Explainable multiobjective optimization

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Overview

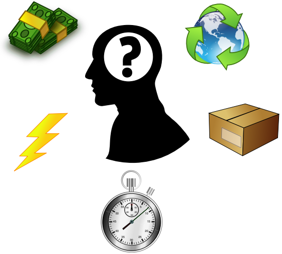
Motivation

Multiobjective optimization

- Real-life problems often consist of multiple conflicting objectives.
- These problems have many compromise, non-comparable solutions with various trade-offs.
- A domain expert, known as the decision maker, is needed to find the *best* solution.
- The decision maker can provide preferences, which are used to find the best solution.

Multiobjective optimization

- Multiobjective optimization methods support the decision maker in finding the best solution.
- The solution is then used in real-life decision-making.
- Often decision makers lack support in providing preferences.
- Can the decison maker *trust* the solution found? Can the solution be *justified* in any way?



Explainability and multiobjective optimization

- Could we make multiobjective optimization methods explainable?
- **Initial idea:** borrow existing techniques from explainable artificial intelligence (XAI).
- In my thesis, I explore a new paradigm: **explainable (interactive) multiobjective optimization**.

Explainable multiobjective optimization

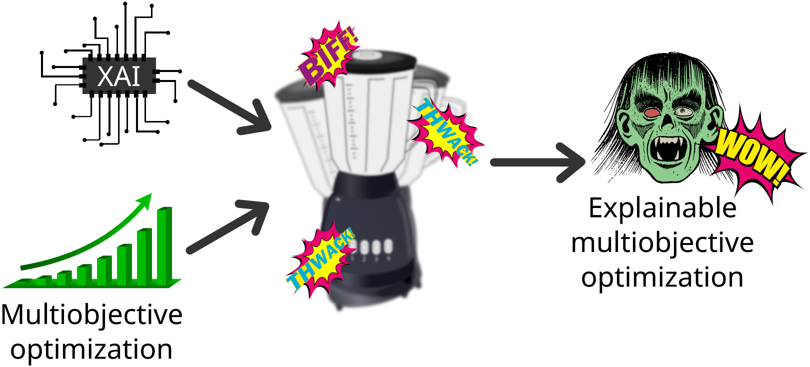


Figure: The main theme of my PhD.

Multiobjective optimization problems

- A multiobjective optimization problem has many conflicting objectives, which are to be optimized simultaneously[1].

Multiobjective optimization problem

A multiobjective optimization problem can be defined as

$$\min F(\mathbf{x}) = (f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_k(\mathbf{x})), \tag{1}$$

where $f_1 \ldots f_i$, $i \in [1, k]$ are objective functions and $\mathbf{x}$ is a decision variable vector. The vectors $\mathbf{x}$ can be subject to both **box-constraints** and **function constraints**. Feasible $\mathbf{x}$ belong to the *feasible variable space* S or $\mathbf{x} \in S$.

[1] Kaisa Miettinen. *Nonlinear multiobjective optimization*. Boston: Kluwer Academic Publishers, 1999.

Box-constraints

$$x_i^{\text{low}} <= x_i <= x_i^{\text{high}}, x_i \in \mathbf{x} \tag{2}$$

Function constraints

$$\begin{aligned} g(\mathbf{x}) - \delta_g &> 0 \\ h(\mathbf{x}) - \delta_h &= 0 \\ \delta_g, \delta_h &\in \mathrm{R} \end{aligned} \tag{3}$$

- In (2) x_i^{low} and x_i^{high} are the lower and higher limits for the ith element in $\mathbf{x}$, respectively.
- In (3) δ_g and δ_h are scalar values which should be exceeded or be exactly matched by $g(\mathbf{x})$ and $h(\mathbf{x})$, respectively.

More definitions

Objective vector

An objective vector $\mathbf{z}$ is the image of the solution $\mathbf{x} \in S$ such that $F(\mathbf{x}) = \mathbf{z}$. The set of objective vectors Z consists of all the images $\mathbf{z}$.

