On the Potential of Multi-Objective Algorithm Configuration on Multi-Modal Multi-Objective Optimisation Problems

Oliver L. Preuß, Jeroen Rook, Heike Trautmann

JOLEA talk, June 19, 2024

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MALEO

Machine Learning and Optimisation

Prof. Dr. Heike Trautmann

ALGORITHMIZATION AND SOCIAL INTERACTION

UNIVERSITY OF TWENTE.

Automated Algorithm Selection and Configuration

Data Stream Mining Social Media Analytics

Trustworthy Artificial Intelligence

Multi-Objective Optimization and Decision Support

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CONSTRUCTING EXPLAINABILITY

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Talk Outline

!! This talk combines three different Multiobjective Perspectives – MOO^3 !!

Multi-Objective Optimisation (Algorithms)

Multi-Objective Performance Measurement

Multi-Objective Automated Algorithm Configuration

… with special focus on **Multi**modality

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In a nutshell: We will present (automatically) optimized hyperparameter settings of evolutionary multiobjective optimizers

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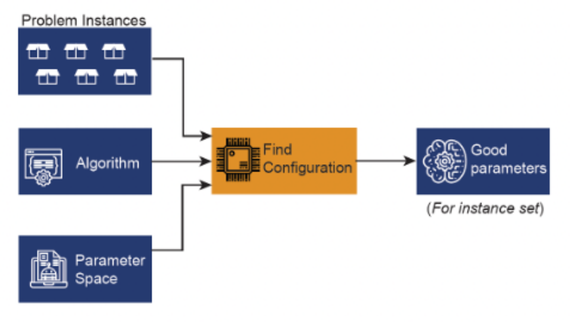
... why is that of crucial importance and why do we need to make this so complicated ??

... we aim to reduce the barrier to building, deploying, maintaining high-quality AI pipelines (predictable, robust, performant)

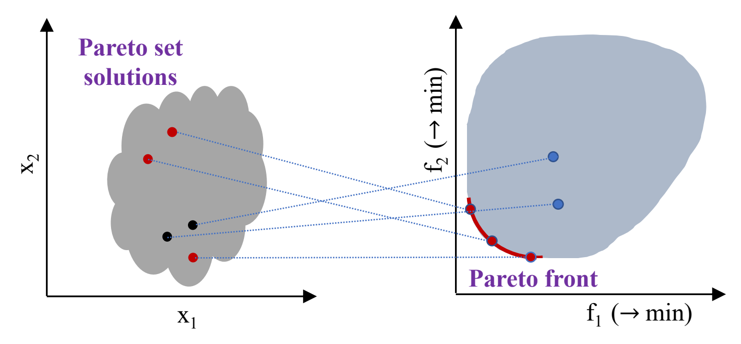
- low-quality algorithmic components are a risk within larger AI pipelines
- use meta-algorithmic (Auto-ML)-frameworks to (help) construct AI systems with robust components
- e.g. automated algorithm selection, automated algorithm configuration



The world is multi-objective ...

Multi-Objective Optimization (MOO)

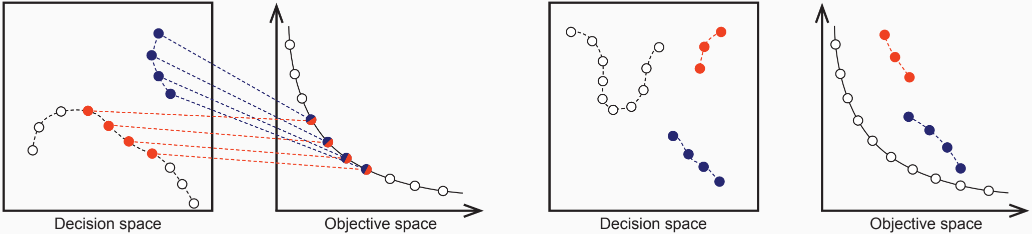
- Multi-objective optimization problems (MOP) have multiple (conflicting) objectives
- Solution is usually a set of trade-offs between objectives
- Find all solutions that are Pareto optimal



Multi-Modal MOPs

Many MOPs are multimodal ...

