elicit expert knowledge to identify decision variables and constraint functions, in addition to the objective functions, to construct a MOO problem appropriately. Our approach also enables the verification and validation of the problem before the actual decision making process.

Keywords: Problem structuring · MOO problem formulation · Eliciting expert knowledge · Identifying objectives · Decision making · Stakeholder interviews.

1 Introduction

The concept of optimization refers to making the best use of a given situation and resources. In particular, optimization is the process of determining the values of decision variables to optimize (minimize or maximize) the values of objective functions since, in real-world problems, we are typically faced with multiple conflicting objective functions, such as decreasing expenses and maximizing profit.

Such problems are known as *multiobjective optimization (MOO) problems*, and they involve two or more conflicting objective functions that must be minimized or maximized simultaneously. Typically, several compromise solutions with varying tradeoffs exist, and the preference information of a decision maker (DM), who is an expert in the problem domain, is required to identify the most preferred solution [37].

A MOO problem typically consists of three main components [41]: *Objective functions* define the mathematical representations of aspects what characterize the goodness of the decision to be made. *Decision variables* represent the choices that must be made. *Constraint functions (constraints)* are, e.g., (in)equality constraints or lower and upper bounds that limit the values of the decision variables. Real-world problems may have many objective functions, decision variables, and constraints. Identifying all these components at once may be difficult for a DM or an analyst (who is an expert in modeling MOO problems and can apply optimization methods to solve MOO problems). Based on experiences (e.g., [13, 23, 44]), several iterations are often needed in which the optimization is performed based on some initial versions of the MOO problem, and some objective functions, decision variables, and (or) constraints are eliminated or modified, or new ones added based on the initial results. Furthermore, some objective functions may sometimes be converted to constraints or vice versa. In this paper, we consider deterministic MOO problems.

For real-world MOO problems, the problem formulation is essential, where the three components mentioned above are to be identified. However, the importance of problem formulation is often neglected in the literature [28] while the focus is on developing methods for solving MOO problems, assuming that the problem has already been formulated. Often, benchmark problems are used to demonstrate the use of the proposed methods. Accordingly, most studies lack information on how the problems have been formulated, i.e., without sufficient information on how the functions involved and decision variables have been identified.

Multiple criteria decision analysis (MCDA) is a sub-discipline of operation research that facilitates the systematic evaluation of alternatives in terms of multiple, conflicting criteria (e.g., [7, 31]). The criteria in MCDA and the objective functions in MOO problems basically mean the same. In practice, however, the problems are very different since alternatives in MCDA are explicitly given, while in MOO, they are implicitly described with objective functions and decision variables. Thus, the approaches developed to structure MCDA problems are not directly applicable to formulating MOO problems.

Modeling an accurate and adequate MOO problem may need many brainstorming sessions between domain experts (whom we here refer to as DMs or stakeholders even though there may be many domain experts involved in the problem formulation) and the analyst. In some cases, it can take a lot of time to formulate an appropriate MOO problem. For example, it is mentioned in [13] that three iterations with different problem formulations were needed to meet the needs of a shape optimization problem in an air intake ventilation system of a tractor cabin. Among other changes, the number of objective functions varied. Besides, some objective functions may be first incorrectly formulated (e.g., [23, 44]). Thus, having a verified and validated MOO problem is crucial, as it directly affects the decision. In other words, a poorly formulated MOO problem may result in erroneous or misleading solutions.

In this paper, we propose a generic systematic way of structuring deterministic real-world MOO problems. Our systematic approach consists of a four-step methodology, with each step showing the corresponding methods and tools for obtaining a verified and validated MOO problem prior to solving it (i.e., conducting the real decision making process). We begin by eliciting the DM's knowledge to identify the decisions that must be made and the objectives that must be met. Importantly, we list explicit questions to be asked in structuring the problem. We then verify and validate the MOO problem after constructing it based on the identified objective functions, decision variables, and constraints. This process is iterative, where the DM and the analyst are involved.

The remainder of this paper is organized as follows: In Section 2, we introduce the basic concepts and provide a brief literature review. Section 3 is devoted to the proposed systematic way of structuring real-world optimization problems. We discuss the possible ways of analyzing the qualitative data gathered through stakeholder interviews and mention the limitations of applying the proposed approach in different application domains in Section 4. Finally, we draw conclusions in Section 5.