Pareto optimality

A solution $\mathbf{x}^* \in S$ is said to be Pareto optimal if, and only if, there does not exist any other solution $x \in S$ such that $f_i(\mathbf{x}) \leq f_i(\mathbf{x}^*) \, \forall i \in [1, k]$ and $f_i(\mathbf{x}) < f_i(\mathbf{x}^*)$ for at least some $i \in [1, k]$.

Pareto front

The Pareto front Z^{Pareto} consists of the images of all the Pareto optimal solutions. The set of Pareto optimal solutions is the Pareto optimal solution set.

More definitions

Ideal and nadir points

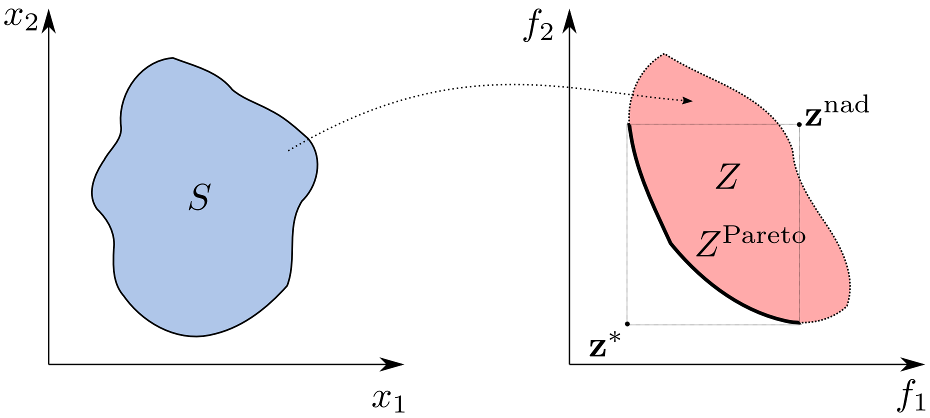
The ideal $\mathbf{z}^*$ and nadir $\mathbf{z}^{\text{nad}}$ points represent the best (lowest) and worst (highest) values of the objective function values on the Pareto front, respectively.

Reference point

A reference point $\bar{\mathbf{z}}$ is a vector of aspiration levels $\bar{z}_i, i = 1...k$. The reference point can be provided by a decisision maker, in which case, the reference point represents the decision maker's preferences.

Important concepts graphically

$$\min_{\mathbf{x}\in S}\{f_1(\mathbf{x}), f_2(\mathbf{x})\}$$



Scalarization

- Multiobjective optimization problems can be scalarized using a scalarizing function $s : \mathrm{R}^k \to \mathrm{R}$.

Scalarized problem

$$\begin{aligned} \min \quad & s(\mathbf{F}(\mathbf{x}); \mathbf{p}) \\ \text{subject to} \quad & \mathbf{x} \in S, \end{aligned} \tag{4}$$

where **p** is a set of additional parameters given to the scalarizing function .

- Scalarizing functions usually have some desiderable properties, such as guaranteeing (weak) Pareto optimality of the solution found.

Scalarization

- Scalarizing function used in STOM[2]:

STOM

$$\mathrm{STOM}(\mathbf{F};\bar{\mathbf{z}},\mathbf{z}^{**}) = \max_{i=1,\dots,k}\left[\frac{f_i(\mathbf{x}) - z_i^{**}}{\bar{z}_i - z_i^{**}}\right] + \rho\sum_{i=1}^{k}\frac{f_i(\mathbf{x})}{\bar{z}_i - z_i^{**}}, \tag{5}$$

where $\mathbf{z}^{**} = (z_1^* - \delta, z_2^* - \delta, \dots, z_k^* - \delta)$ is an utopian point with $\delta \in \mathrm{R}^+$, and $\rho \in \mathrm{R}^+$.

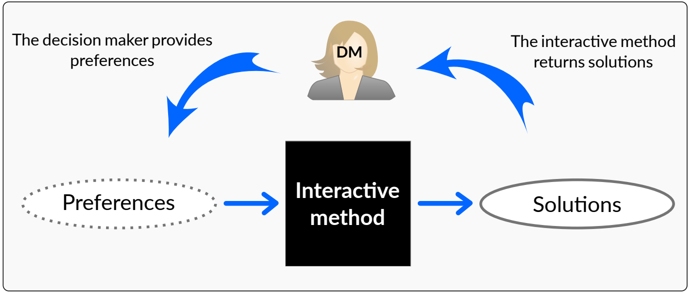
- A reference point $\bar{\mathbf{z}}$ can be incorporated in scalarizing functions.
- More examples of scalarizing functions in[3].

