Report from Dagstuhl Seminar 15031

Understanding Complexity in Multiobjective Optimization

Edited by

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Abstract

This report documents the program and outcomes of the Dagstuhl Seminar 15031 Understanding Complexity in Multiobjective Optimization. This seminar carried on the series of four previous Dagstuhl Seminars (04461, 06501, 09041 and 12041) that were focused on Multiobjective Optimization, and strengthening the links between the Evolutionary Multiobjective Optimization (EMO) and Multiple Criteria Decision Making (MCDM) communities. The purpose of the seminar was to bring together researchers from the two communities to take part in a wide-ranging discussion about the different sources and impacts of complexity in multiobjective optimization. The outcome was a clarified viewpoint of complexity in the various facets of multiobjective optimization, leading to several research initiatives with innovative approaches for coping with complexity.

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1 Executive Summary

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Understanding complexity in multiobjective optimization is of central importance for the two communities, MCDM and EMO, and several related disciplines. It enables us to wield existing methodologies with greater knowledge, control and effect, and should, more importantly, provide the foundations and impetus for the development of new, principled methods, in this area.

We believe that a strong route to further progress in multiobjective optimization is a determination to understand more about the various ways that complexity manifests itself in multiobjective optimization. We observe that in several fields, ranging from engineering to medicine to economics to homeland security, real-world problems are very often characterized by a high degree of complexity deriving from the presence of many competitive objectives to be optimized, many stakeholders expressing conflicting interests and the presence of many technical parameters being unstable in time and for which we have imperfect knowledge. These very complex problems require a specific methodology, mainly based on multiobjective optimization, that, using high computational capacities, takes into account robustness concerns and allows an effective participation of the several stakeholders in the decision process.

The seminar took place January 11th–16th 2015. The main goals of the seminar were the exploration and elucidation of complexity in three fundamental domains:

Focus 1: Complexity in preference

This topic is mainly concerned with elicitation, representation and exploitation of the preference of one or more users, for example: discovering and building preferences that are dynamic and unstable, group preference, complex structure of criteria,non-standard preferences, learning in multiobjective optimization.

Focus 2: Complexity in optimization

This topic is mainly concerned with the generation of alternative candidate solutions, given some set of objective functions and feasible space. The following topics are examples for the wide range of issues in this context: high-dimensional problems, complex optimization problems, simulation-based optimization and expensive functions, uncertainty and robustness, interrelating decision and objective space information.

Focus 3: Complexity in applications

An all-embracing goal is to achieve a better understanding of complexity in practical problems. Many fields in the Social Sciences, Economics, Engineering Sciences are relevant: E-government, Finance, Environmental Assessment, E-commerce, Public Policy Evaluation, Risk Management and Security issues are among the possible application areas.

During the seminar the program was updated on a daily basis to maintain flexibility in balancing time slots for talks, discussions, and working groups. The working groups were established on the first day in highly interactive fashion: at first each participant was requested to write her/his favorite topic on the black board, before a kind of collaborative clustering process was applied for forming the initial five working groups, some of them splitting into subgroups later. Participants were allowed to change working groups during the week, but the teams remained fairly stable throughout. Abstracts of the talks and extended abstracts of the working groups can be found in subsequent chapters of this report.

Further notable events during the week included: (i) a session devoted to discuss the results and the perspectives of this series of seminars after ten years of the first one, (ii) a hike within a time slot with worst weather conditions during the week, (iii) a presentation session allowing us to share details of upcoming events in our research community, and (iv) a wine and cheese party made possible by a donation of UCL's *EPSRC Centre for Innovative Manufacturing in Emergent Macromolecular Therapies* represented by Richard Allmendinger.

Outcomes

The outcomes of each of the working groups can be seen in the sequel. Extended versions of their findings will be submitted to a Special Issue on "Understanding Complexity in Multiobjective Optimization" in the *Journal of Multi-Criteria Decision Analysis* guest-edited by the organizers of this Dagstuhl seminar.

This seminar resulted in a very insightful, productive and enjoyable week. It has already led to first new results and formed new cooperation, research teams and topics. In general, the relations between the EMO and MCDM community were further strengthened after this seminar and we can expect that thanks to the seminar a greater and greater interaction will be developed in the next few years.

Acknowledgements. Many thanks to the Dagstuhl office and its helpful and patient staff; huge thanks to the organizers of the previous seminars in the series for setting us up for success; and thanks to all the participants, who worked hard and were amiable company all week. In the appendix, we also give special thanks to Salvatore Greco as he steps down from the organizer role.

2 Table of Contents

3 Overview of Talks

3.1 Preference learning in EMO: Complexity of preference models

Jürgen Branke (University of Warwick, GB), Salvatore Corrente (Università di Catania, IT), Salvatore Greco (Università di Catania, IT), Roman Słowiński (Poznan University of Technology, PL), and Piotr Zielniewicz (Poznan University of Technology, PL)

Joint work of Branke, Jürgen; Corrente, Salvatore; Greco, Salvatore; Słowiński, Roman; Zielniewicz, Piotr
Main reference J. Branke, S. Corrente, S. Greco, R. Słowiński, P. Zielniewicz, "Using Choquet Integral as Preference Model in Interactive Evolutionary Multiobjective Optimization," WBS Working Papers, Warwick Business School, 2014.
URL http://wrap.warwick.ac.uk/64234/

When learning user preferences from user interactions, one usually has to make a decision on the nature of the preference model to be learned. There is a trade-off: if the preference model is too simplistic (say, linear), it is unlikely to be able to represent perfectly the user's preferences expressed in interactions. On the other hand, if the preference model is too versatile, a lot of preference information is required from the user to narrow down the model's parameters to a useful degree, i.e., such that the preference relation implied by the model is sufficiently richer than the dominance relation. In this talk, we will survey the literature on preference learning in EMO with a special focus on the complexity of the preference model used. We will then move on to some of our recent work where the complexity of the preference model is increased adaptively.

3.2 Computational Complexity in Multi-objective (Combinatorial) Optimisation

Matthias Ehrgott (Lancaster University, GB)

In combinatorial optimisation, the study of worst case complexity of problems is very important. Researchers have also considered the worst case complexity of multi-objective versions of combinatorial optimisation problems. Most results are thoroughly unexciting and negative: MOCO problems have been shown to be NP-hard (their decision versions), #P-hard (the related counting versions, and to have exponentially many efficient solutions and non-dominated points. This is true for multi-objective versions of very easy polynomially solvable, even trivial, single objective combinatorial optimisation problems. This begs the question whether worst case complexity in the standard sense is the right framework for discussing complexity of MOCO problems. On the other hand, recent results in multi-objective linear programming show the theoretical (but far from practical) polynomial solvability of MOLP, and the possibility of computing non-dominated extreme points in MOLP with polynomial delay. Is polynomial delay a better framework and the best one can hope for? Maybe for specific instances? Is there any hope for any polynomiality results? This brief presentation is intended to encourage discussion of these issues which have been largely ignored in multi-objective optimisation to date.

3.3 Variable ordering structures – what can be assumed?

Gabriele Eichfelder (TU Ilmenau, DE)

Main reference G. Eichfelder, "Variable Ordering Structures in Vector Optimization," Springer, 2014.
URL http://www.springer.com/mathematics/book/978-3-642-54282-4

In some real-world applications in multi-objective optimization it cannot be assumed that there is a partial ordering in the image space, i.e. that there exists a binary relation which is reflexive, transitive and compatible with the linear structure of the space. Instead, preferences may vary depending on the current information. This can be modeled by an ordering map which associates sets of improving (or deteriorating) directions with each element of the image space or of the pre-image space. Depending on the point of view (i.e. preference or domination) different optimality concepts are discussed in the literature. In this talk we give some motivating applications and a basic introduction to this topic. We present the various ways given in the literature to model a variable ordering structure and the different optimality concepts which are derived. We collect some basic properties which are often assumed for obtaining theoretical and numerical results. Limitations of the current concepts are also pointed out. This talk aims to be the base for a discussion on how variable ordering structures can be modeled, which assumptions on an ordering map seem to be reasonable, and which optimality concepts are considered to be most practically relevant.

3.4 An Open Problems Project for Set Oriented and Indicator-Based Multicriteria Optimization

Michael Emmerich (Leiden University, NL)

Main reference SIMCO – Open problems webpage
URL http://simco.gforge.inria.fr/doku.php?id=openproblems

In September 2013 the 'Set-oriented and Indicator Based Multicriteria Optimization Open Problems Project' (SIMCO-OPP) was launched during the Lorentz Center Workshop on Multicriteria Optimization in Leiden University, The Netherlands, in order to collect exact results on algorithms and open questions in indicator based multi-criteria optimization. The SIMCO-OP Project maintains a collection of registered positive (exact) results and questions related to problems such as multi-criteria sorting and searching, computation of multi-criteria performance indicators, gradient computations, convergence times of problem-algorithm pairs, and optimal subset computation problems. Computational complexity results are a major theme and state-of-the-art results for the known computational complexity bounds for a large number of problems are maintained.

In our talk, which is related to the topic 'complexity in optimization', an overview of the SIMCO-OP Project will be given, including a brief introduction to its scope and the structure of result records in the repository. The aim is to invite participants to use the repository and to contribute to it by, for instance, registering new published results that they find or that come to their attention. The presentation will also highlight selected open problems on computational complexity of algorithms in multicriteria optimization.

3.5 Pareto-front approximation statistics

Carlos M. Fonseca (University of Coimbra, PT)

Joint work of Fonseca, Carlos M.; Grunert da Fonseca, Viviane; Guerreiro, Andreia P.; López-Ibáñez, Manuel; Paquete, Luis

In this talk, the variation of Pareto-front approximations across multiple multiobjective optimisation runs is considered from a statistical point of view. The attainment function methodology [1] is briefly described as a means of capturing important aspects of algorithm behaviour, such as location, variability, and dependence, through the estimation of the moments of the set-distribution of the corresponding outcome approximation sets. Complexity issues [2] concerning the computation, visualisation, and size of the moment estimates, as the number of objectives, number of runs, and size of the approximations grow are highlighted.

Acknowledgments. This work was partially supported by iCIS (CENTRO-07-ST24-FEDER-002003).

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2 C. M. Fonseca, A. P. Guerreiro, M. López-Ibáñez, and L. Paquete. On the computation of the empirical attainment function. In *Evolutionary Multi-Criterion Optimization. 6th Int'l Conf., EMO 2011* (R. H. C. Takahashi, K. Deb, E. F. Wanner, and S. Greco, eds.), vol. 6576 of *LNCS*, pp. 106–120, Springer, 2011.

3.6 Complex combinatorial problems with heterogeneous objectives

Andrzej Jaszkiewicz (Poznan University of Technology, PL)

An important source of complexity in multiobjective combinatorial optimization that is often overlooked are heterogeneous objectives. By heterogeneous we understand objectives that differ from the point of view optimization, i.e. the tasks of single objective optimization of particular objectives differ significantly.

The objectives may differ by difficulty in optimization. They may of different difficulty from computational complexity point of view, e.g. optimization of some objectives may correspond to simple problem while optimization of other objectives may correspond to NP-hard problems. Probably even more common are differences in practical difficulty, i.e. optimization of some objectives may require much more or less steps of an evolutionary or more generally metaheuristic algorithm. Differences in difficulty may result from different mathematical form of the objective functions, but even if the mathematical form is the same, different objectives may correspond to instances of different difficulty. For example for classical CO problems like TSP or set covering it is well known that various classes of instances, like Euclidean, random, clustered, are of different difficulty.

Another, even more complex aspect, of heterogeneous objectives is that they may require different optimization algorithms, or different operators used in the algorithms, to get very good results. For example, very different recombination operators may perform best for particular objectives.

Quick literature review shows that most theoretical papers focus on problems with homogeneous objectives, while most papers about practical applications of MOCO describe problems with heterogeneous objectives. Thus, naturally existing algorithms are well adapted to homogeneous objectives only.

3.7 Bridging the Gap between Theory and Application in Evolutionary Multi-Objective Optimization

Yaochu Jin (University of Surrey, GB)

This talk aims to bridge the gap between the current hot topics in evolutionary multi-objective optimization (MOO) and the urgent demands from real-world optimization. We will show that, while solving multi-objective optimization problems (MOPs) with a large number of objectives, often known as many-objective optimization, MOPs having a high-dimensional decision space (large-scale optimization) and MOPs having a very complex Pareto front have been very popular in academia, industry is more concerned with complexity in formulating the optimization problems, choosing the right decision variables, defining the most important objectives, and handling different constraints in the conceptual, design and verification phases. We will also point out that some assumptions in the present many-objective optimization and dynamic optimization research are unrealistic; the results are practically of little value, or even misleading. In addition, handling uncertainty and reducing the computational complexity in evaluating the quality of the designs are extremely important in dealing with real-world problems. As a result, incorporating a priori knowledge in various forms will be critical for handling the time constraint and performance requirement in real-world optimization. In the presentation, several application examples from industry, including design of vehicles, natural gas terminals and steel-making processes will be used to illustrate the real-world challenges in multi-objective optimization.

3.8 Machine Decision Makers: From Modeling Preferences to Modeling Decision Makers

Manuel López-Ibáñez (Free University of Brussels, BE)

Joint work of López-Ibáñez, Manuel; Knowles, Joshua D.
Main reference M. López-Ibáñez, J. D. Knowles, "Machine decision makers as a laboratory for interactive EMO," in Proc. of the 8th Int'l Conf. on Evolutionary Multi-Criterion Optimization (EMO'15), LNCS, Vol. 9019, pp. 295–309, Springer, 2015; pre-print available as IRIDIA Technical Report No. TR/IRIDIA/2014-016.
URL http://dx.doi.org/10.1007/978-3-319-15892-1_20
URL http://iridia.ulb.ac.be/IridiaTrSeries/link/IridiaTr2014-016.pdf

Quantitative assessment of any method involving human decision-makers (DMs) is difficult due to the need for a DM from whom preference information is elicited.Not only it is complex to characterize the properties of a human DM, but the DMs considered during experimentation may not have the same characteristics nor the same motivation than the ones for which the method is ultimately designed. Most studies that simulate DMs typically consider them as no more than a utility function. In a few cases, noise is added to this utility function to simulate human mistakes. Such a simple model cannot hope to capture the complexity of human psychological biases. At the same time, it neglects the existence of common characteristics in human DMs that are independent of a particular preference. The existence of such commonalities is more evident when considering DMs within a particular application scenario that may be, for example, risk-averse, risk-seeking or exploratory. Nonetheless, there are several works in the literature that have tried to simulate realistic DMs. In particular, T. J. Stewart proposed simulation models of various cognitive biases and factors that deviate from the ideal model ("non-idealities"), and studied their effect on multi-criteria decision-making (MCDM) methods such as goal programming, aspiration-based methods and additive value functions. Recently, López-Ibáñez and Knowles have applied this simulation model to evaluate an interactive evolutionary multi-objective optimization (EMO)algorithm. This talk discusses the concept of a machine decision-maker as are-usable, parametric, and general model of a realistic DM that can be used to analyze the effect of human factors and other non-idealities on interactive MCDM/EMO algorithms. The ultimate goal is that machine DMs would motivate the development of methods that are able to cope with various human cognitive biases and other non-idealities. Moreover, given enough data about past human interactions, it could be possible to learn the parameters of machine DMs in order to adapt them to particular application scenarios. Theories and results from psychology of judgment and decision-making, behavioral economics, and cognitive science should guide the construction of machine DMs. Nevertheless, there are still many open research questions on how to build, configure and use machine DMs in the context of interactive MCDM/EMO algorithms.

3.9 Sources of Computational Challenges in Multiobjective Optimization

Kaisa Miettinen (University of Jyvaskyla, FI)

Joint work of Luque, Mariano; Ruiz, Francisco; Ruuska, Sauli; Sindhya, Karthik; Steponavice, Ingrida

In this talk we, discuss some reasons why multiobjective optimization problems may be computationally expensive and challenging to solve. We also propose some ways of tackling the challenges. The main focus is on simulation-based optimization. It is important to keep in mind that reliable models are required for optimization but, on the other hand, optimization enables taking full advantage of high-quality models. A high accuracy easily introduces a high computational cost and this implies a need for balancing between accuracy and cost.

In simulation-based optimization we need different tools for handling complexity. When objective and constraint functions depend on the output of simulation models, function evaluations may be time-consuming, which introduces computational cost as a challenge. And as real life problems typically involve several conflicting objectives to be optimized simultaneously, methodological support for decision makers is important in identifying the most preferred solution. This necessitates preference information from the decision maker. Simulation models may have a black box nature and, thus, properties of functions involved may be unknown. For example, global optimization is needed when the convexity of the problem cannot be assumed and this typically increases the computational cost. Finally, stochasticity may have to be taken into account, for example, because the output of simulation models may be random vectors with unknown distributions. Handling this requires sampling the output which increases the computational cost.

We outline a three-stage approach which has been proposed in [1] for solving computationally challenging multiobjective optimization problems involving black-box models and stochasticity. In the pre-decision making stage, a set of Pareto optimal solutions is generated based on which a computationally less expensive surrogate problem is formed. The decision maker can solve the surrogate problem in the decision making stage with an interactive method because of low computing times. Finally, in the post-decision making stage, the final solution of the surrogate problem is projected to the Pareto optimal set of the original problem. The three-stage approach is applied in [1] when solving a joint design and operation problem of a paper plant. Here, the PAINT method [2] is used to generate the surrogate problem and the decision maker solves the problem with the interactive NIMBUS method [3].

We also discuss further method development challenges including high dimensions in decision and objective spaces, need of robustness, different forms of uncertainty, multilevel problems, user interface design and the importance of usability, the added value offered by different disciplines like visual analytics, new devices and platforms enabling a better utilization of the strengths of humans and computers and the potential of hybrid methods where elements of different types of methods are combined.