- Multiple global and local optima
- Different points in the decision space map to the same point in objective space



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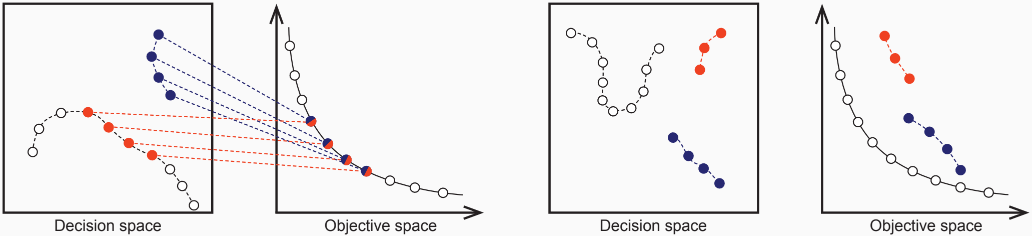


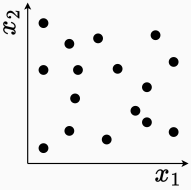
↪ Goal: diverse solution set in decision space and convergence towards Pareto front

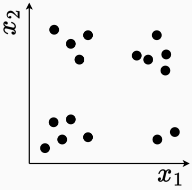
Diversity in Decision Space

Solow Polasky measure (SP)

[Solow & Polasky, ’94]

- Pairwise distances of points
- Measures diversity of decision space
- Should be maximized



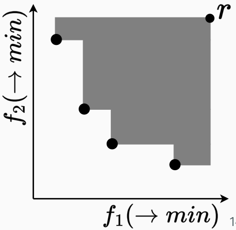


Convergence in Objective Space

Dominated hypervolume (HV)

[Zitzler et. al., ’03]

- Area of non-dominated points and reference point *r*
- Accounts for convergence and spread in objective space
- To be maximized



Solow-Polasky

Diversity: Solow-Polasky Measure

$$SP(P) = \sum_{1 \leq i,j \leq \mu} M_{ij}^{-1} \in [1, \mu]$$

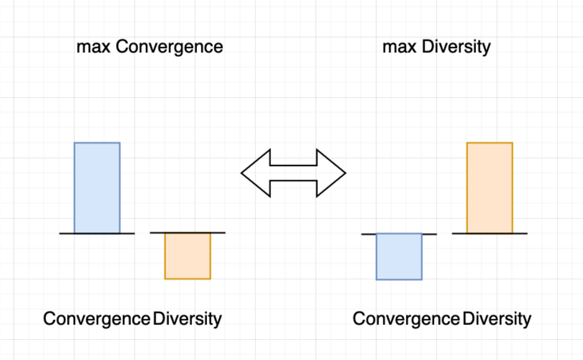
P Population of μ individuals

M^{-1} Moore-Penrose generalised inverse matrix of M with $M_{i,j} = \mathbf{exp}(-d(P_i, P_j))$

d (Euclidean) distance between two individuals

Evolutionary Multi-Objective Optimisation Algorithms

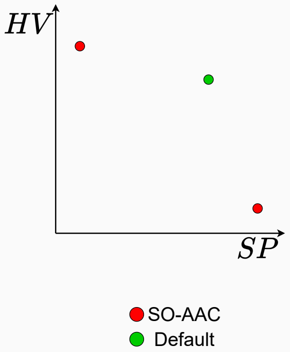
Most Evolutionary Mult-Objective Algorithms (EMOAs) are not designed for diversity in decision space but rather for convergence and diversity in objective space



↪ We will use automated algorithm configuration (AAC) to find EMOA hyperparameters that will (simultaneously) yield decision space diversity [Rook et al., '22]

EMOAs: Diversity-Convergence Trade-Off

- Rook et al., 2022 pointed to hyperparameter sensitivity
- Single-Objective Configurations for SP impacts convergence behavior (HV) and vice versa