[2] Hirotaka Nakayama. "Aspiration Level Approach to Interactive Multi-Objective Programming and Its Applications". In: *Advances in Multicriteria Analysis*. Ed. by Panos M. Pardalos, Yannis Siskos, and Constantin Zopounidis. Boston, MA: Springer, 1995, pp. 147–174. ISBN: 978-1-4757-2383-0. DOI: 10.1007/978-1-4757-2383-0_10.

[3] Kaisa Miettinen and Marko M. Mäkelä. "On scalarizing functions in multiobjective optimization". In: *OR Spectrum* 24.2 (2002), pp. 193–213. DOI: 10.1007/s00291-001-0092-9.

Interactive method

- A decision maker (DM) iteratively provides preference information as a reference point.
  - New solution(s) are computed for the problem after each iteration.
- We focus on reference point based interactive methods.

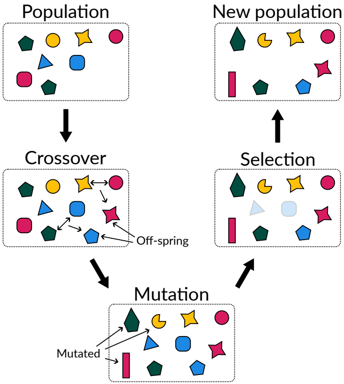


Evolutionary multiobjective optimization

- Instead of scalarizing a multiobjective optimization problem (1), we can also use evolutionary methods.
- In evolutionary methods, genetic algorithms inspired by Darwinian evolution are used to *evolve* a population of solutions over a number of generations with the goal of improving the population after each generation.
- This way, a bunch of *approximate* solutions can be found at once to a multiobjective optimization problem. But we have no guarantee of the Pareto optimality of the solutions...

Evolutionary multiobjective optimization

One generation in an evolutionary method



Improving in each generation

Evolutionary multiobjective optimization

- Interactive evolutionary multiobjective optimization methods exist as well.
- The preferences provided by a decision maker can be used to guide the evolutionary process towards potentially interesting solutions.
- For examples, see[4].

[4] Jussi Hakanen et al. "Connections of reference vectors and different types of preference information in interactive multiobjective evolutionary algorithms". In: *2016 IEEE Symposium Series on Computational Intelligence (SSCI)*. Athens, Greece: IEEE, 2016, pp. 1–8. DOI: 10.1109/SSCI.2016.7850220.

Explainable Artificial Intelligence

- The field of explainable artificial intelligence (XAI)[5] focuses on the study and development of artificial intelligence that is capable of functioning in a way understandable by humans.
- Clear focus on machine learning methods, especially deep neural networks and deep learning in general.
- Usually model interpretability (by humans) and predictive power correlate negatively. I.e., most powerful machine learning models are also black-boxes.
- Roughly two main approaches to explainability: using interpretable models and model agnostic approaches.

[5] David Gunning et al. "XAI–Explainable artificial intelligence". In: *Science Robotics* 4.37 (2019). DOI: 10.1126/scirobotics.aay7120.

Why explainability?

- If we use artificial intelligence (AI) for decision-making, we cannot blindly trust any model.
- How to tell if a model works correctly? How to justify decisions made based on these models?
- Explainability aims to uncover these issues by shedding light on the black-box.
- There is societal pressure in EU as well to consider explainability in AI: GDPR recital 71[6] (right to explanation[7]).

[6] https://www.privacy-regulation.eu/en/r71.htm

[7] Bryce Goodman and Seth Flaxman. "European Union regulations on algorithmic decision-making and a "right to explanation"". In: *AI magazine* 38.3 (2017), pp. 50–57.

Motivating examples

If the field of XAI is new to you and you work with AI/ML, I would highly suggest the following reads:

- Essay published in Nature by Cynthia Rudin on why we should stop explaining black-box models and use interpretable models instead.[8]
- Examples on how usage of AI can do more harm than good in society.[9]
- A very handy reference to start using interpretable AI.[10]
- A more traditional text book on XAI.[11]

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[8] Cynthia Rudin. "Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead". In: *Nature Machine Intelligence* 1.5 (2019), pp. 206–215.