We conclude by outlining the interactive E-NAUTILUS method [4] for computationally expensive problems, which combines the three-stage approach and the philosophy of the NAUTILUS method [5]. In NAUTILUS, solutions of consecutive iterations improve all objectives and, thus, only the final solution is Pareto optimal. In this way, the decision maker can make a free search for the most preferred solution without e.g. anchoring.

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5 K. Miettinen, P. Eskelinen, F. Ruiz, and M. Luque. NAUTILUS Method: An Interactive Technique in Multiobjective Optimization based on the Nadir Point. *European Journal of Operational Research*, 206(2):426–434, 2010.

3.10 Understanding and managing complexity in real-case applications

Silvia Poles (Noesis Solutions, BE)

This presentation will be divided into two parts. In the first part we list all the possible sources of complexity in real-case applications and we analyze how these sources can affect the achievement of a solution in terms of time and effort.

Among other sources of complexity, we can mention the difficulty in integrating external solvers (e.g. simulation software) or the evaluation of time consuming functions (e.g. CFD codes) in the optimization process. Another difficulty can be a limited number of possible function evaluations, this limit is very common when dealing with time consuming functions. As other sources of complexity we can have a highly dimensional problem, a highly constrained problem, an optimization problem many conflicting objectives, or a problem with highly non-linear responses.

In the second part of the presentation we discuss about proposed solutions for managing complexity in real-case applications. For example, we show the use of a "process integration for design optimization" (PIDO) tool such as Optimus for the easy integration of different external solvers into a single platform. We will demonstrate the use of design of experiment approaches for reducing the problem dimension, and the use of models (meta-models) for reducing the number of evaluations of time consuming function. Eventually, the use of hybrid algorithms or a task list of methods will be proposed as an approach for highly non-linear problems. In this second part, all the proposed solutions will be supported by real-case multiobjective optimization problems.

3.11 Perspectives on the application of multi-objective optimization within complex engineering design environments

Robin Purshouse (University of Sheffield, GB)

Joint work of Purshouse, Robin; Giagkiozis, Ioannis; Fleming, Peter

Multi-objective optimization has experienced significant growth as a research field over the last few decades. However there exist very few published examples where multi-objective optimization methods have been used within a real decision-making context for engineering products or services. Whilst this dearth of evidence may be due to disincentives surrounding publication, it may also support a hypothesis that formal methods for multi-objective optimization are incongruent with *in situ* organisational practices and, as a result, are simply not used. This presentation will review the existing optimization frameworks that have attempted to account for the complexity in engineering design environments. Most of these frameworks have arisen in the field of multi-disciplinary design optimization (MDO), and include architectures such as collaborative optimization and analytical target cascading. The presentation will also highlight some of the key challenges as yet unaddressed by the MDO community; specifically: (1) how to handle the asynchronous distributed nature of the engineering design environment to ensure right-first-time design; (2) how to allocate resources to compromise-seeking activities in an environment of shared design variables and conflicting product requirements.

3.12 Advancing Many-Objective Robust Decision Making Given Deep Uncertainty

Patrick M. Reed (Cornell University, US)

Main reference J. D. Herman, P. M. Reed, H. B. Zeff, G. W. Characklis, "How Should Robustness Be Defined for Water Systems Planning under Change?" Journal of Water Resources Planning and Management, 2015.
URL http://dx.doi.org/10.1061/(ASCE)WR.1943-5452.0000509

This talk will demonstrate the many-objective robust decision making (MORDM)framework on a severely challenging real-world application where we are working to facilitate improved coordination across four independent U.S. cities seeking to maintain their region's supply reliability and financial stability given increasingly severe droughts. MORDM combines massively parallel many objective evolutionary optimization under uncertainty (benchmarked on more than 500,000compute cores) with recent decision theoretic work in the area of robust decision making (RDM). MORDM makes extensive use of interactive visual analytics, to facilitate negotiated group decisions and to provide insights on key system uncertainties. In contexts such as urban water supply planning, nontrivial conceptual as well as computational challenge due to the structural uncertainties associated with defining complex management problems (e.g., choosing objectives, management decisions, planning horizons, representations of preferences, etc.) as well as the challenges associated with predicting the impacts of actions (e.g., imperfect knowledge of system dynamics, external forcings, or environmental thresholds). Often in complex infrastructure systems, modelled processes are impacted by deep (or Knightian) uncertainties. Deep uncertainties emerge when planners are unable to agree on or identify the full scope of possible future events including their associated probability distributions. RDM is used in the second stage of this framework to determine the robustness of tradeoff alternatives to deeply uncertain future conditions and facilitates decision makers' selection of promising candidate solutions. MORDM tests each solution under the ensemble of future extreme states of the world (SOWs). Global sensitivity methods are used to identify what assumptions and system conditions pose many-objective performance vulnerabilities if candidate Pareto approximate alternatives are selected.

3.13 Tutorial on Large-Scale Multicriteria Portfolio Selection Leading Up to Difficulties Obstructing Further Progress

Ralph E. Steuer (University of Georgia, US)

Joint work of Hirschberger, Markus; Steuer, Ralph E.; Utz, Sebastian; Wimmer, Maximilian; Qi, Yue
Main reference M. Hirschberger, R. E. Steuer, S. Utz, M. Wimmer, Y. Qi, "Computing the Nondominated Surface in Tri-Criterion Portfolio Selection," Operations Research, 61(1):169–183, 2013.
URL http://dx.doi.org/10.1287/opre.1120.1140

This is oriented toward algorithms for solving large-scale multicriteria portfolio selection problems and visualization methods for conveying the nondominated set. The basic formulation here is a multiple objective linear program other than for one or more of the objectives being quadratic. It is necessary to compute the entire nondominated set because in portfolio selection users are usually not able to select an optimal solution until after seeing that everything else is worse. There are two basic ways of solving for the nondominated set. One is to compute exactly the nondominated set by means of a parametric quadratic programming procedure. The other is to compute a dotted representation of the nondominated set via an e-constraint strategy, but because of covariance matrix difficulties this is not always as easy as it may seem.The simplest portfolio case is a QL problem: two objectives (one quadratic, one linear). In this case the nondominated set graphs as a frontier consisting of a connected collection of curved arcs each coming from a different parabola. With additional objectives, the nondominated set becomes a surface consisting of a connected collection of curved patches each coming from a different paraboloid. While we can also compute the patches of QLL and QLLL problems, problem size drops dramatically. Now we are beginning to see QQL and QQLL problems proposed, but no one knows how to deal with them yet. Whereas it is a struggle to graph the nondominated surfaces of tri-criterion portfolio selection problems, how to employ visualization techniques with the nondominated sets of problems with four criteria is a major challenge. Then there are other types of difficult problems including the cardinality constrained portfolio selection problem.

3.14 Distributed MCDM under partial information

Margaret M. Wiecek (Clemson University, US)

Main reference B. Dandurand, M. M. Wiecek, "Distributed computation of Pareto sets," to appear.

Technological advances and globalization of the world create a need for multiobjective optimization-based decision making for large-scale systems. Such systems are characterized by a number of subsystems and various science or engineering disciplines that demand for specific expertises and multiple teams working in different geographical locations. Subsystems and disciplines are involved in the decision making process as interconnected elements in the physical as well as conceptual sense. The participating teams do not have access to the optimization subproblems of the other teams but may exchange limited information about their own current decisions. Because information flow between the subproblems is limited and requires periodic updating, direct solution approaches are available only at the subproblem level, and not at the level of the entire system.For example, in a large international corporation decisions are made under multiple objectives locally in each country so that the entire corporation performs globally at its best. In a military environment, multiteam planning takes place and multiple missions are executed under partial information due to constraints in the communication bandwidth or due to required communication latencies. Complex engineering design problems involve a system-level design problem and component-level design subproblems that correspond to different design-team organizational structures and require disparate solution methodologies and software interfaces. This decision making scenario requires the development of mathematical models and distributed solution methodologies that are able to capture the presence of different interconnected entities making decisions for different subsystems based on the criteria originated in multiple disciplines.The state-of-art analyses for distributed solution approaches such as the alternating direction method of multipliers (ADMM) and the block coordinate descent (BCD) method had been developed in the context of problem decomposition originating in a single objective setting and are not immediately applicable to multiobjective programs (MOPs). Applying certain scalarization techniques well-suited for nonconvex MOPs, the decomposable MOP is reformulated into a single objective problem (SOP) but the decomposability is not preserved and the SOP is not suitable for the application of ADMM. Furthermore, coupling between the subproblems makes BCD in its current form likewise inadequate. To address these challenges to distributed multiobjective optimization, existing theory is extended for 1) iterative augmented Lagrangian coordination techniques and 2) the block coordinate descent method. Based on this study, a Multi-Objective Decomposition Algorithm (MODA) is developed for the distributed generation of efficient solutions to nonconvex decomposable MOPs. MODA is applied to a bilevel automotive design problem that is formulated as a collection of two subproblems including a vehicle-level subproblem and component-level subproblem. Numerical results of the implementation are presented showing the MODA capability of exploring the tradeoffs generated by the multiple criteria at each level.

4 Working Groups (WGs)

4.1 Modeling Behavior-Realistic Artificial Decision-Makers to Test Preference-Based Multiple Objective Optimization Methods (WG1)

Jürgen Branke, Salvatore Corrente, Salvatore Greco, Miłosz Kadziński, Manuel López-Ibáñez, Vincent Mousseau, Mauro Munerato, and Roman Słowiński

4.1.1 Introduction

Traditionally, in Multiple Objective Optimization (MOO), two separate methodological streams have been developed: evolutionary and interactive ones [2]. On the one hand, the role of Evolutionary MOO (EMO) is to approximate the entire Pareto front. On the other hand, Interactive MOO (IMO) deals with identification of the most preferred solution. IMO techniques require participation of a Decision Maker (DM) who is expected to provide her subjective preference information. The recent trend in MOO consists in merging the interactive and evolutionary approaches (for reviews, see [2, 8, 3]). This is achieved by integrating preference information into the EMO algorithms already during their optimization runs. The appealing effect of such integration consist in focusing the search on the area of the Pareto front which is most suitable to the DM.

Whenever DM preferences are used for guiding the search in MOO methods, the theoretical analysis [4] and experimental assessment of such algorithms is challenging, because it requires setting up a test environment that includes a model of the DM's behavior. Traditionally, artificial DMs have been simulated as a pre-defined value (utility) function for decision making. For example, the two user's functions used in an experimental setting in [3] assumed either linear weighting or a Tchebycheff-like aggregation of the objectives. In some other works, uncertainty of the DM interacting with an algorithm has been modeled by adding noise to an assumed function. In any case, the underlying model of an artificial DM is not known to a tested algorithm, but rather used to derive preference information that is subsequently provided at the method's input.

By contrast, the literature in (multiple criteria) decision making clearly identifies several cognitive biases, psychological phenomena, and inaccuracies occurring at the stage of problem modeling. Obviously, these highly affect preference elicitation and interactive decision making.

Thus, the simple models of DMs most commonly used in the literature for testing IMO algorithms neglect the richness of human behavior and aggregate into a random component a variety of factors that should be rather modeled individually. The important factors that we identified are discussed in the following section. Altogether, they contribute to the idea of implementing a *machine DM* that would take into account the "true" criteria and "true" preference modified appropriately so that to approximate the behavior of real-world DMs.

4.1.2 Modeling cognitive biases, psychological phenomena, and inaccuracies of a machine Decision Maker

We call a machine DM, a model of DM biases and other factors that influence the interaction of the DM with the algorithm by modifying the true criteria and the true preference considered by the DM. This model does not actually specify the criteria and preferences considered by the DM, although different models (different machine DMs) may require them to satisfy certain characteristics. We decided to extend the machine DM from [7], which is based on previous work by Stewart [10], by modeling additional cognitive biases. Stewart [10] assumes a true preference function inspired by prospect theory, that is, a weighted sum of sigmoidals, and the biases modeled are omission of objectives, mixing of objectives and noise. We discuss these phenomena along with the newly considered ones in the following subsections.

Omission of criteria

Omission of criteria consists in neglecting by the algorithm some of the criteria that are internally considered by the DM [10, 11]. For example, attributes of the problem that are modeled as constraints might be considered criteria by the DM. As noted by Stewart [11], the selection of the q criteria among m true ones (with $q < m$) can be conducted as follows:

- assign to each criterion g_j a uniformly generated weight w_j;
- order the criteria from the least ($rank = 1$) to the most important ($rank = m$);
- select q criteria randomly with probabilities proportional to the ranks of criteria so that less important objectives have a higher probability of being omitted.

In this scenario, the machine DM derives its preferences from the m-objective space, whereas the algorithm is allowed to refer the $q < m$ objectives only, i.e.:

$$\vec{g} \in \mathbb{R}^m \quad \text{(DM)} \quad \Rightarrow \quad \vec{\hat{g}} \in \mathbb{R}^{q<m} \quad \text{(algorithm)}. \tag{1}$$

Inversely, the machine DM may neglect some of the m criteria known to the algorithm by constructing its preferences on the basis of $q < m$ criteria only. In this case:

$$\vec{g} \in \mathbb{R}^{q<m} \quad \text{(DM)} \quad \Rightarrow \quad \vec{\hat{g}} \in \mathbb{R}^{m} \quad \text{(algorithm)}. \tag{2}$$

This bias can be modeled analogously to the previous one.

Mixing of criteria

Even if the criteria internally considered by the DM are preferentially independent, they may have been inadvertently corrupted when modeling the problem by mixing them in such a way that violates preferential independence [6, 10, 11]. Stewart suggests to obtain the new criteria in the following way [11]:

$$\hat{g}_k = (1-\gamma)g_j + \gamma g_{j+1}, \tag{3}$$

where $\gamma \in [0, 1]$ is a mixing parameter.

In the same spirit, even if the criteria have been defined so that to satisfy the requirement of preferential independence, one may introduce interaction components to the machine DM's value function. For example, Greco et al. [5] considered two particular types of such components corresponding to "bonus" and "penalty" values for positively or negatively interacting pairs of criteria. A bonus is added to (a penalty is subtracted from) the comprehensive value if a pair of criteria is in a positive (negative) synergy for performances of the considered alternatives on the two criteria. These effects may be considered as mutual strengthening or mutual weakening effects, respectively, which are both easily integratable into the model of a machine DM.

Mental fatigue

A great share of MOO methods require the DM to provide the preference information incrementally. On the one hand, this allows both avoiding the necessity of dealing with a large set of preference information pieces already at the initial stages of the interaction as well as controlling the impact of each piece of information (s)he supplied on the delivered results. On the other hand, a lengthy preference elicitation process may result in a mental fatigue of the DM. Such fatigue is defined as a temporary inability to maintain maximal cognitive performance from prolonged periods of cognitive activity (in our case, answering questions that would guide the search) [http://en.wikipedia.org/wiki/Fatigue_(medical), last accessed: 10/03/2015]. Obviously, its onset depends upon an individual DM, but in general it is considered to be gradual. Thus, we have decided to model it as a noise factor $\sigma(k)$ that depends on the number of queries (k) to the DM. We found an exponential model $\sigma_0 \cdot e^{\alpha \cdot k}$ as appropriate for this purpose. Note that a closely related cognitive bias may consist in modeling mistakes of the machine DM just by negating or inverting the preferences derived from its model at random intervals.

Bounded rationality

The limited abilities of the DMs concerning information manipulation and computation have been accounted in the literature within the extensive studies on *bounded rationality* [9]. Indeed, the observed real-world decisions often violate the normative principles according to which all the relevant information should be taken into account. Various phenomena indicating that only a limited part of the available information is accounted in practical decision problems have been framed within so called *decision strategies* or *choice heuristics*. Using reverse engineering, these heuristics can be used for modeling the behavior of a machine DM with bounded rationality. For example, we may refer to:

- the satisficing heuristic [9] which (1) considers the solutions one after another, in a random way, (2) compares the value on each criterion of the current solution to a predefined level, and (3) selects the first alternative which passes this test; this procedure may potentially neglect a large part of the solution set;
- the elimination by aspect heuristic [12] which compares all solutions to a pre-defined aspiration level at each criterion starting from the most important one until a single alternative remains; thus defined, this approach considers a limited number of criteria.

Anchoring

Anchoring is a cognitive bias that describes the common human tendency to rely too heavily on the first piece of information offered (the "anchor") when making decisions. During decision

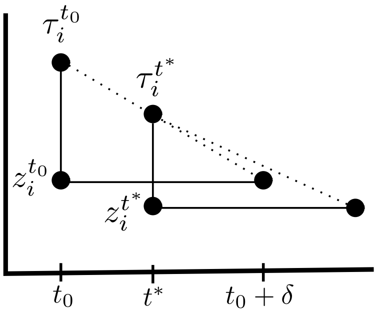

Figure 1 Dynamic model with delayed adjustment of reference point.

making, anchoring occurs when individuals use an initial piece of information to make subsequent judgments [http://en.wikipedia.org/wiki/Anchoring, last accessed: 10/03/2015].

There are two levels of anchoring: a psychological or judgmental level, where there is no notion of gains or losses, and a reference-based level, where the DM defines her reference point according to earlier interactions and resists changing it. As a particular case of anchoring, we considered shifting the reference levels at each interaction according to the median value of each criterion for solutions shown to the DM (or the best solution found). However, we concluded that such a shift may have different interpretations depending on whether dynamic changes in true preference are desirable or not. Thus, we considered two models, where $U()$ is the true preference of the DM and $\hat{U}()$ is the perceived preference that determines the interaction with the algorithm:

- **Static (stable) model**, where interaction does not change the true reference point. In this model, anchoring means that interaction shifts the perceived reference point in $\hat{U}()$ from the true reference point in $U()$. The goal of the algorithm is to minimize the error with respect to the true (static) preference.
- **Dynamic model**, where interaction allows the DM to adjust her reference point (learn), that is, reference point changes in the true preference $U(\vec{z})$. In this model, anchoring means a resistance to change in $\hat{U}()$, when $U()$ changes. The goal of the algorithm is to minimize error with respect to the true preference at the last iteration. Such dynamic model may be treated as an example of evolving DM preferences, when the internal model of the DM changes as a result of the interaction with an algorithm.