2 Background

In this section, we present the basic concepts required to understand the proposed systematic way of structuring MOO problems. In addition, we provide a brief literature review to demonstrate the gap in the literature as well as the differences in problem structuring for the MOO and MCDA problems.

2.1 Basic concepts

In real-world applications, we may have different ways to evaluate the identified objectives. An *analytical objective* function can be described analytically by a mathematical expression and is evaluated by solving the mathematical function formulation. However, this is not always possible in real-world applications, where the objective function may not be known or cannot be represented as a mathematical function [28]. In this case, the collected data (e.g., from physical experiments or from past performance) can be used to formulate objective functions, and we refer to them as *data-driven objective* function. On the other hand, some objectives are evaluated using computer simulations, called *simulation-based objective* functions. This means that the output of a simulator is needed for objective function evaluation. In what follows, we use the shorter term *objectives* instead of objective functions (and the same for constraints).

As previously stated, a MOO problem involves a set of conflicting objectives (to be minimized or maximized) as characteristics of a good decision that the DM wants to make. A set of feasible solutions can be generated by a set of decision variable values in the feasible region, subject to constraints. Constraints are the conditions that should be satisfied and can be represented by mathematical functions. Sometimes, the values of the decision variables are also limited by lower and upper values, known as boundary constraints. A solution is called feasible if it satisfies the constraints. Typically, no solution exists to optimize all objectives simultaneously. Instead, we have so-called *Pareto optimal* solutions [37]. A feasible solution is called Pareto optimal if it is not *dominated* by any other feasible solution, i.e., improving any objective value always implies sacrificing in at least one of the others. Thus, there are tradeoffs among the objectives. Pareto optimal solutions are mathematically incomparable, and to identify the *most preferred solution* as the final decision, we need preference information of a DM. By a solution (decision making) process, we mean finding the most preferred solution.

MOO methods can be divided into three classes based on when preference information is incorporated in the decision making process [26, 37]. In *a priori* methods, the DM first provides preference information before the optimization, and solutions reflecting the DM's preferences are generated. On the other hand, in *a posteriori* methods, a representative set of Pareto optimal solutions is generated first, and then the preference information of the DM is used to select the most preferred one among them. Finally, in *interactive* methods, the DM provides preference information iteratively to direct the solution process and to obtain specific Pareto optimal solutions that reflect their preference information. Interactive methods are useful because they allow the DM to participate in the decision making process iteratively while also learning about tradeoffs among the objectives and available solutions, as well as the feasibility of the preferences [38].

2.2 Brief literature review

Structuring MCDA problems is a well-studied research field. Similar to MOO problem formulation, identifying criteria is an important phase, as different sets of criteria result in different decisions [11]. In problem structuring, analysts (often called facilitators in MCDA) ask DMs to list their criteria. On the other hand, this is often considered *more of an art than a science* [29]. While many MCDA studies have assumed that a well-structured problem is available [8], in the late 1990s, Keeney's work on value-focused thinking emphasized the need for effective problem structuring [30]. Accordingly, the general problem structuring methods presented for rational analysis [42] were integrated with MCDA (e.g., [3, 6, 17]).

Furthermore, experimental studies were conducted to structure MCDA problems in practice (see, e.g., [8, 20], and the survey [36] and references therein). For meaningful analysis, identifying key and fundamental criteria instead of having a large set of criteria was emphasized in [35], and the characteristics of good criteria including, e.g., completeness, conciseness, non-redundancy, understandability, measurability and preferential independence, were listed. Moreover, some recent studies used online surveys to elicit criteria from a large number of individuals without the assistance of an analyst (or facilitator) (see, e.g., [2, 22]).

The proposed methods (e.g., in [36] and references therein) first ask stakeholders to state criteria in the domain in brainstorming sessions. Then, a facilitator shows a master list (pre-generated set of criteria) and asks stakeholders to select and match some of the criteria in the master list with their stated criteria. Finally, they select the final set of criteria from the self-generated criteria in addition to the recognized ones from the master list. To apply this kind of method, we need at least a master list which may not be the case for a new problem domain. How to create a list of criteria from scratch is still an open research question.