[9] Hans de Bruijn, Martijn Warnier, and Marijn Janssen. "The perils and pitfalls of explainable AI: Strategies for explaining algorithmic decision-making". In: *Government Information Quarterly* 39.2 (2022), p. 101666.

[10] Christoph Molnar. *Interpretable Machine Learning. A Guide for Making Black Box Models Explainable*. 2nd ed. 2022. URL: https://christophm.github.io/interpretable-ml-book.

[11] Uday Kamath and John Liu. *Explainable Artificial Intelligence: An Introduction to Interpretable Machine Learning*. Springer, 2021.

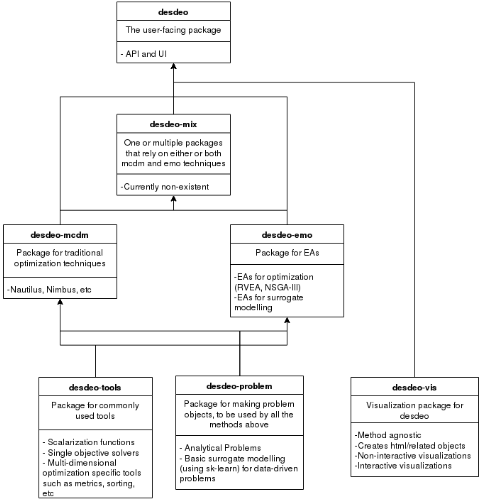
Paper 1: DESDEO

DESDEO

- DESDEO[12] is a Python software framework for interactive multiobjective optimization.
- It is open source and has a modular structure. It consists of four main packages:
  - `desdeo-problem`
  - `desdeo-tools`
  - `desdeo-mcdm`
  - `desdeo-emo`
- DESDEO is very central in my thesis, since my work is very much method development and implementation.
- Anybody is free to use and contribute to DESDEO.

[12] G. Misitano et al. "DESDEO: The Modular and Open Source Framework for Interactive Multiobjective Optimization". In: *IEEE Access* 9 (2021), pp. 148277–148295. DOI: 10.1109/ACCESS.2021.3123825.

DESDEO


desdeo
The user-facing package
- API and UI
desdeo-mix
One or multiple packages that rely on either or both mcdm and emo techniques
-Currently non-existent
desdeo-mcdm
Package for traditional optimization techniques
-Nautilus, Nimbus, etc
desdeo-emo
Package for EAs
-EAs for optimization (RVEA, NSGA-III)
-EAs for surrogate modelling
desdeo-tools
Package for commonly used tools
- Scalarization functions
- Single objective solvers
- Multi-dimensional optimization specific tools such as metrics, sorting, etc
desdeo-problem
Package for making problem objects, to be used by all the methods above
- Analytical Problems
- Basic surrogate modelling (using sk-learn) for data-driven problems
desdeo-vis
Visualization package for desdeo
-Method agnostic
-Creates html/related objects
-Non-interactive visualizations
-Interactive visualizations

DESDEO

IEEE Access
Multidisciplinary | Rapid Review | Open Access Journal

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DESDEO: The Modular and Open Source Framework for Interactive Multiobjective Optimization