We also tentatively discussed an additional *dynamic model with delayed adjustment of reference point* (Fig. 1), where the reference point is updated as:

$$\tau_i^{t^*} = \tau_i^{t_0} + (z_i^{t_0} - \tau_i^{t_0}) \cdot \frac{t^* - t_0}{\delta}$$

where $\delta > 0$ is a delay in adjusting preferences (anchoring). In this model, the goal is to minimize the error with respect to the true preference model at the last iteration $+\,\delta$.

Loss aversion

The best solution identified so far in the course of an interaction with the MOO method may be treated by the DM as a reference point. When further exploring the objective space, the DMs tend to collate the newly constructed solutions with her actual reference. Such comparisons may be affected by a loss aversion bias, which implies that the impact of a difference on a criterion is greater when that difference is evaluated as a loss than when the same difference is evaluated as a gain [13]. Such asymmetry in perception of gains and

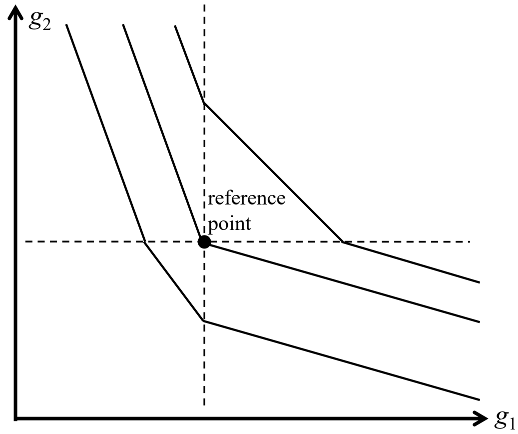

Figure 2 Exemplary indifference curves illustrating loss aversion with respect to the reference point.

losses with respect to the reference point $R = [r_1, \ldots, r_j, \ldots]$ may be easily modeled by transforming the DM's true function u_j in the following way:

$$R_j(x_J) = \begin{cases} u_j(x_j), & \text{if } x_j \geqslant r_j \\ \lambda_j u_j(x_j) - (1-\lambda_j)u_j(r_j), & \text{if } x_j < r_j, \end{cases} \tag{4}$$

where λ_j is a coefficient of loss aversion for criterion g_j. In Figure 2, we provide exemplary indifference curves illustrating the application of thus defined transformation to a two-objective additive linear value function. These isoquants demonstrate that, when observing improvements on both objectives, the perception of the DM is unchanged, whereas the loss in performance at one objective negatively affects the overall quality of the solution from the point of the DM.

4.1.3 Conclusions and future work

The assumption that a true, not directly observable, preference exists is controversial on itself. One consequence of such a model is that, when attempting to avoid biases that distort this function, we are basically telling the DM that her behavior is somehow wrong. We recognize that this is a contentious issue, however, for simulation purposes, the existence of such a true preference is a useful working hypothesis which enables the analysis of how different biases affect interactive algorithms.

When modeling the machine DM, we can draw inspiration from previous literature on theoretical models and empirical studies with human DMs in (multiple criteria) decision making, behavioral economics, judgmental psychology, and cognitive science. In this perspective, we feel that a thorough analysis of how DMs actually behave may gain yet another stream of applied research. That is, apart from having a relevant practice of preference elicitation and designing efficient preference elicitation procedures, we may design the procedures for deriving preference information to be provided at the input of tested algorithms.

Since the ultimate goal of modeling machine DM consists in using them for analysis and comparison of different methods, their models should be extended to various types of preference information, interaction and true preference models, in order to achieve as much generality as possible. During a group discussion, we decided to focus on how to model DM biases in the context of ranking and pairwise comparisons of solutions, nonetheless, we agreed that it is a worthwhile goal to understand how to simulate DM biases in the context of various types of interaction and preference information, including aspiration levels (goal programming), reference points, trade-offs, select 1 of n, sorting into categories, scoring, intensities of preferences, order of objectives, and desirability functions.

Our plan is to apply the proposed machine DM to NEMO-Choquet [1], which is an interactive evolutionary multiple objective algorithm based on the Choquet integral. Our intuition is that NEMO-Choquet should be able to cope with various biases, such as the mixing of objectives. In the medium term, we wish to do experiments that examine the trade-off between number of questions and quality of information, which decreases because of the fatigue, with respect to different types of questions (pairwise vs. ranking vs. aspiration levels vs. …). Future machine DMs should also simulate more biases such as bounded rationality heuristics in order to simulate more realistic behaviors.

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4.2 Computational Complexity (WG2)

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4.2.1 Introduction

As discrete multiobjective optimization is more and more applied in practice, the necessity arises to categorize both computationally easy and computationally difficult problems. This asks for a thorough complexity theory and analysis of discrete multiobjective optimization problems. Some classical complexity concepts have their limitations when applied to multiobjective optimization, since almost all non-trivial multiobjective optimization problems are NP-hard and intractable.

To the best of our knowledge there are only few publications on the topic of computational complexity for multicriteria optimization problems in general ([5, 1, 2, 3]). In [3], different notions of complexity (depending on the solution concept) are proposed and their interrelations are analyzed. However, there is a wide range of articles investigating the complexity issues of several multiobjective optimization problems and/or their approximability.

Some properties determining the complexity of a problem are related to the decision space, like total unimodularity or other polyhedral properties of the feasible set, others are related to the objective space, like the cardinality of $f(X)$ and its dominance structure. Particularly, the construction scheme, usually applied to show intractability of a problem, uses a very special dominance structure, in which all points are pairwise nondominated.

4.2.2 Dominance Structure

Consider the following biobjective integer problem with a cardinality constraint:

$$\begin{aligned} \min f(X) = &\begin{pmatrix} p^1 X \\ p^2 X \end{pmatrix} \\ \text{s.t. } &\|X\|_1 = \ell \\ &X \in \{0,1\}^n \end{aligned} \tag{P1}$$

where $\|\cdot\|_1$ denotes the 1-norm. Note that $(X, \leq)$ is a strict partially ordered set (i.e. a *poset*), where $\leq$ denotes the component-wise ordering. We build a Hasse diagram of $(X, \leq)$ *via* the cover relation with an implied upward orientation, that is,

1. If $f(x_i) \leq f(x_j)$ holds in the poset, then the point corresponding to x_j appears lower in the drawing than the point corresponding to x_i.
2. The edge between the points corresponding to any two elements x_i and x_j of the poset is included in the drawing if and only if x_i covers x_j or x_j covers x_i, with respect to the given cover relation.

We are particularly interested in relating the (dominance) structure of a given instance of Problem (P1), via the Hasse diagram of the set $\{x_1, x_2, \ldots, x_n\}$, with the cardinality of the efficient set.

Let graph $H = (V, E)$, with vertex set $V = \{x_1, \ldots, x_n\}$ and edge set E, correspond to the graph representation of the Hasse diagram of an instance of Problem (P1). Note that graph H may be disconnected. We denote by $V_i \subseteq V$, $1 \leq i \leq k$, the vertex set of the i-th connected component of graph H, and by $V^* \subseteq V$ the set of all vertices that are minimal elements in the Hasse diagram. We obtain a directed graph $G = (V \cup \{x_0\}, A)$ by performing the following transformation in graph H:

1. For each edge $\{x_i, x_j\} \in H$, $f(x_i) \leq f(x_j)$, create an arc (x_i, x_j) in G
2. For each vertex $x_i \in V^*$, create an arc (x_0, x_i) in G
3. For each vertex $x_i \in V^*$ and $x_j \in V$, for which it holds that $f(x_i) \not\leq f(x_j)$, create arcs (x_i, x_j) and (x_j, x_i)

Note that this directed graph is connected, may contain cycles and is rooted in x_0. An upper bound on the number of efficient solutions for an instance of Problem (P1) is given by the number of distinct paths of size $\ell + 1$ in G, starting in vertex x_0. In the following we illustrate this transformation on some particular cases and give the upper bound on the number of efficient solutions.

A trivial example is given in the left plot of Figure 3, for which it holds that

$$f(x_i) \leq f(x_j) \iff i < j$$

The graph transformation is given in the right plot of Figure 3, for which there is only one efficient solution. The second example is given in the left plot of Figure 4 with two connected components. The graph transformation is given in right plot, where the dashed arcs correspond to arcs of type 3. In this case, we have $O(\ell^2)$ efficient solutions. A generalization of the previous example is to consider k connected components, each of which with the same structure as that described in the first example. In this case, the number of efficient solutions is $O(\ell^k)$.

Another example is given in left plot of Figure 5, which connects the two connected components from the example in the left plot of Figure 4. In this case, the number of efficient solutions is $O(2^\ell)$. A generalization of the previous example, which can be obtained by connecting k connected components, gives $O(k^\ell)$ efficient solutions.

Another example is given in left plot of Figure 6, which consists of a binary tree, and corresponding transformation in the right plot. An upper bound on the number of efficient solutions is given by the number of binary trees of size ℓ, which corresponds to the Catalan number $C_\ell = \frac{1}{\ell+1}\binom{2\ell}{\ell}$. Finally, left plot of Figure 7 shows a worst case example with the corresponding transformation in the right plot. An upper bound on the number of efficient solutions is given by the $O(n^\ell)$.

4.2.3 Using Total Unimodularity in Multiobjective Optimization

Total unimodularity (TU) is a well known and widely investigated property to identify a certain class of easy-to-solve optimization problems in single objective integer programming (see e. g. [4]). The special polyhedral structure of totally unimodular problems allows to use linear programming to solve integer problems. So the question arises: *Is total unimodularity also useful in multiobjective optimization?*

▶ **Definition 1.** An $m \times n$ integral matrix A is *totally unimodular (TU)* if the determinant of each square submatrix of A is equal to 0, 1 or -1.

▶ **Property 2** (C.f. [4]). *If A is TU and b is integral, then linear programs of forms like $\{\min cx : Ax \geq b, x \geq 0\}$ have integral optima, for any c and thus can be solved using (continuous) linear programming.*

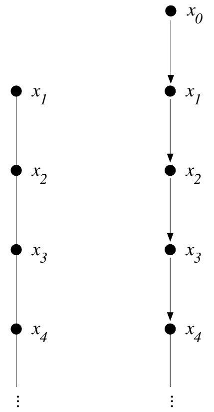

Figure 3 The first example (left) and the graph transformation (right).

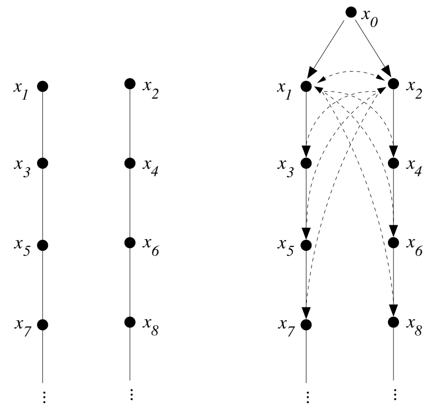

Figure 4 The second example (left) and the graph transformation (right).

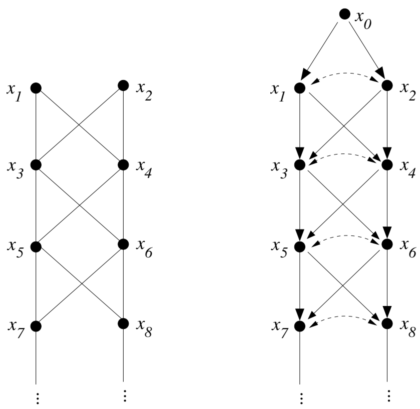

Figure 5 The third example (left) and the graph transformation (right).

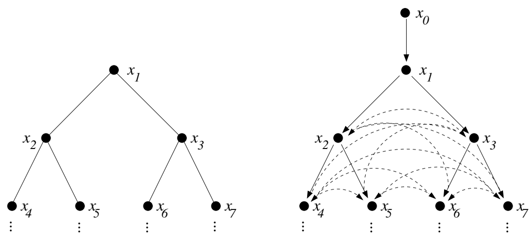

Figure 6 The fourth example (left) and the graph transformation (right).

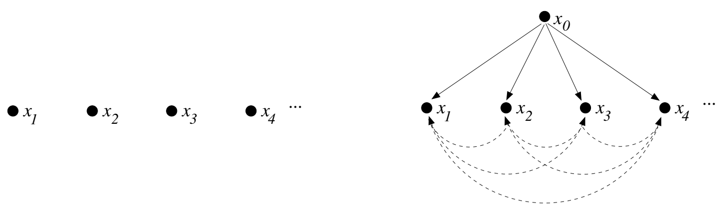

Figure 7 The fifth example (left) and the graph transformation (right).

▶ **Proposition 3.** *The non-dominated set of the following biobjective integer problem*

$$\min \begin{pmatrix} c^1 x \\ c^2 x \end{pmatrix} \qquad \text{(BOIP)}$$
$$s.t.\ A\,x = b$$
$$x \geq 0$$

where A is TU can be enumerated in polynomial delay*, when c^2 is*

- *a unit vector (in polynomial time)*
- *any row A^i of A.*

Moreover, all non-dominated points of (BOIP) *are supported.*

Proof. The problems

$$\begin{aligned} &\min c^1 x \\ &\text{s.t. } A\,x = b \\ &\quad x \geq 0 \quad \text{(integer)} \end{aligned}$$

can be solved in polynomial time, since A is TU. The constraint matrices of the ε-constraint problem, namely

$$A' = \begin{pmatrix} & A & & 0 \\ & & & \vdots \\ 0 & \dots & 1 & 1 \end{pmatrix} \qquad \text{or} \quad A' = \begin{pmatrix} A & 0 \\ & \vdots \\ A^i & 1 \end{pmatrix}$$

are then also TU, c.f. [4], page 540. Consequently, the corresponding ε-constraint problems

$$\begin{array}{ll} \min & c^1 x \\ \text{s.t.} & A'\,x' = \begin{pmatrix} b \\ \varepsilon \end{pmatrix} \\ & x' \geq 0 \end{array} \iff \begin{array}{ll} \min & c^1 x \\ \text{s.t.} & A\,x = b \\ & c^2 x \leq \varepsilon \\ & x' \geq 0 \quad \text{(integer)} \end{array} \qquad \text{(EC)}$$

can also be solved in polynomial time using linear programming.

There is still to show, that all nondominated points are supported, i. e. every nondominated point can be obtained by solving a weighted-sum scalarization

$$\begin{aligned} &\min \lambda c^1 x + (1-\lambda)\, c^2 x \\ &\text{s.t. } A\,x = b \\ &\quad x \geq 0 \quad \text{(integer)} \end{aligned} \qquad \text{(WS)}$$

for a value of $\lambda \in [0, 1]$.

We can reformulate (WS) and interpret it as the Lagrange dual of (EC) relaxing the constraint $c^2 x \leq \varepsilon$:

$$\begin{aligned} &\min c^1 x + \mu\,(c^2 x - \varepsilon) \\ &\text{s.t. } A\,x = b \\ &\quad x \geq 0 \quad \text{(integer)} \end{aligned} \qquad \text{(LD)}$$

with Lagrange multiplier $\mu \geq 0$. Furthermore we apply the result ([4], page 329), that strong duality holds, i. e. $\exists \mu \geq 0$: the optimal values of (EC) and its Lagrange dual (LD) coincide, iff

$$\text{conv}\{x \in \mathbb{R}^n : Ax = b, c^2 x \leq \varepsilon\} = \text{conv}\{x \in \mathbb{R}^n : Ax = b\} \cap \{x \in \mathbb{R}^n : c^2 x \leq \varepsilon\}.$$

This equality holds since all considered polyhedra are TU, and thus we can conclude that every nondominated point can be obtained by weighted sum scalarization with a certain value of $\lambda \in [0, 1]$. ◀

Since all the non-dominated points are supported the problem can be solved even more efficiently using dichotomic-search.

Application to the Transportation Problem

Let I be the set of suppliers with capacities to deliver up to an amount of s_i product units, and J be the set of customers with demands d_j. As in the single objective transportation problem we consider the minimization of transshipment costs and additionally we introduce a second objective of the form given in Proposition 2, which corresponds to the minimization (or maximization) of product flow between one supplier and one customer (a) or the minimization (or maximization) of the number of units provided by one supplier (b).

a)
$$
\begin{aligned}
&\min \sum_{ij} c_{ij}\, x_{ij} \\
&\min x_{12} \\
&\text{s.t.} \sum_i x_{ij} = d_j \qquad \forall j \in J \\
&\sum_j x_{ij} \leq s_i \qquad \forall i \in I \\
&x_{ij} \geq 0 \text{ (integer)} \quad \forall (i,j) \in I \times J
\end{aligned}
$$

$$
\begin{aligned}
&\min \sum_{ij} c_{ij}\, x_{ij} \\
&\text{s.t.} \sum_i x_{ij} = d_j \qquad \forall j \in J \\
&\sum_j x_{ij} \leq s_i \qquad \forall i \in I \\
&x_{12} \leq \varepsilon \\
&x_{ij} \geq 0 \text{ (integer)} \quad \forall (i,j) \in I \times J
\end{aligned}
$$

$$
\begin{array}{|ccccccccc|l}
\hline
1 & \dots & 1 & & & & & & & = d_1 \\
 & & & 1 & \dots & 1 & & & & = d_2 \\
 & & & & & & 1 & \dots & 1 & = d_3 \\
1 & & & 1 & & & 1 & & & \leq s_1 \\
 & 1 & & & 1 & & & 1 & & \leq s_2 \\
 & & 1 & & & 1 & & & 1 & \leq s_3 \\
\hline
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \leq \varepsilon \\
\hline
\end{array}
$$

b)
$$
\begin{aligned}
&\min \sum_{ij} c_{ij}\, x_{ij} \\
&\min \sum_j x_{1j} \\
&\text{s.t.} \sum_i x_{ij} = d_j \qquad \forall j \in J \\
&\sum_j x_{ij} \leq s_i \qquad \forall i \in I \\
&x_{ij} \geq 0 \text{ (integer)} \quad \forall (i,j) \in I \times J
\end{aligned}
$$

$$
\begin{aligned}
\min \; & \sum_{ij} c_{ij}\, x_{ij} \\
\text{s.t.} \; & \sum_{i} x_{ij} = d_j \qquad \forall j \in J \\
& \sum_{j} x_{ij} \leq s_i \qquad \forall i \in I \\
& \sum_{j} x_{1j} \leq \varepsilon \\
& x_{ij} \geq 0 \text{ (integer)} \quad \forall (i,j) \in I \times J
\end{aligned}
$$

$$
\begin{array}{|ccccccccc|l}
\hline
1 & \dots & 1 & & & & & & & = d_1 \\
& & & 1 & \dots & 1 & & & & = d_2 \\
& & & & & & 1 & \dots & 1 & = d_3 \\
1 & & & 1 & & & 1 & & & \leq s_1 \\
& 1 & & & 1 & & & 1 & & \leq s_2 \\
& & 1 & & & 1 & & & 1 & \leq s_3 \\
\hline
1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & \leq \varepsilon \\
\hline
\end{array}
$$

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4.3 Heterogeneous Functions (WG3)

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4.3.1 Introduction

Observing the literature on real-world multiobjective optimization problems, one might notice that many practical applications exhibit considerable heterogeneity regarding the involved objective functions. This working group collected examples of such problems, characterized the kind of heterogeneity that may be found, and identified suitable benchmarks and potential challenges for respective optimization algorithms.