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- Rook et al., 2022 pointed to hyperparameter sensitivity
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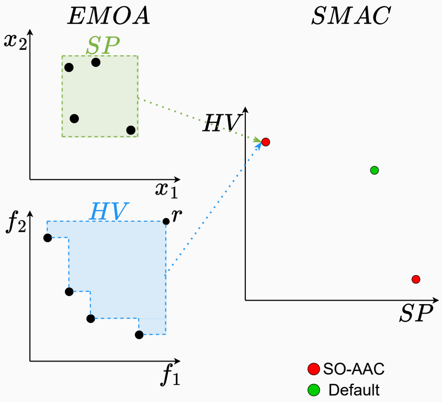
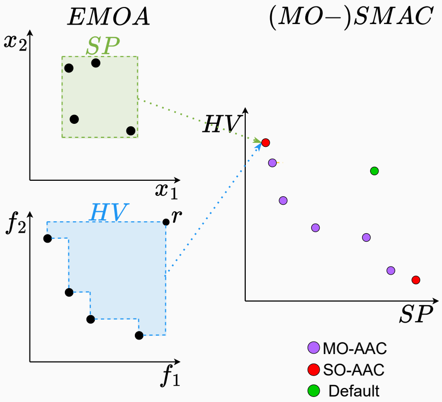
- Can we mitigate the trade-off between SP and HV?



EMOAs: Diversity-Convergence Trade-Off

- Rook et al., 2022 pointed to hyperparameter sensitivity
- **Single-Objective Configurations for SP impacts convergence behavior (HV) and vice versa**
- Can we mitigate the trade-off between SP and HV?
- **Use multi-objective AAC (MO-AAC) for HV and SP simultaneously**



(Multi-Objective) Automated Algorithm Configuration

Automated Algorithm Configuration (AAC)

Find a configuration for an algorithm that optimises its overall performance

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$$\theta^* = \underset{\theta \in \Theta}{\mathbf{argmax}}\, p(A_\theta, \mathcal{I})$$

- Θ Configuration space
- A Algorithm
- $\mathcal{I}$ Problem domain (usually represented by a set of instances (N))
- p Performance measure

Automated Algorithm Configuration (AAC)

Find a configuration for an algorithm that optimises its overall performance

$$\theta^* = \operatorname*{\mathbf{argmax}}_{\theta \in \Theta} p(A_\theta, \mathcal{I})$$

Θ Configuration space

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Challenges

- **Large and mixed-type search spaces**
- Expensive evaluations

Algorithm Configurators

- **SMAC**, ParamILS
- iRace, GGA, ...

Multi-Objective AAC

Find a set of configurations for an algorithm that approaches the trade-off surface of the overall performances

Formulated as multi-objective optimisation problem:

$$\Theta^* = \{\theta \in \Theta \mid \nexists_{\theta' \in \Theta / \{\theta\}} \; p(A_{\theta'}, \mathcal{I}) \prec p(A_\theta, \mathcal{I})\}$$

Algorithm Configurators

- **MO-SMAC**
- MO-ParamILS
- (ParEGO)

MO-SMAC

- Does not aggregate objectives
- **Predicted Hypervolume improvement**
- Returns set of configurations

SMAC: Key Steps

- **Initialization:**
  Generate initial configurations and evaluate their performance.
- **Model Building:**
  Construct a probabilistic model of the performance across the configuration space.

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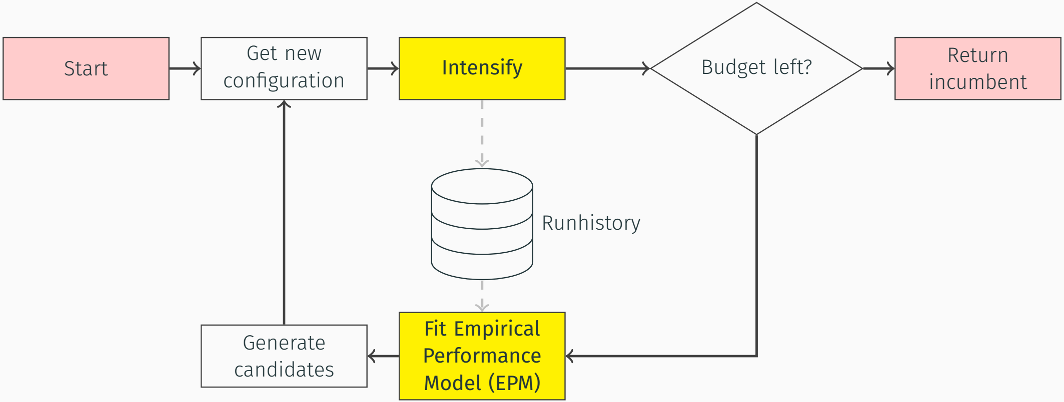
- **Initialization:**
  Generate initial configurations and evaluate their performance.
- **Model Building:**
  Construct a probabilistic model of the performance across the configuration space.
- **Acquisition Function:**
  Use an acquisition function to select new configurations to evaluate, balancing exploration and exploitation.
- **Iteration:**
  Evaluate the selected configurations, update the model with the new data, and repeat the process.