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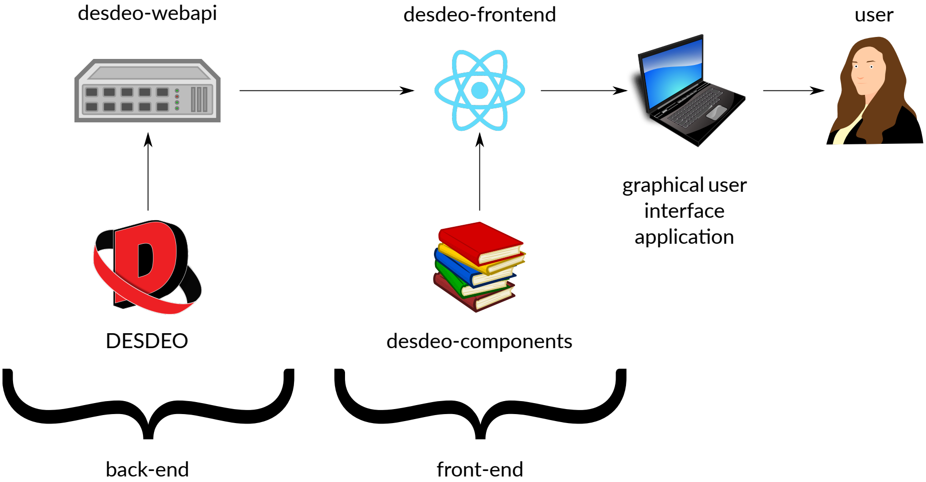
ABSTRACT Interactive multiobjective optimization methods incorporate preferences from a human decision maker in the optimization process iteratively. This allows the decision maker to focus on a subset of solutions, learn about the underlying trade-offs among the conflicting objective functions in the problem and adjust preferences during the solution process. Incorporating preference information allows computing only solutions that are interesting to the decision maker, decreasing computation time significantly. Thus, interactive methods have many strengths making them viable for various applications. However, there is a lack of existing software frameworks to apply and experiment with interactive methods. We fill a gap in the optimization software available and introduce DESDEO, a modular and open source Python framework for

DESDEO web stack



Paper 2: R–XIMO

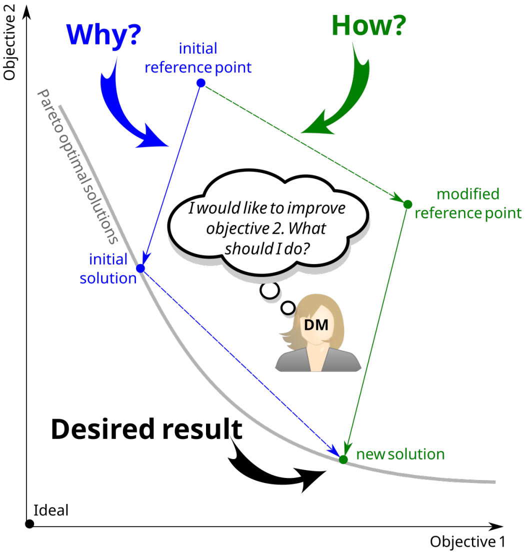
R–XIMO

- R–XIMO[13] is a method that can be used to explain how a reference point given by a decision maker has affected the computed solution(s) in a reference point based interactive multiobjective optimization method.
- R–XIMO can also provide the decision maker with suggestions on how to change the reference point to reach better solutions.
- Based on SHAP values[14], which in turn are based on Shapley values, a concept from game theory.

[13] Giovanni Misitano et al. "Towards explainable interactive multiobjective optimization: R-XIMO". In: *Autonomous Agents and Multi-Agent Systems* 36.2 (2022), pp. 1–43.

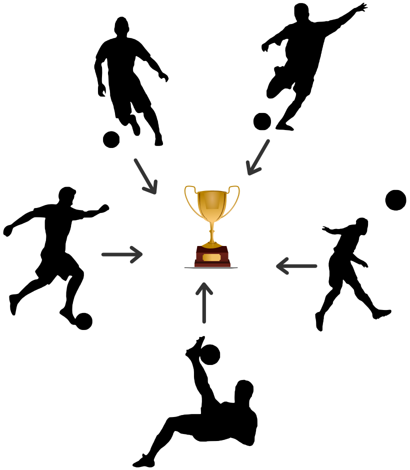
[14] Scott M Lundberg and Su-In Lee. "A Unified Approach to Interpreting Model Predictions". In: *Advances in Neural Information Processing Systems 30.* Ed. by I. Guyon et al. California: Curran Associates, Inc., 2017, pp. 4765–4774.

R–XIMO



Objective 2
Why?
How?
initial reference point
Pareto optimal solutions
modified reference point
I would like to improve objective 2. What should I do?
initial solution
DM
Desired result
new solution
Ideal
Objective 1

R–XIMO



R–XIMO

Decision maker: I would like to improve the first objective.