4.3.2 An example

Let $f^1, f^2 : \mathbb{R}^n \to \mathbb{R}$ be nonlinear (objective) functions and let $f^3 : \mathbb{R}^n \to \mathbb{R}$ be a linear objective function. Moreover, let $\Omega \subseteq \mathbb{R}^n$ be the constraint set. Based on these let us consider two multi-objective optimization problems:

$$\min\,(f^1(x), f^2(x)), \quad \text{s.t. } x \in \Omega \text{ and} \tag{P1}$$

$$\min\,(f^1(x), f^3(x)), \quad \text{s.t. } x \in \Omega. \tag{P2}$$

It is clear that both (P1) and (P2) are classified as nonlinear multi-objective optimization problems. If one applied a *weighted sum method* the scalarized single-objective function remains nonlinear. Therefore, there is no added difficulty (or simplicity) due to the heterogeneity of the objectives in (P2) compared with (P1). *Homotopy-based methods* [13], on the other hand, can use the linearity of objective f^3 in an efficient way, and therefore, (P2) can be solved using such methods in an easier way (compared to the nonlinear problem (P1)). (P2) can also be easier to solve using *population-based heuristics*. A well-known example is the benchmark problem ZDT1 (or ZDT4) where NSGA-II first finds the individual minima of the first, linear objective function, and then spreads along the efficient front.

4.3.3 Motivating Applications

Multiobjective capacitated arc routing problem. Lacomme et al. [19] and Mei et al. [23] consider the multiobjective version of capacitated arc routing problems (CARP). These find application in optimization of salting and removing the snow in the winter or in waste collection by a fleet of vehicles. They consider two objectives, namely the total cost (time) of the routes, which is related to minimization of the total operational costs, and the makespan, i. e., the length of the longest route, which is related to the satisfaction of the clients. Clearly the two objectives differ by mathematical form – sum or maximum of the routes' costs. This difference may also influence the landscapes of these objectives and thus influence their practical difficulty. Consider for example the typical insertion or swap moves for CARP. Such moves modify two routes at a given step. In order to improve the makespan objective the longest route has to be improved, so it has to be one of the modified routes. This means that there are in general less potential moves that could improve this objective and local search may stop at a local optimum very fast. For the total cost objective, on the other hand, many moves may result in an improvement. Please note that this situation is similar to the optimization of either linear (weighted sum) or Chebycheff scalarizing functions. The latter type of functions use a maximum operator. Jaszkiewicz [17] observed that linear functions are easier to optimize than Chebycheff ones in the framework of a multiple objective genetic local search algorithm.

Multiobjective chemical formulation problem. Based on communications with Unilever plc., Allmendinger and Knowles motivated their recent work on heterogeneous evaluation times of objectives [1] using an example from a chemical formulation problem: "We wish to optimize the formulation of a washing powder, and our two objectives are washing excellence and cost. In this case, [...] assessing washing excellence may be a laborious process involving testing the powder, perhaps on different materials and at different temperatures. By contrast, the cost of the particular formulation can be computed very quickly by simply looking up the amounts and costs of constituent ingredients and performing the appropriate summation". Earlier work by the same authors [2] stated that heterogeneous evaluation times could be associated with other lengthy experimental processes such as fermentation, or might occur because of a need for subjective evaluations from experts. In both studies (ibid.), the authors consider a variety of algorithmic approaches to handling objectives with different "latency", including use of pseudofitness values, and techniques based on interleaving evaluations on the slower and the faster objective(s).

Multiobjective traveling salesman problem with profits. Jozefowiez et al. [18] consider the multiobjective traveling salesman problem with profits. The two objectives are minimization of the tour length and maximization of the collected profits. The tour does not have to include all nodes. TSP with profits is a well known combinatorial problem with multiple applications [10]. Although it is multiobjective by nature, it is usually solved by aggregation of the two objectives, which not only differ by mathematical form but also have different domains. The tour length depends on both the selected cities and the chosen tour, while the profit depends only on the selected cities. Furthermore, the two objectives correspond to two different classes of combinatorial problems. The authors used two sets of moves. The first set optimizes the tour while the second set modifies the set of visited nodes. An interesting observation is that the higher the number of selected nodes, the more difficult is the related TSP subproblem, i. e., optimization of the tour.

Multi-objective optimization in the Lorentz force velocimetry framework. Lorentz force velocimetry (LFV) is an electromagnetic non-contact flow measurement technique for electrically conducting fluids. It is especially suited for corrosive or extremely hot fluids (glass melts, acidic mixtures, etc) that can damage other measurement setups [30]. The magnetic flux density B is produced by permanent magnets and an electrically conducting (σ) fluid moves with a velocity v through a channel. The magnetic field interacts with the fluid and eddy currents develop. The resulting secondary magnetic field acts on the magnet system. The Lorentz force F_L breaks the fluid and an equal but opposite force deflects the magnet system, which can be measured. It holds that $F_L \sim \sigma \cdot \bar{v} \cdot \bar{B}^2$. Fluids with a small electrical conductivity produce only very small Lorentz forces. Thus, a sensitive balance system is necessary for measurement. This limits the weight of the magnet system (we use the magnetization M as surrogate) and causes external disturbances to have a high influence on the force signal. In order to increase the force to noise aspect ratio, the objective function has to take into account two conflicting goals: maximize the Lorentz force and minimize the magnetization.

$$\min \begin{pmatrix} f_1(x) \\ f_2(x) \end{pmatrix} = \begin{pmatrix} -F_L(\Phi, \Theta, M) \\ \sum_{k=1}^{8} M_k \end{pmatrix}$$
$$\text{such that}$$
$$\Phi_i \in [-\pi, \pi],\ i = 1, \ldots, 8,$$
$$\Theta_j \in [0, \pi],\ j = 1, \ldots, 8,$$
$$M_k \in [0, 10^6],\ k = 1, \ldots, 8$$

The Lorentz force is thereby calculated by a time consuming (20–120 s) simulation run while the magnetization can be calculated analytically. In the above optimization problem $\Phi \in \mathbb{R}^8$ and $\Theta \in \mathbb{R}^8$ describe the direction of the magnetization vector. Both functions are assumed to be smooth. The derivatives of the second objective can be easily determined while already the first derivative of the first objective can only be approximated by numerical differentiation. As this requires in general many functional evaluations, it should be avoided. The second objective is even linear and also the feasible set is a linearly constrained set (there are only box constraints). The first objective is nonlinear and has locally optimal solutions which are not globally optimal.

Portfolio optimization. The portfolio optimization problem is formulated as a bi-criterion optimization problem, where the reward (mean of return) of a portfolio is maximized, while the risk (variance of return) is to be minimized. Practical portfolio optimization problems use extensions to the Markowitz model, and these often use several risk measures, e. g., quantile-based risk measures [3]. These measures replace variance in the standard mean-variance model, thus leading to an entire family of mean-risk portfolio selection models. This makes the problem heterogeneous as the first objective is linear and the second objective has stochastic terms. Many other practical portfolio optimization formulations even use a tri-objective problem so as to find trade-offs between risk, return, and the number of securities in the portfolio [4], which is even more heterogeneous (continuous, stochastic, and integer-valued functions are involved). An overview on extended Markowitz models for further reading can be found in [29]. Conditional values at risk and satisficing constraints can also be incorporated.

Multi-objective inventory routing. The *inventory routing problem* (IRP) describes a generalization of the classical vehicle routing problem (VRP), in such that delivery volumes, i. e., the quantities of the products delivered to customers in a logistics network, are considered to be additional variables. While early research on this problem can be traced back to the 1980s [9], it has only recently been investigated in its true formulation as a multi-objective problem [12]. The bi-objective formulation of [12] introduces two objectives: the inventory levels held by the customers in the network are to be minimized (a typical consideration in just-in-time logistics), and the costs for transporting the goods to the customers are minimized. Obviously, the two criteria are in conflict with each other. A decision support system for this biobjective IRP is visualized in [16]. There, it could be observed that the minimization of the inventory levels is of lower practical difficulty than the minimization of the routing costs. The reasoning behind this is based on the observation that delivery volumes simply are the setting of a single variable value for each customer, and the subsequently held inventories are directly affected by the amount of delivered products. However, the solution of the resulting VRP is difficult even for small data-sets, and in practical cases with reasonable running time restrictions, only (meta-)heuristics appear to be promising solution approaches [15].

Interventional radiology in medical engineering. An essential component of interventional radiology is the procedure of minimally invasive therapeutic interventions, for example in the vasculature. Since the line of sight is interrupted, the interventional material used in these procedures, e. g., catheters, guide wires, stents, and coils, are tracked by imaging techniques. In this application we consider the deformable 3D-2D registration for CT. With the considered method the patient motion during the intervention can be corrected. Only such a procedure can reconstruct artifact-free volumes showing the true position of the interventional material. A bicriterial approach is taken in [11], which is based on raw data and adapts the position of the prior volume immediately to the position included in the raw data without a reconstruction. One objective is the sum of squared differences in raw data domain and the other is a regularization term which originates from physical models for fluids and diffusion processes. An application of a gradient method to this bicriterial problem would require the solution of an implicit differential equation for the computation of a gradient direction. In order to reduce the inhomogeneity of the objectives the bicriteria optimization is done in an alternating manner. The raw data fidelity is minimized by a conjugate gradient descent and the resulting vector fields are then convolved with Gaussian kernels to realize regularization. This alternation between the two objectives is only possible using a special linking term combining both objectives. With this technique one gets the required images with high quality in a faster way.

4.3.4 Aspects of Heterogeneity

Functions of multi-objective problems may differ in several, usually interconnected aspects, of which the following could be identified:

Scaling. An objective function's range of values may be quite different from the range for other objective functions of the problem.

Landscape. Objective functions may differ quite considerably in basic features, as their degree of multi-modality, presence of plateaus, separability, or smoothness. An even richer description can be achieved by calculating empirical summary characteristics such as fitness-distance correlation, auto-correlation, or the numerous features developed under the term exploratory landscape analysis (ELA) [24]. These require evaluating a space-filling sample drawn from the domain of the multi-objective problem. Such features may be less intuitive than theoretical properties, but nonetheless they are designed to correspond to the practical performance of heuristic optimization methods, and thus provide valuable information about the function. However, current ELA features are designed for individual objectives and the design of specific features capturing the multiobjective problem characteristics, like e.g. front shape, local fronts etc., is still an open research topic. The relationship between the individual ELA features and multiobjective problem characteristics would be very helpful in assessing the influence of objective heterogeneity.

Evaluation time. Each objective or constraint function of a multi-objective problem may take a different amount of time to evaluate. These differences may result from different theoretical complexity of the functions, different size of the domain of the functions (see Domains below), or other differences. In practical problems, the heterogeneity of evaluation times could be large, for example if one objective function was a simple sum while the other one was evaluated by conducting a physical experiment [1, 2]. A further point related to evaluation time is that some functions may be computed more quickly if another solution, whose function value is known and differing in the values of a small number of decision variables, is available. In some cases the ability to evaluate efficiently the objective functions by computing the difference (or delta) from an existing solution is very important (e. g. in symmetric TSP) for local search methods.

Theoretical and practical difficulty. Some functions may be more or less difficult to optimize in terms of the number of solutions that must be explored in order to find an optimum (e. g., using a local search or other iterative search method). Differences in practical difficulty between the objectives could be a result of different theoretical complexity of the functions, or different domain sizes, or different properties of the fitness landscape.

Domains. Let us consider the binary relation "intersects with" between all pairs of domains of the objective functions and constraints as a graph. This graph may have only one connected component, or there would be no conflict between some of the functions. However, the domains do not necessarily have to be completely identical, either. This holds especially for constraints, which usually concern only a subset of the variables. Consequently, not all functions have to be defined on variables of the same data type.

Parallelization. Each objective function could have different restrictions regarding the amount of parallelization. E. g., some objective functions might require physical equipment or software licenses, which restrict the number of function evaluations that can be executed in parallel.

Problem class. It may be known that some objective belongs to a different problem class than another. Examples are the aforementioned TSP and shortest path.

Analytic form vs. black box. Some objective function may be available in analytic form, while another may be available only as a black box. This usually implies that the evaluation time differs considerably between the objective functions (see above). Moreover, while for the analytic functions the derivatives can be calculated, they can only be approximated for black-box functions using numerical differentiation.

Determinism. Some objective functions of a problem may be stochastic, while others might be deterministic.

4.3.5 Benchmarks

For investigating this topic in controlled experiments, "artificial" benchmark problems are a useful tool. Here we argue which existing benchmarks exhibit heterogeneity and how even more heterogeneous ones could be constructed.

Continuous benchmarks. In the area of evolutionary multi-objective optimization a large number of continuous test instances are collected in [14]. These have different landscapes as for instance one objective is linear and the second one is highly nonlinear. This is used to create convex, non-convex, mixed convex-concave, and multi-modal problems. The objectives in ZDT, SZDT, RZDT, and WFG test problem instances are heterogeneous. One of the test functions is linear (or piecewise linear) while the other objective(s) are highly nonlinear and multi-modal. DTLZ test problem instances, on the other hand, use similar objective functions (using sine and cosine terms) and hence are not heterogeneous at first sight. They might differ in terms of ELA features, however. Simple benchmark functions like e.g. the Schaffer or Binh problems are homogeneous, though. Instances with differing evaluation times can be easily constructed by inserting a time delay in the respective functions. Moreover, noise can be added to a subset of the objectives in order to address heterogeneity in terms of determinism as discussed above.

KP benchmarks. We carried out some preliminary experiments to construct heterogeneous discrete problems. The bi-objective unidimensional 01 knapsack problem (KP) was used as a basis for these investigations. Its objective is to optimize $\vec{f} = (\max \sum_{j=1}^{n} c_j^1 x_j,$ $\max \sum_{j=1}^{n} c_j^2 x_j)^T$ under the side constraints $\sum_{i=1}^{n} w_j x_j \leq \omega$ and $x_j \in \{0, 1\}$. Four families (A/B/C/D) of instances are already provided by the MOCOlib [25]. Among them are family A, where c_j^1, c_j^2 are randomly generated for $i = 1, \ldots, n$ ($1 \leq c_j^1, c_j^2 \leq 100$), and family C, which contains patterns (plateaus where l_i is the length and v_i is the value) created by choosing v_i randomly in $\{1, \ldots, 100\}$, $c_1^1 = c_2^1 = \ldots = c_{l_1}^1 = v_1$, and $c_{l_1+1}^1 = c_{l_1+2}^1 = \ldots = c_{l_1+l_2}^1 = v_2$. In [8] it was observed that the patterns tend to make the MOCO problem harder to be solved. So, our preliminary impression is that the patterns provide a way to introduce a form of heterogeneity in functions.

We also constructed some new families by combining different existing ones, e. g., by taking objective 1 and resource constraint from family A and objective 2 from family C. This way, we obtained five new families, called AC, AL, AZ1, AZ12, and AZ3. In preliminary experiments with a solver taken from [5, 6], the comparison of results obtained on A, AZ12, and AZ3 indicated that the presence of "null" plateaus seems to affect the performance of the solver negatively. More research on this topic shall follow.

Constraint satisfaction benchmarks. Max-SAT-ONE [28, 22] is an example of a bi-criterion constraint satisfaction problem with objectives heterogeneous in their (assumed) computational complexity class. The first objective is NP-hard, while the other objective is a simple sum over variables and is hence linear.

Max-SAT-ONE is a relative of the logical Satisfiability (SAT) problem, an archetypal decision problem with a central role in theoretical computer science as the first to be proved NP-Complete [7]. In an instance of the SAT problem a number c of logical clauses involving a number n of Boolean variables are presented. The problem is to determine whether there is an assignment to the variables that satisfies all the clauses. The optimization form of the problem, known as MAX-SAT, is also well-known. The problem, the subject of intensive research for a number of years, follows the same form as SAT but for the objective, which is now to maximise the number of satisfied clauses. The problem is NP-hard, and examples of techniques developed for the problem can be found in [20, 27].

Max-SAT-ONE has been studied in the context of constraint programming [22] and decomposition methods in multiobjective optimization [28]. The first objective is that of MAX-SAT, while the second one is to maximize the number of variables with an assignment of TRUE. This leads to a discrete Pareto front with at most n distinct Pareto optimal points.

TSP benchmarks. One of the possibilities is to use a MOCO problem with objectives defined mathematically in the same way, but with different distribution of parameters. Paquete [26] and Lust and Teghem [21] proposed a set of travelling saleperson (TSP) instances with various classes of objective functions:

- Euclidean instances: the costs between the edges correspond to the Euclidean distance between two points in a plane, randomly located from a uniform distribution.
- Random instances: the costs between the edges are randomly generated from a uniform distribution.
- Clustered instances: the points are randomly clustered in a plane, and the costs between the edges correspond to the Euclidean distance.