A few real-world studies focusing on MOO problem formulation have been published. The authors of [48] proposed a holistic approach allowing the reformulation of the constructed initial optimization problem by adding or removing objectives and (or) decision variables. Their approach was applied to a complex real-world problem for the conceptual design of indoor sports buildings. They utilized simulators in building design, and the objectives were identified according to the output data of the simulators. Similarly, in [47], the objectives of the MOO problem were identified for chemical processes by utilizing the available data, and machine learning model(s) for some or all objectives are fitted whenever applicable.

In [24], several (semi)structured interviews with stakeholders were used to formulate a preliminary design problem of wood-based insulating materials. In [5], the same method was applied in formulating the MOO problem of microfiltration of skim milk. Unfortunately, the complete set of questions used in stakeholder interviews was not shared. Thus, published studies in the MOO literature lack information on how the MOO problem was formulated through stakeholder interviews. To advance research in structuring MOO problems, the procedures must be fully published and reported in detail in order to increase reliability and reproducibility so that others can utilize them in other application domains.

3 Systematic Way of Structuring MOO Problems

We propose a generic systematic way of structuring MOO problems, which is not application-specific. With the proposed approach, one can identify the components of MOO problems through structured interviews with stakeholders and then construct the MOO problem by utilizing the existing knowledge in the domain. Since ensuring the correctness of the MOO problem at once is not easy, especially for large-scale problems, i.e., with many objectives and decision variables, we propose an iterative process that is repeated until the MOO problem is verified and validated. In what follows, we first present the main steps in general and then provide further details for each step. Overall, the main steps of the proposed systematic approach are the following:

- **Step 1:** Identify components of the MOO problem (objectives, decision variables, and constraints) through stakeholder interviews.
- **Step 2:** Construct the MOO problem. (It should be noted that some constraints can also be constructed using the options indicated below.)
  - **Analytical objectives:** Formulate the mathematical functions representing the objectives.
  - **Data-driven objectives:** Construct surrogate models based on the data available to derive data-driven objectives.
  - **Simulation-based objectives:** Configure the simulator using identified components of the MOO problem. Basically, the input of the simulator is decision variables, and simulation results are used to evaluate objectives.
- **Step 3:** Verify the (overall) applicability of the MOO problem via a preliminary assessment by the analyst. (The analyst generates random points in the feasible region for the decision variables, evaluates objectives and constraints, and checks the generated results.) If verification fails, go to Step 2.
- **Step 4:** Validate the MOO problem until the DM is convinced of the correctness of the MOO problem. (The analyst generates nondominated solutions via some selected (a posteriori) MOO methods and presents them to the DM. The analyst then asks if the tradeoffs among the objectives are clear and meaningful.) If the validation fails, go to Step 2. Otherwise, terminate the process.

In what follows, we discuss each step of the proposed approach. For **Step 1**, we propose a list of interview questions in Table 1 to be used in the structured interviews with the domain experts (or stakeholders) to identify the objectives, decision variables, and constraints. We cannot ask for these details directly (it would be highly difficult to verbalize and define the problem to be solved straight as objectives, decision variables, and constraints), but we need to elicit the knowledge of domain experts and understand their needs and requirements. The key aim is to understand the decision to be made and the data availability. Typically, analysts ask casual (informal) questions to domain experts and try to formulate the MOO problem based on their understanding. However, this process is up to the analysts' capabilities and the way they ask questions. We, therefore, propose a systematic and comprehensive list of interview questions. We have selected some of the questions proposed in [30] and added some new ones to obtain information for decision variables and constraints (they are not considered in structuring MCDA problems). The interview questions first aim to get a general overview and understanding of the problem and then seek to formulate the problem technically. For example, the decision to be made is an abstract thought at a general level at the beginning; on the other hand, decision variables try to capture the decision to be made at a technical level.

Step 1 starts with a round of interviews. First, we propose to apply these interview questions to each stakeholder individually to ensure that each stakeholder's perspectives are considered in structuring the problem. The interview method utilized can vary if changes to the order of the questions are to be made

Table 1. Proposed list of interview questions to be used in stakeholder interviews. Note: Questions written in italics are from [30].