Example explanation:

Objective 1 was most improved in the solution by the second component and most impaired by the third component in the reference point.

Example suggestion:

Try improving the first[15] *component and impairing the third component in the reference point.*

[15] We always improve the component that matches the objective the decision maker wishes to improve.

Autonomous Agents and Multi-Agent Systems (2022) 36:43
https://doi.org/10.1007/s10458-022-09577-3

Check for updates

Towards explainable interactive multiobjective optimization: R-XIMO

Giovanni Misitano[1] · Bekir Afsar[1] · Giomara Lárraga[1] · Kaisa Miettinen[1]

Accepted: 6 July 2022 / Published online: 13 August 2022

Abstract
In interactive multiobjective optimization methods, the preferences of a decision maker are incorporated in a solution process to find solutions of interest for problems with multiple conflicting objectives. Since multiple solutions exist for these problems with various trade-offs, preferences are crucial to identify the best solution(s). However, it is not necessarily clear to the decision maker how the preferences lead to particular solutions and, by introducing explanations to interactive multiobjective optimization methods, we promote a novel paradigm of *explainable interactive multiobjective optimization*. As a proof of concept, we introduce a new method, *R-XIMO*, which provides explanations to a decision maker for reference point based interactive methods. We utilize concepts of explainable artificial intelligence and SHAP (Shapley Additive exPlanations) values. R-XIMO allows

Paper 3: XLEMOO

- Learnable evolutionary models[16] (LEMs) are a class of evolutionary algorithms that combine evolutionary algorithms with machine learning.
- The point is to utilize machine learning to learn what makes a population member good or not, and then use the learned model to instantiate new good population members. The goal is to make the population converge faster and more "intelligently".
- LEMs have been used occasionally in multiobjective optimization in the past.

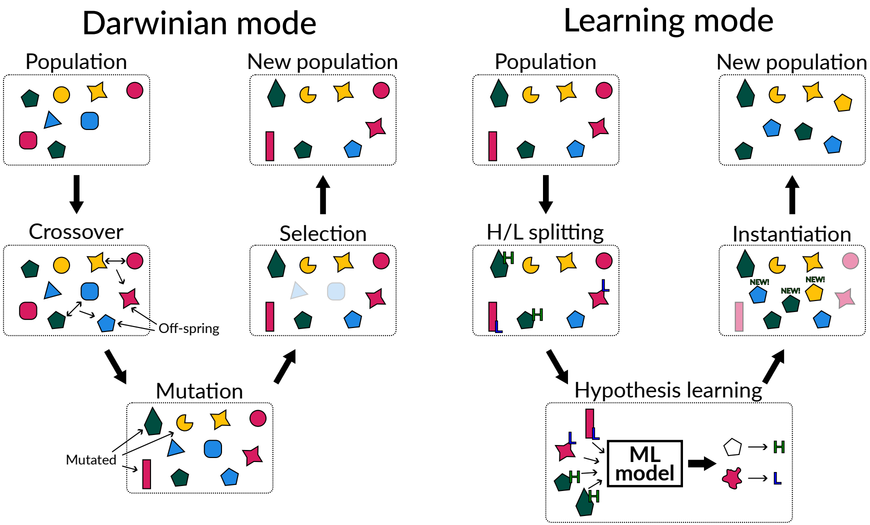
[16] Ryszard S. Michalski. "LEARNABLE EVOLUTION MODEL: Evolutionary Processes Guided by Machine Learning". In: *Machine Learning* 38 (2000), pp. 9–40.

XLEMOO

- **Idea**: what if we use explainable (interpretable) machine learning to not just boost the evolutionary process, but to also try and learn something useful about the population of solutions to further support decision makers?
- This gave raise to the concept of *explainable and learnable evolutionary multiobjective optimization* (XLEMOO) and my third paper[17].

[17] Giovanni Misitano. "Exploring the Explainable Aspects and Performance of a Learnable Evolutionary Multiobjective Optimization Method". In: *Transactions on Evolutionary Learning and Optimization* (2022). Under review.