They also proposed mixed instances: the first cost comes from the Euclidean instance while the second cost comes from the random instance. They observed some differences in behavior of the multiobjective algorithms for these instances. The Lin-Kerninghan heuristic used in the first phase required significantly more time for random than for Euclidean instances. The Pareto local search used in the second phase was on the other hand faster on Euclidean instances due to much lower number of efficient solutions. The time performance of mixed instances was in between in both cases.

The above mentioned multiobjective traveling salesman problem with profits [18] is an interesting candidate for discrete benchmark problem with heterogeneous objectives. It is relatively simple in definition, based on well studied TSP problem, and contains several aspects of heterogeneity – different mathematical definitions, different difficulty, different domains.

4.3.6 Conclusions and Outlook

Our study suggests that heterogeneity between the objectives of a multiobjective optimization problem is both common and yet little understood (or even considered) in the literature. We have made a modest start on providing motivating examples and beginning a characterization of this complex feature. There seems to be a rich vein to investigate further, and much work to do in proposing and testing suitable methods.

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4.4 Visualization in Multiobjective Optimization (WG4)

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4.4.1 Introduction

Visualization is useful and needed for many purposes in multiobjective optimization. Roughly speaking, we can identify three main uses for visualization: as a tool for analyzing either sets of solutions or individual solutions, as part of decision support in applying interactive methods, and as a tool for analyzing performance of algorithms. One can say that visualization itself has multiple objectives. On one hand, visual representations or graphics should be easy to comprehend so that no relevant information is lost but, on the other hand, no additional, unintentional information should be included as a byproduct. Whichever way visualization is used, it is closely connected to graphical user interface design.

People are familiar with e.g. simple bar charts or pie diagrams and understanding them is not regarded demanding. However, as soon as the dimensions or the amount of the information to be visualized increases [34], there are many challenges involved. In both developing visualizations and interpreting them, one should avoid introducing biases like having unintentional meanings associated to colors (which may be culture-dependent) or assignment of axes to represent different dimensions of the information being visualized. It may not be possible to generate self-explanatory visualizations but cognitive training is needed. Overall, contextual awareness of all parties involved is important.

As mentioned, visualization has many purposes and has a lot to offer for various needs. Surveys of visualization techniques for multiobjective optimization and multiple criteria decision making are given in [21, 25, 29, 43]. The work [29] also contains many further references relevant for visualization. When analyzing sets of solutions or individual solutions, it is beneficial to exploit the geometric structure of Pareto front approximations or the connection between the decision and the objective space. As part of decision support, new ways can be provided to decision makers for directing the progress of interactive methods. When analyzing the performance of algorithms, one can exploit recent algorithm advances. Furthermore, new technologies like virtual or augmented reality and 3-D printers etc. give a new meaning to visualization.

In what follows, we briefly consider different visualization problems and tools and provide further references.

4.4.2 Open problems

Visualization is generally seen as a powerful means of conveying information to humans by harnessing the strong information processing capabilities associated with human vision and cognition. However, while humans are usually quite comfortable with two-dimensional data, effective visualization rapidly becomes more difficult as the number of dimensions increases, due to a combination of human and technical factors. Indeed, multidimensional data visualization is intimately tied to the features and limitations of the computing and display technologies available and to the cognitive limitations associated with the high numbers of dimensions and high volumes of data.

In this section, some of the challenges posed by visualization in the context of multiobjective optimization are discussed, from selecting the information to be visualized, through to the visual representation of individual solutions and of families of solutions, possibly under uncertainty, and finally to user interaction.

Selecting information to be visualized

Large amounts of high-dimensional data impose both a computational burden (on equipment) and, more importantly, a cognitive burden on users that may simply render visualization ineffective or even impossible. Therefore, information (data and/or dimensionality) reduction techniques are often required, the goal being to provide the user with a sufficiently accurate representation of the data which highlights the most relevant features without introducing unintended artifacts. In practice, as elaborate representations are often used to embed multiple dimensions into two- or three-dimensional representations, cognitive training is often required before users can usefully process such representations.

Particularly in multiobjective optimization, users (as decision makers) are usually concerned both with the values and with the relations among the various data points. Appropriate notions of Pareto front approximation quality and of the relative importance of the different objectives are, therefore, required. Once such concepts are established, selecting the information to be visualized reduces to solving the corresponding computational problems, which is often another challenge in itself, especially as the number of objectives increases.

Identifying representative sets. For many continuous, discrete or mixed discrete-continuous multiobjective optimization problems, one can compute a large set of Pareto optimal or nearly Pareto optimal solutions. In such a case, it becomes more difficult to compare solutions in the decision space and identify the possible tradeoffs between them in the objective space.

For visualization, one can follow two approaches, possibly combined, to deal with the large size of a set of computed solutions. First, given a set of solutions, one can identify a subset of solutions which (1) has a smaller size and (2) satisfies some quality criterion. Two widely used criteria are the hypervolume indicator, to be maximized, and the additive or multiplicative ε-coverage. Satisfying both (1) and (2) seems to be difficult above the bi-objective case (see e.g. [6] for the ε-coverage criterion), but optimal subset selection can now be performed rather efficiently based on the hypervolume indicator and ε-dominance [7, 22], but also uniformity and coverage [46].

Second, one can try to group together solutions that behave similarly in the decision space or in the objective space. Clustering techniques are used to this end. In the objective space, the Euclidean distance is relevant for quantitative objectives. In the decision space, the distance between solutions has to be chosen according to the context, in order for the result of the clustering to be meaningful. An interesting recent approach, found in [45], attempts to generate clusters of solutions that are "compact and well separated" both in the decision space and in the objective space. To this end, two validity indexes are defined to minimize intracluster distances and maximize intercluster distances, in the decision and objective spaces, respectively. Therefore the clustering problem is itself a bi-objective problem for which one seeks compromise solutions, i.e. clusters of solutions that are good both in the decision and objective spaces..

Reducing objective space dimensionality. Dimensionality reduction is a fundamental task in data visualization. In particular, all data must be projected on two dimensions to be displayed e.g. on a computer screen. Such a physical limitation may be alleviated to some extent by 3D display technologies (whether stereoscopic, volumetric or holographic) and/or by resorting to animation, but ultimately the number of dimensions that can be used directly is low.

At a more abstract level, the number of visualization axes may be extended further, e.g. by associating them with properties of the different graphical objects displayed, as with bubble charts. In addition to the cognitive training required to interpret such representations, a fundamental limitation of those techniques is that the representation of a point may then occlude that of another point. Thus, the amount of data displayed, as discussed in the previous subsection, the number of dimensions actually represented, or both, need to be reduced.

As pointed out by Brockhoff and Zitzler [8], there are two distinct approaches to dimensionality reduction: feature extraction and feature selection. Considering the visualization of the objective space in multiobjective optimization, feature extraction consists in producing a (small) set of arbitrary axes, possibly by non-linearly combining the original objectives, so as to represent the given data as well as possible. Principal component analysis and maximum variance unfolding have been used for objective reduction [41], and are are examples of such techniques. Unfortunately, although they may preserve certain types of relationships in the data, dominance relationships are usually not preserved [38], and unwanted biases may be introduced in the representation of Pareto front approximations. The cognitive burden imposed on the decision maker, who has to accommodate additional, artificial, objectives, and deal with potentially misleading dominance information, is also increased.

A feature selection approach to objective space dimensionality reduction, on the other hand, consists in selecting a subset of the original objectives to be visualized allowing dominance information to be more strictly preserved. Since conflicting objectives are at the heart of multiobjective optimization, it is natural to see non-conflicting objectives as good candidates to be discarded. More specifically, objectives that do not affect the set of Pareto optimal solutions are termed redundant, and can be safely omitted from the optimization, although they may be of semantic interest to the decision maker [2].

Several interpretations of what conflicting objectives are have been proposed. For Purshouse and Fleming [38], there is conflict between two objectives when improvement in one objective leads to deterioration with respect to the other. A similar view is adopted also by other authors [23, 41], although the actual definition of conflict may vary. Brockhoff and Zitzler [8], on the other hand, define conflict as a relation between sets of objectives, based on the structure of the corresponding weak Pareto dominance relations. Since such a notion of conflict is often too strict, they extend it using the concept of ε-dominance to arrive at a measure of degree of conflict, and at a subset selection formulation of objective reduction.

Assigning objectives to visualization axes. Prior to visualization, one needs to decide how to map the objectives to visualization axes. While this might seem straightforward and is often done implicitly by assigning objectives to visualization axes in their existing order, many visualization methods are order-sensitive and produce significantly different visualizations for different arrangements of objectives. Consider, for example, bubble charts, parallel coordinates [18], radar charts (or star plots) [10], radviz [17], interactive decision maps [24], hyper-space diagonal counting [1], heatmaps [37], hyper-radial visualization [11] and prosections [43].

A lot of research on this topic, called also axes (re-)ordering, has been devoted to parallel coordinates. Assigning the objectives to parallel coordinates so that a similarity measure is maximized is an NP-complete problem [4]. While the similarity between adjacent objectives/axes seems to be the focal point of most work, our working group has agreed that in multiobjective optimization we often need to show conflicts between objectives. These conflicts can be difficult to observe if similarity between adjacent objectives is enforced. We are also missing more research of other methods such as bubble charts, where one needs to determine which of the objectives is going to be represented with color (or size), and discussions on how decision maker's preferences influence such choices.

Visualizing solutions and surfaces

The illustration of solutions and surfaces in objective space plots is a valuable tool not just for dynamically elucidating the progress of the algorithms but also exploiting the results in applications (e.g. enabling to shed light on some features of the problem). Meaningful graphical displays should offer domain experts information about the range of Pareto optimal solutions and the assessment of the trade-offs between the competing objectives, thus conveying relevant information to aid the selection of a final recommendation or a reduced set of solutions for further screening. Human information processing strongly relies on visual processes to deal with large amounts of data and unveil patterns that lead to sounder decisions, thus minimizing cognitive effort.

Different types of plots, namely scatter plots, are used to visualize 2-D and 3-D (approximations of) Pareto optimal sets. These plots are quite informative in 2-D problems and in most cases provide useful information in 3-D problems, although in this case visualization challenges may already arise due to the complexity of the surfaces or sets of solutions to be displayed. Additional information may be portrayed in scatter plots using size or color (e.g. bubble charts). Whenever the problem has more than three objective functions, sometimes projection techniques may be of help, but no general technique exists offering straightforward visualization in higher dimensions ensuring clarity, intuitiveness, and intelligibility. Dimension reduction approaches to obtain 2-D or 3-D mappings include, among others, self-organizing maps [20] and interactive decision maps [24], which attempt to highlight different features of data under analysis. Self-organizing maps are unsupervised neural networks that generate a mapping of the high dimension data into cells (array of nodes) usually in 2-D, which may then be clustered according to some similarity measure. Nodes are associated with weighting vectors (one vector per node), which are sorted and adapted such that similar data are mapped to the closest node. Interactive decision maps approximate the feasible objective set (and the objective points dominated by it) by developing frontiers of bi-objective slices that display as "topographical" maps (i.e. avoiding intersections). Animation, or its snapshots, can be used to deal with problems with more than three objectives.

Techniques aimed at encompassing the whole information include parallel coordinates [18] and heatmaps [37]. In parallel coordinate plots each evaluation dimension is visualized on a vertical axis and each data point is represented as a line connecting the corresponding values on those axes. A high number of dimensions to be visualized using parallel coordinate plots and too many data points may result in a dense and unclear view. Heatmaps organize data in rows (solutions) and columns (objective function or other feature under analysis). An extensive use of color is made to convey information of the matrix elements, although some color schemes are criticized with the arguments of the lack of a natural perceptual ordering or erroneous perceptions of color gradients due to color changes between matrix cells. In some way, enabling the interchange of rows or columns may circumvent these issues.

In general, in projection schemes there is no Pareto dominance preserving mapping from a higher- to a lower-dimensional space, i.e. erroneous dominance relations may appear in lower-dimensional displays that are not present in original points. [43] use the projection of a section ("prosection") to visualize 4-D points in 3-D in an intuitive manner, in such a way that the shape, range and distribution of points are reproduced.

Empirical attainment functions (EAF) [15, 14], which are associated with the probabilistic distribution of the (approximation of) Pareto sets, can also be used to offer visualizations, by using cutting planes to cut through the 3-D objective space of the EAF values and display the resulting intersections in 2-D [44].

Visualizing uncertainty

Uncertainty is an inherent characteristic of real-world problems arising from multiple sources of distinct nature. It is generally unfeasible that mathematical and decision aid models could capture all the relevant inter-related phenomena at stake, get through all the necessary information, and also account for the changes and/or hesitations associated with the expression of the decision makers' preferences. In addition to structural uncertainty associated with the knowledge about the overall system being modeled, input data (model coefficients and parameters) may suffer from imprecision, incompleteness or be subject to changes.

Preferences are often ill-specified at the outset of a decision support process and they should be progressively strengthened through experimentation and learning for increasing the confidence in a final recommendation. Once a final solution is selected for execution, the decision variables may drift from the computed values, e.g. in case they are associated with some components of an engineering design project. That is, uncertainty may arise in the model structure, in the mathematical model coefficients, in preferences and in the behavior of the decision variables after implementation.

Therefore, it is of utmost importance to provide decision makers with robust conclusions. The concept of robust solution is not uniformly defined in the literature but it is generally linked to the guarantee of a certain degree of "immunity" to data perturbations and adaptive capability (or flexibility) regarding an uncertain future and ill-shaped preferences, leading to an acceptable performance even under a plausible set of unfavorable conditions [12, 5, 19]. In this setting, uncertainty visualization techniques may have a role in influencing decisions and decision makers' confidence in the recommendations to be adopted. Several approaches have been proposed to communicate to decision makers the effects of uncertainty upon solution quality, which should be tailored to the context of the study in order to convey useful information to decision makers. In general, uncertainty adds further dimensions to the visualization to display the uncertain outcomes. How this is operationalized also depends on how uncertainty is captured (e.g., probability distribution functions, fuzzy sets, intervals).

The most common approach is juxtaposition, i.e. providing a visualization of the effects of uncertainty in a separate display together with a crisp representation. This approach can be extended by means of a toggle capability, thus enabling swapping between the crisp representation and the uncertain ones possibly controlled by a "perturbation" parameter. This technique also enables to offer a dynamic view of the uncertain outcomes associated with model coefficients or preferences uncertainty. For instance, dynamic bars juxtaposed to a crisp solution representation may help in distinguishing the relationship between desirable and undesirable outcomes according to uncertainty parameters and user-defined thresholds of acceptability. Overlay techniques are also used on top of the visualization of crisp outcomes, by combining different types of displays. Colors can be added to represent degrees of uncertainty associated with solutions.

These approaches can be combined with pictorial solution displays, for instance in network optimization problems in which solutions can be shown on a (real or schematic) map. In these cases both value uncertainty and positional uncertainty would be at stake as information to be conveyed to decision makers. Some approaches have been specifically designed to assist decision makers in dealing with uncertainty visualization in multiobjective optimization models. In this context, the main issues stated in the previous sections regarding visualization in high dimensional spaces apply, with even more significance since additional dimensions should be taken into account. The hyper-space diagonal counting method maps the n-dimensional Pareto front to two- or three- dimensional data thus enabling to visualize it in a succinct way [1]. However, as reported in [35] this method does not preserve all neighborhoods when collapsing the n-dimensional data onto two or three dimensions, i.e. different grouping schemes of the n-dimensional neighborhoods may lead to different visualizations. In [35], the hyper-radial visualization method proposed in [11] is used to incorporate into the analysis random and epistemic uncertainty associated with preference choices.

Visualization in Interactive Solution Processes

In interactive multiobjective optimization methods, a solution pattern is formed and repeated so that a decision maker iteratively takes part and provides preference information to direct the solution process (see, e.g. [26, 27, 33, 39]). Her/his preference information is used to generate one or more new Pareto optimal solutions. In this way, only those Pareto optimal solutions that are interesting to the decision maker are generated and the decision maker considers a small set of Pareto optimal solutions at a time. If visualization is used to provide preference information or feedback to guide the interactive method, we can call it visual steering.

It is important to utilize visualization in both providing preference information and analyzing the solutions generated. This should enable the decision maker to express one's wishes of what kind of solutions are more desirable and understand the consequences of these preferences and compare the solutions obtained. Different methods utilize different preference information and offer different types of information to the decision maker which naturally means that different visualizations are needed. The dimensions and the complexity of the problem also set their own requirements on the visualization techniques to be applied.

As mentioned in the introduction, visualization is closely connected to graphical user interface design. Examples of studies in user interface design for the WWW-NIMBUS implementation [31] of the interactive NIMBUS methods [32] are given in [30, 40]. Further example of user interface design are given in [42] for the interactive Pareto Navigator method [13] and in [16] involving heatmap visualizations and particle swarm optimization.

Different people prefer different visualizations and, thus, it is desirable not to use only one but different visualizations that the decision maker can compare and combine or switch between them. The objective space typically has a lower dimension than the decision space and that is why the consideration of preferences often takes place in the objective space but the connection between the two spaces can be important. It may, e.g. be necessary to consider the corresponding solution in the decision space to be able to evaluate the goodness of a solution in the objective space. In this, the visualizations in the decision space are typically problem-specific whereas objective vectors can be visualized with problem-independent visualizations. Further research is still needed to enable steering in both decision and objective spaces.

One can think of taking full advantage of visualization in connection of interactive methods from at least two perspectives: starting from what the method needs or starting from what visualization techniques can offer. This will likely lead to new method development and new software implementations. Examples of software implementations including visualizations are Grapheur [9], IND-NIMBUS [28, 36] and iMOLPe [3].

When visualization and the interaction are successful, it may also lead to reformulating the problem instead of solving it. The challenge of making the most of the expertise of the decision maker is crucial in the success of applying interactive methods. Visualizations can be a key in not only expressing preference information but enabling insight gaining and learning.