Aim	**Questions**
A wish list	*What do you want? What do you value? What should you want?*
Decisions	What is the nature of the decision you must make? What kind of actions are to be taken?
Available information	What information is needed for you to take the decision? How do you get that information? What kind of data is available?
Goals	What perspectives characterize the goodness of your decision? *What are your aspirations?*
Strategic objectives	*What are your ultimate objectives? What are your values that are fundamental?*
Generic objectives	*What environmental, social, economic or safety objectives are important?*
Structuring objectives	*Why is that objective important? How can you achieve it? What do you mean by this objective?*
Quantification of objectives	*How would you measure achievement of an objective?*
Decision variables	How can these objectives be accomplished? What kind of information do you need to evaluate your objectives? What factors/variables affect your objective values?
Structuring decision variables	Which decision variables influence which objectives?
Constraints	What are the limiting factors of your objectives and (or) decision variables? Are there any lower and (or) upper bounds for decision variables?

to be able to elicit the required expert knowledge. If the question list is utilized in the depicted order, a method of a structured interview can be used (e.g., [21]). The output lists problem characteristics from each stakeholder's point of view once the qualitative data (responses given to the interview questions) are analyzed. The interview data needs to be transcribed into the textual format and can be analyzed with various analysis methods depending on the context of the study, such as with conventional, directed, or summative qualitative content analysis [25] or with thematic analysis, e.g., [10]. We then propose to have a joint workshop, including all the stakeholders, to adjust and finalize the components of the MOO problem.

In **Step 2**, the analyst constructs the MOO problem utilizing the output of Step 1. According to the responses given to the question of available information, the analyst can understand which objectives and constraints have to be modeled based on 1) mathematical function formulations, 2) the available data, or 3) calling a simulator. For the first option, 1), the analyst writes a piece of programming code that represents the mathematical function. In the second option, 2), if we have data originating from the problem domain for some objectives and constraints, the analyst constructs surrogate models based on the data available. In this, the analyst first pre-processes the data since it can be incomplete, noisy, and heterogeneous [28] and then needs to select the best-suited surrogate model based on their previous experiences. Another option is to apply an automatic surrogate model selector (e.g., [43]) on the available data. In [43], the authors use the data from known optimization problems to train several surrogate models (e.g., polynomials [34], neural networks [4], radial basis functions [12], support vector machines [45] and stochastic models such as Kriging [33] or Bayesian modeling [46]) and extract features from the trained surrogate models. These features are then used to identify the best surrogate modeling technique for a given new data set. If some of the objectives and constraints are to be evaluated based on the output of a simulator, 3), the analyst may set up the simulator based on the identified components for the objective and constraint in question, which may involve pre- and post-processing. Pre-processing is needed to configure the input of the simulator using the decision variables, while post-processing is necessary to evaluate the corresponding objective and constraint values from the output of the simulator.

Step 3 is applied to technically verify the MOO problem before solving it. First, the analyst generates random decision variable values (e.g., uniform random distribution or normal distribution with some mean and standard deviation in the feasible region) and evaluates and checks the feasibility of objectives and generated results to verify the MOO problem. Here, a MOO problem is said to be verified if the MOO problem is correctly programmed, different types of objectives and constraints (e.g., analytical, data-based, or simulator-based) are appropriately constructed, and generated results are meaningful considering the given input values. If this step fails, the analyst goes to Step 2, checks the details of the MOO problem to see whether there is an error, and fixes errors (e.g., the code is corrected or the post-processing of the simulator is restored). This process terminates when the MOO problem appears to be constructed correctly to the best knowledge of the analyst.

Finally, in **Step 4**, the analyst generates a set of nondominated solutions using some optimization methods (e.g., a posteriori evolutionary MOO methods [14, 28]) and presents these solutions to the DM. The DM can select some solutions to study the tradeoffs among the objectives. A MOO problem is said to be validated if the tradeoffs among the objectives are meaningful. If the DM is not happy with the generated solutions, the DM can decide to ask the analyst to revisit the constructed MOO problem. If any error is found, the analyst fixes the MOO problem formulation. Furthermore, if the DM so desires, the analyst converts some objectives into constraints (or vice versa). The analyst then generates new nondominated solutions using the revisited MOO problem. Besides validating the MOO problem, the analyst can also study the time spent in generating nondominated solutions. If the MOO problem is computationally demanding, computationally inexpensive surrogate models can be used to replace expensive (objective or constraint) functions. This process continues until the DM is happy with the generated solutions and sure about the correctness of the solutions to the best of their knowledge.