XLEMOO



Darwinian mode
Population
New population
Crossover
Off-spring
Selection
Mutation
Mutated
Learning mode
Population
New population
H/L splitting
H
L
Instantiation
NEW!
Hypothesis learning
ML model
H
L

Paper 4 (WIP): XADM

XADM

- One big issue in the field of interactive multiobjective optimization is the lack of tools and methods to compare interactive methods with each other.
- So-called artificial decision makers (ADMs) have been proposed to be used in place of humans so that interactive methods could be compared without real decision makers.
- However, ADMs hardly capture human like behavior and limits, like learning, exploring, memory, and cognitive load.

- Computational rationality[18] gives a nice theory on how human interaction with computers can be modeled quite accurately by modeling the limitations of cognition and assuming humans do the best they can with what they have available. This is a contrasting approach to assuming certain behavioral patterns.
- Decision making, and to some extent, decision makers, can be modeled as partially observed Markov decision processes (POMDPs)[19], which can be used to learn an optimal policy to model optimal decisions under noisy and uncertain conditions (like human decision making in multiobjective optimization).

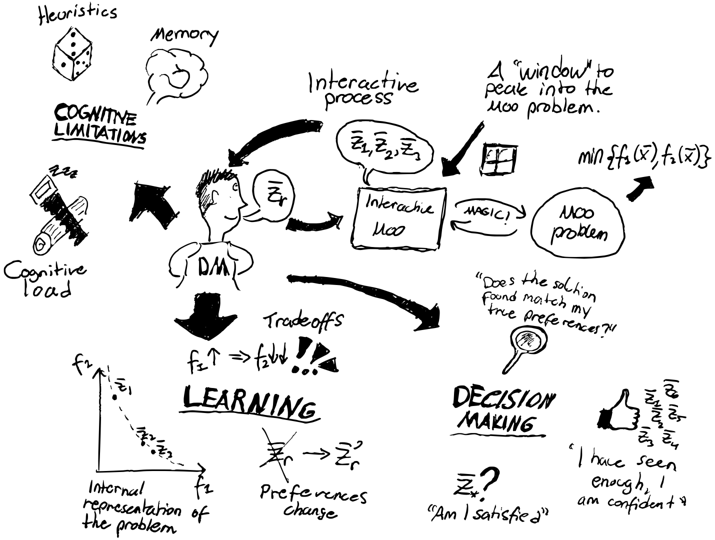
[18] Antti Oulasvirta, Jussi P. P. Jokinen, and Andrew Howes. "Computational Rationality as a Theory of Interaction". In: *CHI Conference on Human Factors in Computing Systems*. ACM, 2022, pp. 1–14. DOI: 10.1145/3491102.3517739.

[19] Leslie Pack Kaelbling, Michael L. Littman, and Anthony R. Cassandra. "Planning and acting in partially observable stochastic domains". In: *Artificial Intelligence* 101.1-2 (1998), pp. 99–134. DOI: 10.1016/S0004-3702(98)00023-X.

XADM

- Optimal policies are traceable, therefore, they can be explained.
- Could computational rationality and POMDPs be combined into a new kind of explainable ADM, an XADM, that can be used to compare interactive methods and support decision makers? Remains to be seen...

XADM



Heuristics
Memory
COGNITIVE LIMITATIONS
Cognitive load
Interactive process
A "window" to peak into the MOO problem.
$\bar{z}_1, \bar{z}_2, \bar{z}_3$
$\bar{z}_r$
Interactive MOO
MAGIC!
MOO problem
$\min\{f_1(\bar{x}), f_2(\bar{x})\}$
DM
"Does the solution found match my true preferences?"
Tradeoffs
$f_1\uparrow \Rightarrow f_2\downarrow\downarrow$!!
LEARNING
f_2
f_1
Internal representation of the problem
$\bar{z}_r \rightarrow \bar{z}_r'$
Preferences change
DECISION MAKING
$\bar{z}_*$?
"Am I satisfied"
"I have seen enough, I am confident"

Other works in our group

Other papers and co–authored papers

- Integration of lot sizing and safety strategy placement using interactive multiobjective optimization[20].
- Designing empirical experiments to compare interactive multiobjective optimization methods[21].
- Interactivized: Visual interaction for better decisions with interactive multiobjective optimization[22].
- Interactively learning the preferences of a decision maker in multi-objective optimization utilizing belief-rules[23].