4.4.3 Tools

Many tools for visualization of multidimensional data exist. This working group wanted to to provide a (non-exhaustive) list of tools that are especially suitable for visualization in multiobjective optimization and are often used by the researchers in this field.

Free and/or open-source software

Visualization Tool Kit (VTK) (http://www.vtk.org/) is a software system for 3-D computer graphics, image processing and visualization. The VTK library is used by a number of scientific data visualization tools, such as Mayavi (http://code.enthought.com/projects/mayavi/), ParaView (http://www.paraview.org/) and VisIt (https://wci.llnl.gov/simulation/computer-codes/visit).

A separate (non VTK-based) environment for scientific computation, data analysis and data visualization is SCaVis (http://jwork.org/scavis/). The data visualization tool XmdvTool (http://davis.wpi.edu/xmdv/) supports a variety of interaction modes and tools, including brushing, zooming, panning, and distortion techniques, and the masking and reordering of dimensions.

Two powerful high-level programming languages that include numerical computation and optimization in addition to visualization are Scilab (http://www.scilab.org/) and GNU Octave (https://www.gnu.org/software/octave/).

Some basic tools that can be used to produce publication quality figures comprise gnuplot (http://www.gnuplot.info/), matplotlib (http://matplotlib.org/), GLE (http://www.gle-graphics.org/), and PGFPlots (http://pgfplots.sourceforge.net/). When producing such plots, the online tool ColorBrewer (http://colorbrewer2.org/) can be used to help select good color schemes.

Proprietary software

Tools, such as Optimus (http://www.noesissolutions.com/Noesis/), modeFRONTIER (http://www.esteco.com/modefrontier/), OptiY (http://www.optiy.eu/) and DecisionVis (https://www.decisionvis.com/) use advanced and interactive visualization methods to aid the engineering design and optimization process.

MATLAB (http://www.mathworks.com/products/matlab/) is a high-level language and interactive environment that can be used for optimization as well as visualization of multidimensional data.

Finally, Trade Space Visualizer (http://www.atsv.psu.edu/) is a data visualization program designed to help users explore multidimensional data sets to discover relationships between features.

Note that while these tools are generally not free, some offer free academic licenses.

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4.5 Multiobjective Optimization for Interwoven Systems (WG5)

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4.5.1 Introduction

Complex systems' optimization is responsive to the demand that computational sciences solve more and more complex problems. A complex system is defined to be a natural or engineered system that is difficult to understand and analyze because it may (1) involve interactions among many phenomena; (2) have multiple and dissimilar components or subsystems that may be connected in a variety of ways and as a whole exhibit one or more properties not obvious from the properties of the individual parts; (3) be characterized by noncomparable and conflicting criteria. Indeed, many entities of interest to humans are complex systems. In the literature, these systems are also referred to as interwoven systems or systems of systems [23]. Natural complex systems such as human body, oceans, climate, and many more have been around since ever and their understanding have been of great significance to people. Energy or telecommunication infrastructures, manufacturing systems, service sector systems are examples of man-made or engineered complex systems. In the modern global world, man-made systems become more and more widespread and omnipresent, and therefore of growing importance to the society.

For complex systems, the overall decision-making goal is to harmonize local requirements and goals to attain the objectives required of the entire system. The overall system performance depends on the interactions and synergy of all its parts, and human preferences are not always captured in the mathematical model. In the presence of multiple components and criteria, a unique decision optimal for the system does usually not exist but rather many or even infinitely many decisions are suitable. Because of the synergy among the components, the overall system performance is not implied by the simple sum of their performances but is enriched by the synergy among them. Furthermore, when the complex system achieves an “optimal” solution, the system may not have been optimized as a whole because its overall mathematical model may not exist, or if it exists, it makes computations prohibitively expensive. In this case, a solution to the complex system is achieved by optimizing only its components and coordinating their optimal solutions. In effect, due to the features and demands of complex systems, decision-making for them requires tools originated from multiobjective optimization that additionally account for the coupling among the components and the coordination of subsystem optimal solutions into an overall system optimal solution.

Literature on complex systems with multiple criteria is rather limited. The first studies in multiobjective complex problems are undertaken for hierarchical systems in [19, 20, 21, 14, 28, 22] and later continued in [12, 3]. Large-scale hierarchical multiobjective systems are studied in [20, 21, 14]. Other papers propose (i) decomposition of the original problem modeled as one integrated multiple objective problem (MOP) into a collection of smaller-sized sub-problems, for which the development of a solution procedure becomes a more manageable task, and (ii) coordination of the solutions of the sub-problems to obtain the solution of the original problem. A large number of such approaches exists for specific applications in the management sciences, engineering, and multidisciplinary optimization (see [19, 29] among many others). Other papers deal with decomposition and coordination due to a large number of criteria in the original problem [18, 14, 2, 12, 3]. Finally some papers study objective decompositions from a predominantly mathematical perspective [30, 24, 5, 25].

Multidisciplinary design optimization (MDO) had been developed within the engineering community to coordinate results of various disciplines involved in design. The MDO focus has been to either encapsulate disciplinary optimizations into subproblems that are coordinated by a super-optimizer or use sensitivity information to relate the effect of one disciplinary optimization on another. Multiobjective optimization has been introduced to strengthen MDO techniques attempting to deal with noncomparable and conflicting design objectives that are characteristic for each design discipline. Numerous papers present applications of multiobjective MDO in various areas of engineering design, however, formal methodologies such as Multiobjective Collaborative Optimization [29, 27], Multiobjective Concurrent Subspace Optimization (CSSO) [16, 15] and a bilevel method [35] are also proposed.

The discipline-based decomposition of a system, the driving force for MDO, has also been replaced with other types of decomposition such as scenario-based or object-based decomposition, each leading to studying a collection of multiobjective problems. If a system performs in multiple scenarios and each of them is driven by different objective functions, the resulting collection represents a set of multiobjective problems where each of them models the performance of the system in a scenario. Refer to [8, 31, 32] for multiscenario multiobjective optimization in engineering design. An effort to quantify trade-offs between disciplines or scenarios is undertaken in [6, 7]. Physical or object-based decomposition leads to studying a system composed of subsystems and components that can interact with each other in various ways, which additionally increases the complexity of the overall problem. A collection of multiobjective problems naturally emerges because each of the elements may perform according to multiple criteria. Calculation of the Pareto sets of such complex systems is studied in [9, 10, 11].

In this preliminary study, we consider interwoven systems that can be modeled as two interacting subsystems, each modeled as a multiobjective optimization problem (cf. Sec. 4.5.2). The goal is to develop an initial mathematical model of this system and approaches to its optimization. Several examples of such interwoven systems are presented in support of the proposed modeling paradigm (cf. Sec. 4.5.3). Notions of optimality that recognize the overall system optimality as well as local subsystem optimality are introduced, cf. Sec. 4.5.4. Optimization-based solution approaches are proposed as the composition architectures allowing the computation of the optimal solutions (cf. Sec. 4.5.5). Finally in Sec. 4.5.6, connections of the proposed approach to other areas of optimization and systems science are discussed.

4.5.2 Model

A simple yet non-trivial setup of an interwoven system consists of three parts: two subsystems and the interaction between them. The subsystems come in the form of the following optimization subproblems.

Subproblem 1:

$$\begin{aligned} &\min\ f_1(x_0, x_1, y_{21}) \\ &\text{s.t.}\ \ g_1(x_0, x_1, y_{21}) \leqq 0 \\ &\qquad x_0 \in X_0,\ x_1 \in X_1 \end{aligned}$$

and Subproblem 2:

$$\begin{aligned} &\min\ f_2(x_0, x_2, y_{12}) \\ &\text{s.t.}\ \ g_2(x_0, x_2, y_{12}) \leqq 0 \\ &\qquad x_0 \in X_0,\ x_2 \in X_2 \end{aligned}$$

where $X_i \subseteq \mathbb{R}^{n_i}$ for $i = 0, 1, 2$ and $y_{21} \in \mathbb{R}^{n_{21}}$, $y_{12} \in \mathbb{R}^{n_{12}}$ for some $n_0, n_1, n_2, n_{21}, n_{12} \in \mathbb{N}$. Each subproblem has objective functions $f_i : \mathbb{R}^{n_0} \times \mathbb{R}^{n_i} \times \mathbb{R}^{n_{ji}} \to \mathbb{R}^{p_i}$, and constraint functions $g_i : \mathbb{R}^{n_0} \times \mathbb{R}^{n_i} \times \mathbb{R}^{n_{ji}} \to \mathbb{R}^{q_i}$, $i, j = 1, 2,\ i \neq j$, for some $p_i, q_i \in \mathbb{N}$. Note that Subproblems 1 and 2 share some common decision variables $x_0 \in X_0$ while they also comprise model-specific decision variables x_1 and x_2, respectively.

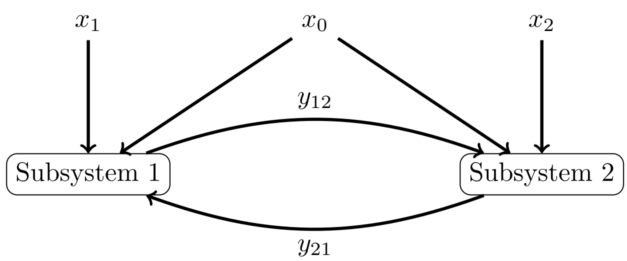
The interaction between the subsystems is modeled with *linking functions* ℓ_1 and ℓ_2 that yield the values of the *linking variables* y_{21} and y_{12}. The interaction is then typically expressed by a system of *interaction equations*:

$$y_{12} = \ell_1(x_0, x_1, y_{21}) \qquad \text{and} \qquad y_{21} = \ell_2(x_0, x_2, y_{12}).$$

where $\ell_i : \mathbb{R}^{n_0} \times \mathbb{R}^{n_i} \times \mathbb{R}^{n_{ji}} \to \mathbb{R}^{r_i}$ for some $r_i \in \mathbb{N}, i, j = 1, 2, i \neq j$. This system of interaction equations has the form of *implicit representation* of linking variables y_{12} and y_{21} by means of linking functions ℓ_1 and ℓ_2. However, an explicit representation of y_{12} and y_{21} of the following form may also exist:

$$\begin{aligned} y_{12} &= y_{12}(x_0, x_1, x_2) \\ y_{21} &= y_{21}(x_0, x_1, x_2) \end{aligned}$$

A graphical exemplification of this setup is given in the following figure:



Feasibility of decision variables may refer to either of the two subsystems or to the interwoven system. This observation motivates the following definitions.

▶ **Definition 1.** A solution (x_0, x_i, y_{ji}) $(i \neq j)$ is said to be *i-subsystem feasible* if $x_0 \in X_0$, $x_i \in X_i$, $g_i(x_0, x_i, y_{ji}) \leqq 0$ and y_{ji} satisfies the interaction equations $y_{ji} = \ell_j(x_0, x_j, y_{ij})$ for some $x_j \in X_j$, where $y_{ij} = \ell_i(x_0, x_i, y_{ji})$.

▶ **Definition 2.** A pair of solutions (x_0, x_1) and (x_0, x_2) is said to be *multisystem feasible* if they are feasible for each system respectively and x_0, x_1, x_2 satisfy the system of interaction equations given by the implicit representation.

In other words, given (x_0, x_1, x_2) such that (x_0, x_1) and (x_0, x_2) are multisystem feasible, the resulting $(x_0, x_1, x_2, y_{21}, y_{12})$ is feasible for the two subproblems.

4.5.3 Examples

An interwoven system consists of interacting subsystems. In some areas of human activity, the susbsystems are developed independently from each other. For example, in engineering design the subsystems of an automotive vehicle such as an engine or a suspension are designed by different companies. Even that each company's designers anticipate that these subsystems will work together within one system (vehicle), the subsystem designs are carried out with limited or even without any information about the future interaction between the subsystems. In other applications, such as location of facilities, subsystems were not even meant to work together when they were being developed but later, due to new circumstances, they necessarily start to interact with each other as an interwoven system.

A countless number of interwoven systems are encountered in daily life and numerous examples can be identified e. g., in traffic systems, multidisciplinary design, or evacuation planning to name just some areas. Nonetheless, some comprehensible examples shall be listed in the following for the sake of intended exemplification of the proposed model.

An Academic Example

Let $X_i = \mathbb{R}$, $i = 0, 1, 2$ and, let $x_i, y_{12}, y_{21} \in \mathbb{R}$, $i = 0, 1, 2$. The scalar-valued objective functions f_1 and f_2 of the subproblems are defined as

$$f_1(x_0, x_1, y_{21}) = x_0^2 + x_1^2 y_{21}$$
$$f_2(x_0, x_2, y_{12}) = (x_0 - 5)^2 + x_2^2 y_{12}$$

The values of the linking variables y_{21} and y_{12} are specified by the following linking functions ℓ_1 and ℓ_2:

$$y_{12} = 2x_0 - 3x_1 + y_{21} = \ell_1(x_0, x_1, y_{21})$$
$$y_{21} = -x_0 + 4x_2 - y_{12} = \ell_2(x_0, x_2, y_{12})$$

For this problem, the following explicit representations can be calculated:

$$y_{21} = -\frac{3}{2}x_0 + \frac{3}{2}x_1 + 2x_2$$
$$y_{12} = \frac{1}{2}x_0 - \frac{3}{2}x_1 + x_2.$$

Integrated Location Problem

Let a finite set of customer locations $A = \{a_1, \ldots, a_M\}$ be given in the plane $\mathbb{R}^2$. Suppose that some group of decision makers, referred to as DM 1, wants to locate an airport at a location $x_1 \in X_1 \subseteq \mathbb{R}^2$. Suppose that for some given weights $w_m^1 \geq 0$, $m = 1, \ldots, M$, the sum of weighted distances between the customers and the airport is to be minimized. Another group of decision makers, say DM 2, wants to locate a hospital at a location $x_2 \in X_2 \subseteq \mathbb{R}^2$ which should (among others) also serve the same set of customers. Given some weights $w_m^1 \geq 0$, $m = 1, \ldots, M$, the maximum weighted distance between the customers and the hospital is to be minimized. The hospital acts as a repulsive facility for the airport (due to noise) which is expressed by some weight $-\lambda_2 < 0$. The airport acts as an attractive facility for the hospital since emergencies occurring at the airport have to reach the hospital quickly. This aspect is modeled by a weight $\lambda_1 > 0$. Staff of the airport and of the hospital will jointly use a service facility, e. g., providing childcare, which has to be located at a location $x_0 \in X_0 \subseteq \mathbb{R}^2$.

The resulting interwoven system can again be specified by identifying the two subproblems corresponding to the two subsystems and by expressing the linking functions.

Subproblem 1: Location of the Airport

$$
\begin{aligned}
&\min\ f_{11}(x_0, x_1, y_{21}) = \sum_{m=1}^{M} w_m^1 d(x_1, a_m) - \lambda_2 d(x_1, y_{21})\\
&\min\ f_{12}(x_0, x_1, y_{21}) = d(x_0, x_1)\\
&\text{s.t.}\ \ x_0 \in X_0,\ x_1 \in X_1
\end{aligned}
$$

Subproblem 2: Location of the Hospital

$$
\begin{aligned}
&\min\ f_{21}(x_0, x_2, y_{12}) = \max\left\{\max_{m=1,\ldots,M} w_m^2 d(x_2, a_m);\ \lambda_1 d(x_2, y_{12})\right\}\\
&\min\ f_{22}(x_0, x_2, y_{12}) = d(x_0, x_2)\\
&\text{s.t.}\ x_0 \in X_0,\ x_2 \in X_2
\end{aligned}
$$

Interaction Equations. The interaction equations are given by the linking functions ℓ_1 and ℓ_2 as

$$
\begin{aligned}
y_{12} &= \ell_1(x_0, x_1, y_{21}) := x_1\\
y_{21} &= \ell_2(x_0, x_2, y_{12}) := x_2,
\end{aligned}
$$

which is again an explicit representation of the linking variables.

Traveling Thief Problem

The traveling thief problem (TTP) consists of two well-known, interacting combinatorial subproblems, the Traveling Salesman Problem (TSP) and the Knapsack Problem (KP). This interaction can be described as follows.

Subproblem 1: Knapsack Problem. A subset of m items numbered $1, \ldots, m$ has to be packed into a knapsack. Each item has a value $b_j \geq 0$ and a weight $w_j \geq 0$, $j = 1, \ldots, m$. The knapsack has a limited capacity Q and it is filled by a thief who wants to maximize the total (additive) value of the items packed while not exceeding the knapsack's capacity. Using binary decision variables $z_1, ..., z_m$, the problem can be modeled as follows:

$$\max f_1(z, b) = \sum_{j=1}^{m} b_j z_j$$

$$\text{s.t.} \sum_{j=1}^{m} w_j z_j \leq Q$$

The solution of the knapsack problem is a binary vector called picked items $z = (z_1, \ldots, z_m)$. Each element z_j, $j \in \{1, \ldots, m\}$ is a binary variable being 1 if the corresponding item is picked and 0 otherwise.

Subproblem 2: Traveling Salesman Problem. The TSP subproblem is one of the classic NP-hard optimization problems. In this problem, there are n cities and the distances between the cities are given by a distance matrix $D = (d_{ij})$ (d_{ij} is the distance between city i and j, $i, j = 1, \ldots, n$). There is a salesman who must visit each city exactly once and minimize the time of the complete tour. While it is usually assumed that the speed v of the salesman is constant throughout every tour, we consider also varying velocities $v(\pi_i)$ of the salesman that depend on the last visited city $\pi_i \in \{1, \ldots, n\}$. Then the TSP subproblem can be formulated as:

$$\min f_2(\pi, v) = \sum_{i=1}^{n} \frac{d(\pi_i, \pi_{i+1})}{v(\pi_i)}$$

$$\text{s.t. } \pi = (\pi_1, \pi_2, \ldots, \pi_n) \in \mathbb{P}_n,$$

where we set $\pi_{n+1} := \pi_1$ to simplify notation. Here, $\mathbb{P}_n$ denotes the set of all permutations of the set $\{1, \ldots, n\}$. The solution of the TSP subproblem is called a tour $\pi = (\pi_1, \cdots, \pi_n)$ where π_i is the i^{th} visited city.