Once these steps in the proposed systematic approach are carried out successfully, we have a verified and validated MOO problem, which can be trusted and used in the actual decision making process. After this, the analyst and the DM can decide which type of method is applied to solve the problem. They can apply, e.g., any interactive multiobjective optimization method [39], including interactive evolutionary ones [27] if the DM wants to direct the solution process with one's preference information.

One can also apply interactive methods as a part of the verification process as proposed in [44]. There, a so-called augmented interactive MOO method is introduced, which incorporates verification and solution processes.

4 Discussion

The results of the qualitative content analysis based on the listed interview questions can be further considered to be analyzed with different method combinations to support the structuring of the problem. One possibility is to utilize cognitive mapping and causal maps. Next, we discuss the logic and main benefits of these kinds of approaches.

After obtaining results from the stakeholder interview transcripts with a chosen qualitative content analysis method, the results (commonly in the form of descriptive categories with sub-categories) can be further elaborated with causal maps for the group discussion (negotiation) purposes to enable understandability and fluency within the group in structuring the MOO problem. Causal maps are efficient in structuring problems as they enable rich representation of ideas modeled as exhaustive networks of argument chains [40]. A causal map can be constructed with the aid of an analyst (or a facilitator) directly from the negotiation process. However, for a detailed understanding of the problem and its reliable formulation, a more in-depth data collection and analysis method combination can be used [16]. As causal maps are often constructed in a group setting, they can precede the procedure of cognitive mapping and construction of individual cognitive maps [15]. A cognitive map is a representation of thoughts of a problem that is derived from the process of cognitive mapping (i.e., mapping an individual's thinking structure and contents about a problem [15]). Cognitive mapping is based on Kelly's personal construct theory [32] (for instructions on how to conduct cognitive mapping, see [1]). Usually, cognitive maps are based on interview data [15] and are presented as networks of nodes and arrows indicating relations represented by an individual.

Thus, the whole procedure of formulating MOO problems could benefit from utilizing a combination of research methods, for example, from interviews to different mappings. The starting point of the problem structuring procedure is beneficial to be based on eliciting expert knowledge of the problem domain through verbalizations to gain a reliable understanding of the phenomenon under investigation. Often this is done via expert interviews (see, e.g., [9]). In addition, thinking-aloud protocols are an efficient way of eliciting expert knowledge through verbalizations [18, 19], from which cognitive maps can be created for further problem formulation. Also, from interview data, cognitive maps can be created via cognitive mapping from each interviewee separately and then via integration into an initial group map to be elaborated as a causal map in a group discussion, searching for a consensus for structuring the problem.

The applicability of the proposed approach in different application domains depends on the resources dedicated to the problem structuring. We assume that the stakeholders are convinced that having a verified and validated MOO problem to get reliable results is more important than merely solving the problems based on unstructured foundations that might not reflect the problem in real-life. However, since the main foundation of the proposed approach is getting the experts' knowledge to identify the components of the MOO problem, it is limited by the experts' reliability and willingness to participate in different steps. In addition, analysts lacking enough knowledge of qualitative data analysis (e.g., in compiling cognitive maps) may be another challenge to applying the proposed approach.

5 Conclusions

We have observed that structuring a MOO problem has not been studied enough in the literature. In this paper, we have proposed a systematic way of structuring verified and validated MOO problems. The proposed approach identifies which objectives to optimize and how decision variables and constraints affect each objective. We first identify the objectives, decision variables, and constraints of a MOO problem through structured stakeholder interviews. To support this interview in a concrete manner, we have proposed a list of interview questions. In the second step, the analyst constructs the MOO problem utilizing the results of the qualitative analysis of the interview responses. We have also proposed possible qualitative content analysis methods to be utilized as well as further analysis methods of cognitive mapping and causal maps to structure the problem based on the interview data. Third, the analyst verifies the MOO problem with randomly generated values for decision variables. Finally, the DM validates the MOO problem by studying some generated solutions with the help of the analyst. This is an iterative process. In this way, the DM gains enough confidence in the formulated MOO problem as it is verified and validated.

This paper is aimed at supporting the task of structuring MOO problems. Our approach covers all aspects of constructing MOO problems, from identifying components to modeling and testing before the actual solution process. We have presented our approach in a general manner, and it can be applied in any real application domain. Because of space limitations, we could not consider an example to apply the proposed approach. However, we plan future studies on applying it in different case studies to demonstrate its applicability.

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