[20] Adhe Kania et al. "Integration of lot sizing and safety strategy placement using interactive multiobjective optimization". In: *Computers & Industrial Engineering* 173 (2022), p. 108731. DOI: https://doi.org/10.1016/j.cie.2022.108731.

[21] Bekir Afsar et al. "Designing empirical experiments to compare interactive multiobjective optimization methods". In: *Journal of the Operational Research Society* (2022), pp. 1–12.

[22] Jussi Hakanen et al. "Interactivized: Visual interaction for better decisions with interactive multiobjective optimization". In: *IEEE Access* 10 (2022), pp. 33661–33678.

[23] Giovanni Misitano. "Interactively Learning the Preferences of a Decision Maker in Multi-objective Optimization Utilizing Belief-rules". In: *2020 IEEE Symposium Series on Computational Intelligence (SSCI)*. IEEE. 2020, pp. 133–140. DOI: 10.1109/SSCI47803.2020.9308316.

Other works

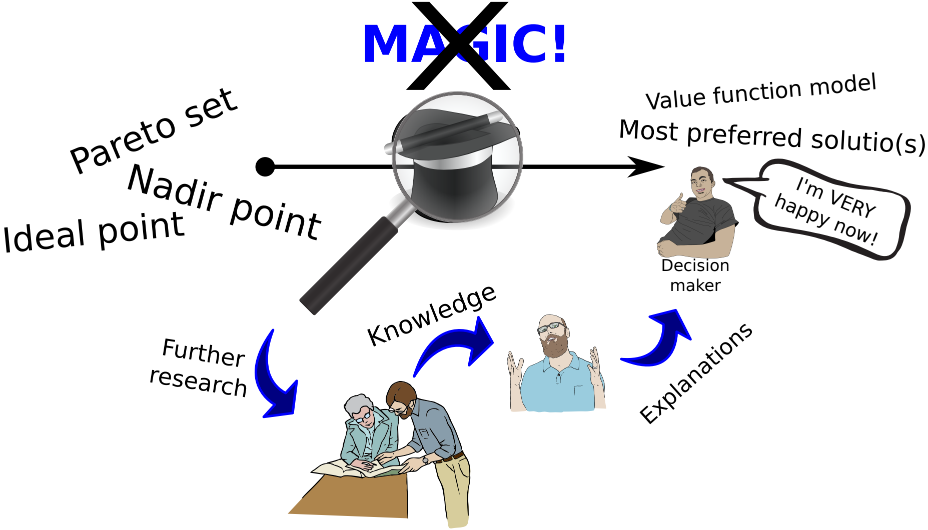
- Group decision-making in multiobjective optimization.
- Hybridization of scalarization and evolutionary methods in an interactive setting.
- Data-driven multiobjective optimization.
- Uncertainty and robustness in multiobjective optimization.
- Scenario-based multiobjective optimization.
- More experiments with human participants to assess various aspects of interactive multiobjective optimization (e.g., a study on the semantic distance of icons).
- Case-studies in various fields.

Conclusions

Conclusions

- Explainability is an exciting and important concept to be studied in the context of and applied to multiobjective optimization.
- Makes the life of decision makers easier.
- Very much an unexplored area in the field of multiobjective optimization.
- New and wild ideas are needed!

Conclusions



Appendices

Links and resources

- DESDEO website[1]
- Multiobjective Optimization (research) Group[2]
- Follow me on LinkedIn[3]
- If Twitter does not burn down, then you can find me there as well: `@misitano_g`

[1] https://desdeo.it.jyu.fi

[3] http://www.mit.jyu.fi/optgroup/

[4] https://linkedin.com/in/misitano

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[1] Kaisa Miettinen. *Nonlinear multiobjective optimization*. Boston: Kluwer Academic Publishers, 1999.

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[6] Bryce Goodman and Seth Flaxman. "European Union regulations on algorithmic decision-making and a "right to explanation"". In: *AI magazine* 38.3 (2017), pp. 50–57.

[7] Cynthia Rudin. "Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead". In: *Nature Machine Intelligence* 1.5 (2019), pp. 206–215.

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