Interaction Equations. In the TTP, there are two objectives, namely maximizing the total value of the knapsack and minimizing the total travel time. We assume that each item is located at one city and that the traveling thief can decide to pick an item or not when visiting the respective city. The more items the thief has picked, the lower his travel speed becomes. In other words, the velocity $v(\pi_i)$ after leaving city π_i depends on the items picked so far. This is modeled using two interconnecting variables:

1. The speed $v(\pi_i)$ of travel when leaving city π_i is related to the knapsack's current weight at city π_i, $i = 1, \ldots, n$:

$$v(\pi_i) = \ell_{1,\pi_i}(z, \pi, b) := v_{\max} - \left(\frac{v_{\max} - v_{\min}}{Q}\right) \sum_{k=1}^{i} \sum_{j=1}^{m} a_j(\pi_k) w_j z_j.$$

   The parameter $a_j(\pi_k)$ is equal to 1 if item j is located in city π_k, and zero otherwise. $v_{\max}$ and $v_{\min}$ are the maximum and minimum velocity of the thief, respectively, and Q is the capacity of knapsack. According to this formulation, the speed of the thief decreases when the weight of the knapsack increases, i.e., the speed captures the impact of the KP on the TSP.

2. The value b_j, $j = 1, \dots, m$, of the picked item j drops over time. In fact, the final value of the item at the end of the travel is not the same as its value when the thief picked the item. This value is dependent on travel time:

$$b_j = \ell_{2,j}(\pi, v) := b_j^{\text{init}} - \rho_j T_j(\pi, v)$$

where $T_j(\pi, v)$ is the time between the moment when item j located at city π_k (i.e., $a_j(\pi_k) = 1$) is picked and the end of the tour:

$$T_j(\pi, v) = \sum_{i=k}^{n} \frac{d(\pi_i, \pi_{i+1})}{v(\pi_i)}.$$

Moreover, ρ_j is a rate of decline in the value of b_j so that $b_j \geq 0$ for all possible values of T_j. The time-dependent value of the items captures the impact of the TSP on the KP.

4.5.4 Notions of Optimality

It is of interest to establish a concept of optimality for the interwoven system presented above. Note that such a concept could recognize all three parts of the system or just a subset of them. We propose three notions of optimality depending on the level of engagement of each subsystem in the overall system.

Assuming that each subsystem would like to perform best to the common good of both subsystems, we define cooperative Pareto solutions that are feasible for both systems.

▶ **Definition 3.** A multisystem feasible solution $(x_0, x_1, x_2, y_{12}, y_{21})$ is said to be *cooperative Pareto optimal* if it is Pareto optimal with respect to all objective functions.

Under the scenario that each subsystem would like to operate at its best for itself regardless of the values of the linking variables passed from the other system, we define individually Pareto-optimal solutions for each system.

▶ **Definition 4.** A solution (x_0, x_1, y_{21}) is said to be *individually Pareto optimal for Subsystem 1* if it can be extended to a multisystem feasible solution $(x_0, x_1, x_2, y_{12}, y_{21})$ and if there is no other multisystem feasible solution $(x'_0, x'_1, x'_2, y'_{12}, y'_{21})$ such that

$$f_1(x'_0, x'_1, y'_{21}) \quad \leq \quad f_1(x_0, x_1, y_{21}). \tag{5}$$

A solution (x_0, x_2, y_{12}) is said to be *individually Pareto optimal for Subsystem 2* if it can be extended to a multisystem feasible solution $(x_0, x_1, x_2, y_{12}, y_{21})$ and if there is no other multisystem feasible solution $(x'_0, x'_1, x'_2, y'_{12}, y'_{21})$ such that

$$f_2(x'_0, x'_2, y'_{12}) \quad \leq \quad f_2(x_0, x_2, y_{12}). \tag{6}$$

The third notion of optimality reflects that both systems might want to perform at their best simultaneously even if one of them could perform better while the other system is ignored.

▶ **Definition 5.** A pair of multisystem feasible solutions (x_0, x_1, y_{21}) and (x_0, x_2, y_{12}) are said to be *mutually Pareto optimal* if there is no other pair of multisystem feasible solutions (x'_0, x'_1, y'_{21}) and (x'_0, x'_2, y'_{12}) such that

$$\begin{pmatrix} f_1(x'_0, x'_1, y'_{21}) \\ f_2(x'_0, x'_2, y'_{12}) \end{pmatrix} \leq \begin{pmatrix} f_1(x_0, x_1, y_{21}) \\ f_2(x_0, x_2, y_{12}) \end{pmatrix} \tag{7}$$

4.5.5 Composition Approaches

We discuss some possible ways of composing the interwoven subsystems.

Biobjective All-in-One System

This approach imposes the least additional structure upon the interwoven system while composing it by bringing together the two subsystems in a natural biobjective way as follows.

$$\begin{aligned}
\min\ & \begin{pmatrix} f_1(x_0, x_1, y_{21}) \\ f_2(x_0, x_2, y_{12}) \end{pmatrix} \\
\text{s.t.}\ & g_1(x_0, x_1, y_{21}) \leqq 0 \\
& g_2(x_0, x_2, y_{12}) \leqq 0 \\
& x_0 \in X_0,\ x_1 \in X_1,\ x_2 \in X_2
\end{aligned}$$

where $y_{12} = \ell_1(x_0, x_1, y_{21})$ and $y_{21} = \ell_2(x_0, x_2, y_{12})$.

The term biobjective is used in relation to the two subsystems involved. Note that if f_1 or f_2 is a vector-valued function, the number of objectives in the above formulation will be more than two. Therefore, in general, this is a multiobjective optimization formulation. The Pareto-optimal solutions to this multiobjective problem can be considered as the solutions to the interwoven system.

As an example, consider again the academic example introduced in Section 4.5.3. The corresponding biobjective all-in-one system is in this case given by

$$\begin{aligned}
& \min f_1(x_0, x_1, y_{21}) = x_0^2 + x_1^2 y_{21} \\
& \min f_2(x_0, x_2, y_{12}) = (x_0 - 5)^2 + x_2^2 y_{12} \\
\text{s.t.}\ & y_{21} = -\frac{3}{2}x_0 + \frac{3}{2}x_1 + 2x_2 \\
& y_{12} = \frac{1}{2}x_0 - \frac{3}{2}x_1 + x_2.
\end{aligned}$$

An approximation of the nondominated set of this all-in-one system is illustrated in Figure 8. The points shown are obtained by sampling feasible solutions and filtering for dominated points.

Bilevel All-in-One System

In some situations, the interactions between the two subsystems may be modeled in a hierarchical way. In such cases, a bilevel programming framework may best describe the composed system. Such a composition does not need to utilize the variables x_0.

$$\begin{aligned}
\min\ & f_1(x_0, x_1, y_{21}) \\
\text{s.t.}\ & g_1(x_0, x_1, y_{21}) \leqq 0 \\
& y_{21} = \ell_2(x_0, x_2, y_{12}) \\
& x_0 \in X_0,\ x_1 \in X_1 \\
& x_2 \in \arg\min f_2(x_0, x_2, y_{12}) \\
& \qquad \text{s.t.}\ g_2(x_0, x_2, y_{12}) \leqq 0 \\
& \qquad\qquad y_{12} = \ell_1(x_0, x_1, y_{21}) \\
& \qquad\qquad x_2 \in X_2.
\end{aligned}$$

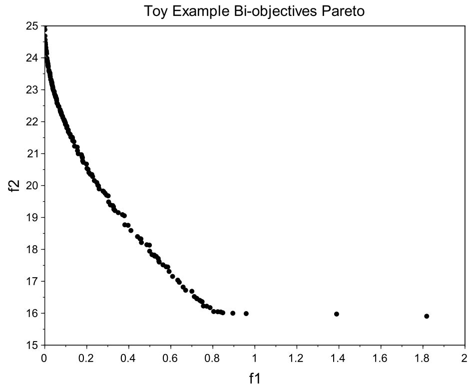


Figure 8 Approximation of the images of the cooperative Pareto solutions of the all-in-one system for the academic example introduced in Section 4.5.3.

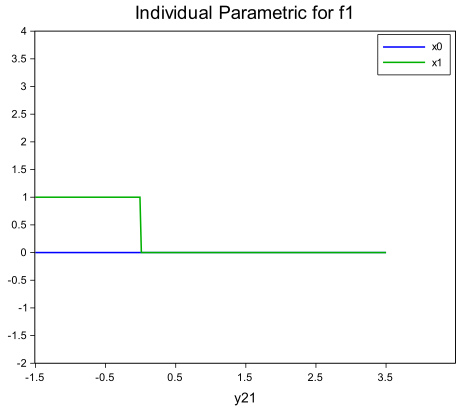


Figure 9 Dependence of the upper level variables x_0, x_1 on the output y_{21} of the lower level problem for the academic example introduced in Section 4.5.3.

In this bilevel problem the objective functions f_1 and f_2 can be scalar and/or vector-valued. Solutions to the interwoven system are solutions to this (possibly multiobjective) bilevel programming problem. The optimal (Pareto-optimal) solutions to this bilevel problem can be considered as optimal (Pareto-optimal) solutions to the interwoven system.

Considering again the academic example problem introduced in Section 4.5.3, Figure 9 shows the dependence of the upper level variables x_0 and x_1 from the value of the linking variable y_{21} that directly depends on the optimal solution x_2 of the lower level problem.

Individual Systems with Parameterized Interactions

The two subsystems may be decoupled by letting each subsystem treat the linking variables as parameters. The idea can be expressed as follows.

$$\min_{x_0, x_1} f_1(x_0, x_1; y_{21})$$

s.t. $g_1(x_0, x_1; y_{21})$ where $y_{21} \in [t_L, t_R]$ is a parameter.

$$\min_{x_0, x_2} f_2(x_0, x_2; y_{12})$$

s.t. $g_2(x_0, x_2; y_{12})$ where $y_{12} \in [u_L, u_R]$ is a parameter.

It is anticipated that best solutions to the two subsystems will be found by solving the subproblems independently. However, since the two subsystems must agree on the linking variables y_{21} and y_{12} and the common variable x_0, a solution mechanism that ensures such a conversion must be employed. This can lead to quite different implementations of the individual systems approach. Below, we describe two possibilities.

Analytical Target Cascading. Analytical target cascading (ATC) is a hierarchical, multi-level multidisciplinary methodology to optimize complex engineering design problems, see, for example, [17]. A system is hierarchically decomposed into individual design problems at each level, possibly in multiple subproblems. Once a higher-level problem is solved, solutions are propagated (cascaded) as targets to the lower-level and then solved at that level. The new solutions (responses) are in turn passed back up to the higher level. The solution process continues iteratively until solutions at every level are within a tolerance level of or as close as possible to the desired targets.

The approach is described in Algorithm 1 below in the form of a pseudocode for the simpler case of the interwoven system without the global variable x_0. However, more general cases can also be addressed with ATC. In the presented case, the linking variable y_{12} is treated as a target being sent down from subproblem 1 to subproblem 2, while the other linking variable y_{21} acts as a response to be send up from subproblem 2 to suproblem 1. In particular implementations, acceptable stopping criteria must be specified.

Algorithm 1 ATC for two subproblems without global variables

Initialize y_{21}^0
$k \leftarrow 0$
repeat
  $k \leftarrow k + 1$
  $x_1^k \leftarrow \arg\min_{x_1}\{f_1(x_1, y_{21}^{k-1}) | g_1(x_1, y_{21}^{k-1}) \leqq 0\}$
  $y_{12}^{k-1} \leftarrow \ell_1(x_1^k, y_{21}^{k-1})$
  $x_2^k \leftarrow \arg\min_{x_2} f_2(x_2, y_{12}^{k-1}) | g_2(x_2, y_{12}^{k-1}) \leqq 0\}$
  $y_{21}^k \leftarrow \ell_2(x_2^k, y_{12}^{k-1})$
until solution (x_1^k, x_2^k) is of acceptable quality

Bayesian Updates. The parameters in the individual systems can be treated as uncertain, although more accurately, these are "presently undetermined" for the particular subsystem in consideration. Since as in the above case, this is true for both subsystems, an iterative optimization mechanism must be employed to converge to a joint solution. At the start of the optimization process, subsystem 1 would formulate a prior distribution for the uncertainty in y_{21} – this could be uninformative or based on some initial estimates coming from subsystem 2. Subsystem 2 does the same. Then either hierarchically or simultaneously, some information sharing that leads to belief updates takes place. The iterative process is repeated until an acceptable solution is obtained.

4.5.6 Connection to Other Disciplines

Game Theory

The structure of interwoven systems can encompass game theoretic models by modeling subsystem behavior. This can be achieved by incorporating anticipation of other subsystem's responses into the objective function or the value function. It is also possible to incorporate different information sharing strategies of subsystems via linking variables. When subsystems exhibit some hierarchical structure as modeled in the bilevel formulation introduced in Section 4.5.5 (Bilevel All-in-One System), a Stackelberg game is relevant. When all subsystems are considered as simultaneous players, a Nash game may be implied [13, 33].

Robust Design

The structure defined in Section 4.5.5 (Bayesian Updates) can relate to robust optimization if a robustness-related metric is chosen as the value function in the sense that each subsystem's individual solution can be regarded as a robust solution where the interaction with the other subsystem is modeled as uncertain. In particular, each subsystem of an interwoven system could treat the interaction variable as an *uncertain* parameter although the interaction variables are *undetermined* rather than uncertain. This concept is embodied in the notion of *Type II Robust Design* [4] when interpreted in the context of coupled variables in a distributed problem [1].

Co-Evolutionary Algorithms

Studies in co-evolutionary computation investigate how separate subpopulations solve their own subproblems as a means of solving the complete problem – an approach known as *c*ooperative-co-evolution [26]. The sub-populations exchange their information at certain intervals, e.g., at a certain number of generations in an evolutionary algorithm. Although subpopulations try to optimize their own objectives, they have to cooperate to solve the overall problem [34].

4.5.7 Summary and Outlook

In this report a mathematical model for an interwoven system consisting of two subproblems was introduced. Different concepts defining the optimal performance of such an interwoven system were proposed, and the relation to associated multiobjective and bilevel optimization models was discussed. Several existing optimization methodologies were suggested as tools for generating optimal solutions to interwoven systems.

This research raises a variety of challenging and interesting questions. This includes generalizations to interwoven systems with more than two subproblems, an in-depth analysis of the similarities and the differences between different notions of optimality and between the associated optimization models, and the development and critical evaluation of efficient solution methods. The example problems mentioned in this report may serve as a first benchmark for such approaches.

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4.6 Surrogate-Assisted Multicriteria Optimization (WG6)

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4.6.1 Introduction

In real-world optimization it is very common to use either physical experimentation or simulators to evaluate solutions (see e.g. [39, 22, 43]). Such evaluation procedures can be costly and time-consuming, and there only a limited budget of evaluations is available. Surrogate-assisted optimization [23] (sometimes also referred to as metamodel-assisted optimization) is a common technique for solving such problems. There are many (specific) research questions that arise when studying this methodology, some of them specific to surrogate-model assisted multiobjective optimization. In this report we summarize sources of complexity and challenges to be met in this field and then discuss recently proposed solutions or prospective solution ideas on how to analyze complexity and how to deal with it.

The report is divided into two main sections: First, Section 4.6.2 discusses challenges and sources of complexity, distinguishing between problems specific to multicriteria surrogate-assisted problems and challenges that are inherited from more general optimization problem settings. Then, Section 4.6.3 proposes some initial ideas on how to meet open challenges related to problem complexity in this research field.

4.6.2 Challenges and Sources of Complexity

In this section, we review common and emerging challenges and sources for complexity. We divide them into two categories: challenges specific to optimization in general and challenges specifically relevant to surrogate-assisted optimization. In both of these categories, there are challenges that are relevant for multiobjective optimization and we will highlight them where applicable.

General challenges in optimization

The following challenges and sources of complexity can be encountered generally in optimization and are not specific to surrogate-assisted optimization. However, these issues can become even more relevant when using surrogates.

- **Functional landscape.** The structure of the fitness landscape has a huge impact on optimization. Examples of challenging landscape features include nonlinearity of objective functions, discontinuity in the objective space, and multimodal (deceptive) functions [25].
- **Decision variables and constraints.** Typical challenges in solving optimization problems include a large number of decision variables as well as a large number of constraints [9]. Recently, problems with dynamic constraints [5] and changing decision variables [3] arose, particularly in the experimental optimization community. Furthermore, problems with mixed-integer variables pose a general challenge in evolutionary optimization [30, 37, 19].
- **Objectives.** In addition, in multiobjective optimization, a high number of objective functions [16, 21] and heterogeneous functions (see e.g. [4, 2]) can provide additional challenges for both the algorithms and post-processing or decision making. Dynamically changing objective functions can increase the complexity further [8, 36].
- **Noise and uncertainty.** Noise and uncertainty are byproducts that are common in simulation-based and experimental optimization, and appropriate methods are needed for solving such problems [24]. Uncertainty can exist both in the decision space and the objective space. An example of noise are measurement errors typically present in experimental optimization [43], whilst imprecise knowledge about the model used in simulation-based optimization would represent a classical example of uncertainty [16].
- **Optimal use of many-core computers.** Recent problems in simulation-based optimization may feature time consuming objective function evaluations (simulations). Those problems can be solved by using general optimization algorithms, but often, algorithms tailored for such problems are needed if, for example, there exist a time limitation. One approach could be to utilize parallelization of the algorithm or the function evaluations [1].

Challenges specific to surrogate-assisted optimization

The following challenges and sources of complexity are directly related to approaches where surrogates are utilized and, thus, are not encountered generally in optimization.

- **Training time.** An important aspect in surrogate-assisted optimization is how much time it takes to train the metamodels used. If training takes too long, then it can significantly reduce the time saved by metamodelling. For example, if the data used in training is large, then matrix inversion needed in some metamodels could be time consuming [27].
- **Metamodel selection.** Many different types of metamodels have been developed over the years and it is not a straightforward task to choose the best one for the problem in question. One approach of overcoming this difficulty is to utilize multiple metamodels or ensembles of metamodels where the best metamodel can be dynamically selected during the optimization run, similar to [17, 29, 52]. Sometimes in multiobjective optimization different metamodels have to be used for different objective functions due to e.g. complexity of the objectives [48].
- **Surrogates for the Pareto front.** It is also possible to use surrogates for the Pareto front instead of the individual objective functions [14, 18, 34]. In that case, the input for training the surrogate is a (small) set of precomputed Pareto optimal solutions. The resulting surrogate can then be used for example for fast decision making with interactive multiobjective optimization methods. Typically in multiobjective optimization the number of objective functions is smaller than the number of decision variables and, therefore, building a surrogate for the Pareto front can be beneficial.
- **Discrete search spaces.** While applications with both discrete and continuous decision variables feature a general challenge to optimization, their presence can become a serious issue for surrogate-assisted optimization. Recent work aiming at overcoming these issues can be found in [31, 6, 47, 35].
- **Multi-fidelity models.** An approach to solve optimization problems with time consuming objective function evaluations is to use a collection of (meta)models that have different fidelity. In these approaches, one has to identify which (meta)model to use in which phase of the solution process. Controlling the model fidelity can be made dynamic by having an automated way of managing this at runtime [32].
- **Additional measurements/outputs.** Simulation-based and experimental optimization can produce a large amount of data although only a tiny fraction of it is utilized to compute the objective function values. It is an open question whether the remaining data can be utilized meaningfully to enhance search [22].

4.6.3 Prospective Solutions

Within the discussion of the workshop some interesting directions for prospective solutions were identified. They will be elaborated in the following.

Model learning for different objective and constraint functions

As outlined in the previous section, different objective and constraint functions can have different characteristics, such as computational effort, types of nonlinearity, e.g. multimodality and discontinuities, and noise. In this context we would like to point to the fact that such heterogeneity in multi-objective optimization is an emerging research topic in itself, discussed in another workgroup of the Dagstuhl Seminar, and here we will limit our discussion only to aspects relevant to surrogate models.

In [40] an automatic procedure for improving the accuracy of metamodels in an adaptive and iterative way is implemented. During the optimization process different modelling techniques are competing for modelling each single function. The performance assessment of metamodels is done independently for the different objective and constraint functions. Also, the evaluation takes place repeatedly during the run. In every iteration it is decided anew which model type is the best one to use for modeling a function. The last run's performance is decisive in this approach: Basically, the winning model on the data points evaluated in the last round will perform surrogate based optimization in the next round. Only, if one model becomes dominant in multiple runs it is taking over the task without further considering the other models (to save computation time).

This idea can be further elaborated by considering different online update schemes of the model-function assignment. An idea that seems to be straightforward in the machine learning context would be to use reinforcement learning [46] here, in order to learn by reward and punishment gradually the frequency of models to be used. It is known that reinforcement is robust, but adapts the frequencies relatively slow. This is, why we render this strategy to be promising only if the budget of function evaluation is moderate (say $\gg 100$) and not very small. A variation of the reinforcement paradigm that seems to lend itself well to online model selection is the multi-armed bandit paradigm [13], which has recently been used in operator selection for multi-criteria optimization. The reward function could take into account the achieved improvement (for instance in (hypervolume) set-performance indicators) or in average errors (model improvement).

Fast linear algebra techniques for large point sets

One of the main challenges specific to metamodeling is that the cost for training metamodels, in particular Gaussian processes (or Kriging) and to a smaller extend Radial Basis Function networks, becomes prohibitively high when the number of training instances (evaluated design points) becomes large.

Recall, that the computational cost of commonly used metamodels is related to the time required to invert the matrix of correlations based on the pairwise distances between design point. Therefore, the size of the matrix grows quadratically with the number of design points.

A solution to this problem that is often proposed is to use *fast approximate matrix inversion*. Although there are efficient algorithms for approximate matrix inversion available in the literature, they are to our knowledge not widely used in the surrogate-assisted optimization community. An interesting research topic would therefore be to compare these techniques in the context of surrogate-assisted optimization. As a first step in this direction we looked in the literature for some relevant techniques and overview papers.

The problem of approximate matrix inversion has been studied since the 70ties in applied mathematics [15], and has received recently increased attention in the machine learning research community. A good survey paper for approximate techniques for matrix inversion in the context of Gaussian processes is [38]. A state of the art method, that was implemented recently in mathematical packages is called Fully Independent Training Conditional (FITC), originally called Sparse Gaussian Processes using of Pseudo-Inputs (SGPP) [44]. These methods make use of the positive definiteness of the correlation matrix. Moreover, they select a relevant subset of the training points and perform the matrix inversion only on the submatrix for these point, while the other points still contribute to the computation of the final result. However, the selection of a subset of points is still based on simple heuristic and it will be interesting to investigate this deeper.

Another technique that is already used in metamodel-assisted evolutionary computation is called *local metamodelling*, where, as stated in [26], 'models are trained separately for each new population member on its closest data among the previously evaluated solutions'. Here the term population members refers to new candidate design points. This method has the advantage of smaller training time, but also to provide metamodels that are more based on the regional characteristic of the response surface rather than on its global structure. This is of particular importance if there is non-stationarity and hyperparameters that lead to good performance in one region but do not perform well in other regions.

A problem that occurs in this context is that discontinuities arise, when the set of nearest neighbors changes, causing problems for gradient-based optimization methods that require smooth surfaces. Moreover, artifacts such as local optima might be created – although this has hardly been studied up to now. In addition to this, if only the nearest neighbors are considered, clustering of sets might lead to ill-conditioned matrices or introduce a bias (e.g. considering points in one direction only). An interesting technique could be to use an adaptive archiving technique, similar to those proposed in [28] in the context of global robust optimization. The idea is to generate a design of experiments, for instance a Latin Hypercube Design [7], around the new design point and collect a nearest neighbors for each design point from the database. If there is no near neighbor to one of the design points, then a new evaluation is scheduled at this point. This strategy is a variant of an *active learning* approach [10], but more targeted towards the needs of optimization. In the context of multi-criteria optimization the amount of information and the radius of the design of experiments should be based on the characteristics of the function, which in first approximation can be derived from the hyperparameters of the model (for instance the estimated auto-correlation(s) and variances in Kriging/Gaussian process models). Already in the classical book on spatial statistics by Cressie [12] some advise for the radius in which relevant training points can be found was given, albeit for rather low dimensional data sets (2, 3 dimensions).

Exploiting dependences between objective and constraint functions

Nowadays, the common approach to use metamodels in multicriteria optimization is to train independent models for each objective and (implicit) constraint function. This makes computations simpler, for instance to compute multiobjective expected improvement [11, 42, 49], but on the other hand these models cannot exploit the possible correlation between different response variables. Hence, there are two difficulties that arise when using dependence information and we will briefly describe which techniques look promising in order to meet them:

Firstly, the computation of metamodels needs to be adapted. In the statistical community, it was dealt with using a technique called multi-output nonparametric regression [33]. More specifically, in the context of Kriging metamodels, it has been recently discussed under the term *multi-response metamodels* [41]. The idea in both approaches is to exploit the covariance between output variables (which could be objective function values or constraint function values). Also the computation of metamodel indicators will become more difficult.

Secondly, in order to compute measures, such as expected improvement, based on multivariate response formula, exact computation schemes [20] need to be modified. The block decomposition schemes right now need to be adapted by computing truncated multivariate Gaussian distributions. Recently, a package on truncated multivariate Gaussian distributions became available [50], which could be a good starting point in this direction.

Creating a benchmark

A recommendation for well referenced test problems was recently released by Surjanovic and Bingham [45]. It is available under the link http://www.sfu.ca/~ssurjano and contains a representative set of popular benchmark problems, including the Branin function, which became a standard test problem in surrogate-assisted optimization. However, a similar benchmark specific for simulator-based *multi-objective* optimization is to our knowledge still missing so far.

Metamodels for mixed-integer and combinatorial optimization

A first approach to use metamodels in mixed-integer and discrete parameter optimization is described in Li et al. [31]. It uses a heterogeneous metric that was developed for radial-basis function neural networks [51]. In the context of combinatorial optimization and permutations a comparison of distance measures was recently conducted by Zaefferer et al. [53]. Although using distances is an approach that works on more parametric problems, it could be interesting to look at machine learning approaches that can model discrete decision variables in a more problem specific way. Often the meaning and impact of a discrete decision variable can be estimated a-priori (e.g. switching on and off a process alternative in a flowsheet). In such cases modeling a problem specific graph metric could be a promising direction, e.g. by defining a transition graph and computing path distances in it. Also, as opposed to neural networks, the theory of Gaussian processes is more heavily based on the assumption of learning continuous functions. In this case we suggest to instead consider Markov random field models, when it comes to combinatorial search spaces. These also model local correlations, but are more natural to the problem and by introducing edge weights (transition probabilities) a neighborhood in terms of design point similarity can be modeled in a more intuitive manner. An open question, to our knowledge, is however to generalize the theory of Gaussian processes to mixed-integer spaces and fundamental research needs to be done in this direction.

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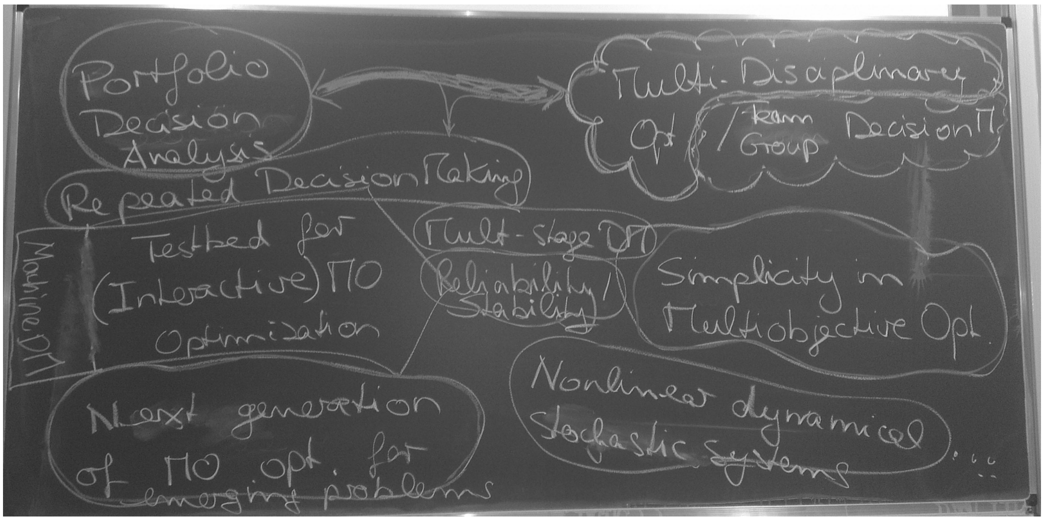
5 Topics of interest for participants for next Dagstuhl seminar

Photograph of topics of interest for participants for next Dagstuhl seminar.



6 Changes in the seminar organization body

6.1 Salvatore Greco steps down as co-organizer

On behalf of all the participants of the seminar, JK, KK and GR would like to extend our warm thanks to Salvatore Greco for his contributions to this Dagstuhl seminar series on Multiobjective Optimization as he steps down from the role of co-organizer, which he has held for three terms of office.

Salvo's passion and enthusiasm for research in multiobjective optimization made the seminars even more vivid and joyful than they are anyway. We are thankful for his advice and activities in the preparation and conduction of the seminar. Thank you, Salvo!

6.2 Welcome to Margaret M. Wiecek

We are pleased that our esteemed colleague Margaret M. Wiecek has agreed to serve as co-organizer for future editions of this Dagstuhl Deminar series on Multiobjective Optimization.

7 Seminar schedule

Monday, January 12, 2015

09:00–10:30: Welcome Session
- Welcome and Introduction
- Short presentation of all participants (3 minutes each!)

Coffee Break

11:00–12:00: Introduction to Complexity in Applications
- Robin Purshouse: Perspectives on the application of multi-objective optimization within complex engineering design environments
- Kaisa Miettinen: Sources of computational challenges in multiobjective optimization

Lunch

13:30–14:30: Introduction to Complexity in Preference
- Jürgen Branke, Salvatore Corrente, Salvatore Greco, Roman Slowinski, Piotr Zielnewicz: Preference learning in EMO: Complexity of preference models
- Manuel López-Ibánez: Machine Decision Makers: From Modeling Preferences to Modeling Decision Makers

Coffee Break

15:00- 16:00: Introduction to Complexity in Optimisation
- Matthias Ehrgott: Computational Complexity in Multi-objective (Combinatorial) Optimisation
- Michael Emmerich: An Open Problems Project for Set-Oriented and Indicator-Based Multicriteria Optimization

Break

16:15–18:00: Group Discussion about Hot Topics and Working Groups

Tuesday, January 13, 2015

09:00 – 10:00: Complexity in MO optimization Chair: Daniel Vanderpooten
- Carlos Fonseca: Pareto front approximation statistics
- Andrzej Jaskiewicz: Complex combinatorial problems with heterogeneous objectives

Coffee Break

10:30–12:00: Working Groups

Lunch

13:30–14:30: Complexity in Applications Chair: Sanaz Mostaghim

- Silvia Poles: Understanding and managing complexity in real-case applications
- Patrick M. Reed: Many-objective robust decision making under deep uncertainty: A multi-city regional water supply example

Coffee Break

15:00–17:00: Working Groups

17:00–18:00: Reports from Working Groups
- 6 minutes / 3 slides per working group
- General discussion and working group adaptations

Wednesday, January 14, 2015

09:00–10:00: Complexity in Applications Chair: Carlos Coello Coello

- Ralph Steuer: Tutorial on large-scale multicriteria portfolio selection leading up to difficulties obstructing further progress
- Yaochu Jin: Bridging the gap between theory and application in multi-objective optimization

Coffee Break

10:30–12:00: Working Groups

Lunch

14:00: Group Foto (Outside)

14:05–16:00: Hiking Trip

16:30–18:00: Reports from Working Groups
- 15 minutes / 5 slides per working group

Thursday, January 15, 2015

09:00–12:00: Working Groups

Lunch

13:30–14:30: Complexity in Optimization Chair: Serpil Sayin

- Margaret M. Wiecek: Distributed MCDM under partial information
- Gabriele Eichfelder: Variable ordering structures – what can be assumed?

Coffee Break

15:00–16:00: General Discussion: 10 Years of MCDM-EMO Dagstuhl Seminars. What do we Expect for the Future?

Break

16:30–18:00: Working Groups

20:00: Wine & Cheese Party (Music Room)

Friday, January 16, 2015

09:00–11:00: Presentation of Working Group Results

Coffee Break

11:30–12:00: Summary, Feedback, and Next Steps

Lunch & Goodbye

Participants

- Richard Allmendinger
University College London, GB
- Jürgen Branke
University of Warwick, GB
- Dimo Brockhoff
INRIA – University of Lille 1, FR
- Carlos A. Coello Coello
CINVESTAV, MX
- Salvatore Corrente
Università di Catania, IT
- Matthias Ehrgott
Lancaster University, GB
- Gabriele Eichfelder
TU Ilmenau, DE
- Michael Emmerich
Leiden University, NL
- José Rui Figueira
IST – Lisbon, PT
- Carlos M. Fonseca
University of Coimbra, PT
- Xavier Gandibleux
University of Nantes, FR
- Martin Josef Geiger
Helmut-Schmidt-Universität – Hamburg, DE
- Salvatore Greco
University of Portsmouth, GB
- Jussi Hakanen
University of Jyväskylä, FI
- Carlos Henggeler Antunes
University of Coimbra, PT
- Hisao Ishibuchi
Osaka Prefecture University, JP
- Johannes Jahn
Univ. Erlangen-Nürnberg, DE
- Andrzej Jaszkiewicz
Poznan Univ. of Technology, PL
- Yaochu Jin
University of Surrey, GB
- Miłosz Kadziński
Poznan Univ. of Technology, PL
- Kathrin Klamroth
Universität Wuppertal, DE
- Joshua D. Knowles
University of Manchester, GB
- Renaud Lacour
Universität Wuppertal, DE
- Manuel López-Ibáñez
Free University of Brussels, BE
- Luis Marté
PUC – Rio de Janeiro, BR
- Kaisa Miettinen
University of Jyväskylä, FI
- Sanaz Mostaghim
Universität Magdeburg, DE
- Vincent Mousseau
Ecole Centrale Paris, FR
- Mauro Munerato
ESTECO SpA – Trieste, IT
- Boris Naujoks
FH Köln, DE
- Luís Paquete
University of Coimbra, PT
- Silvia Poles
Noesis Solutions – Leuven, BE
- Robin Purshouse
University of Sheffield, GB
- Patrick M. Reed
Cornell University, US
- Enrico Rigoni
ESTECO SpA – Trieste, IT
- Günter Rudolph
TU Dortmund, DE
- Stefan Ruzika
Universität Koblenz-Landau, DE
- Serpil Sayın
Koc University – Istanbul, TR
- Pradyumn Kumar Shukla
KIT – Karlsruher Institut für Technologie, DE
- Roman Słowiński
Poznan Univ. of Technology, PL
- Ralph E. Steuer
University of Georgia, US
- Michael Stiglmayr
Universität Wuppertal, DE
- Heike Trautmann
Universität Münster, DE
- Tea Tusar
Jozef Stefan Institute – Ljubljana, SI
- Daniel Vanderpooten
University Paris-Dauphine, FR
- Simon Wessing
TU Dortmund, DE
- Margaret M. Wiecek
Clemson University, US
- Xin Yao
University of Birmingham, GB