SMAC → MO-SMAC



Intensification: Process of selecting and re-evaluating promising configurations more frequently to ensure their performance is accurately assessed.

Empirical Performance Model: Gaussian Process Model (Bayesian Optimisation)

Modification 1: Intensification

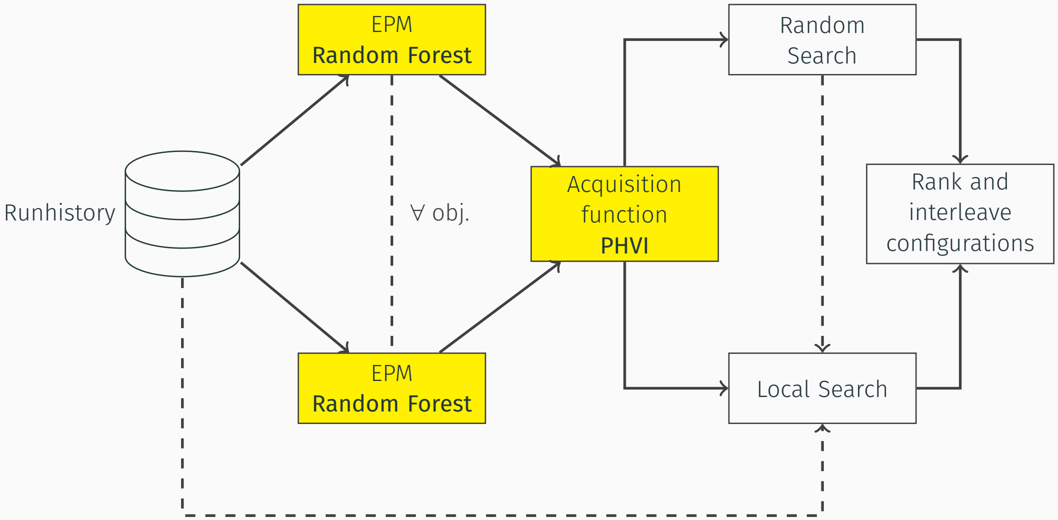
- Incumbent is a population of configurations
- Racing continues until closest[1] configuration $\theta \in \Theta_{inc}$ dominates the challenger

Modification 2: Empirical performance model

- EPM based on Predicted Hypervolume Improvement

[1] Based on the Euclidean distance between the aggregated performance on the overlapping instances

Modification 2: Empirical performance model



Experiments

Experimental Setup (adapted from Rook et al., 2022)

Configurators: SMAC-SP, SMAC-HV, MO-SMAC

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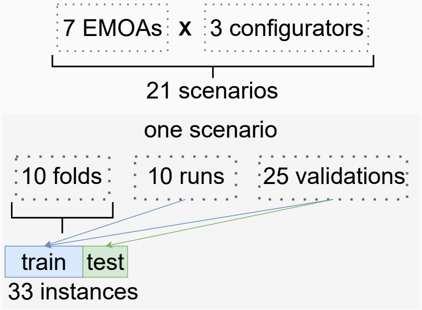
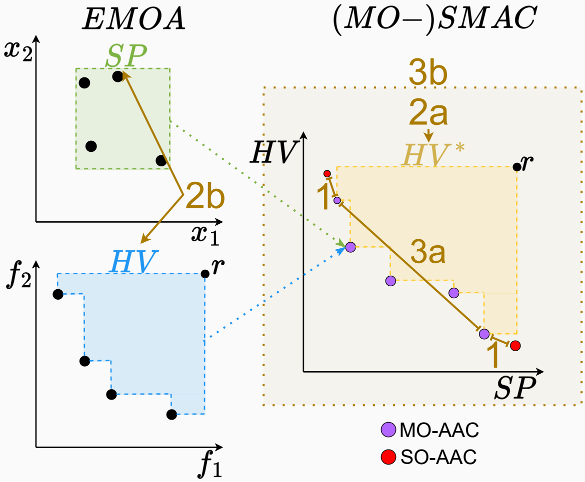
Configurators: SMAC-SP, SMAC-HV, MO-SMAC

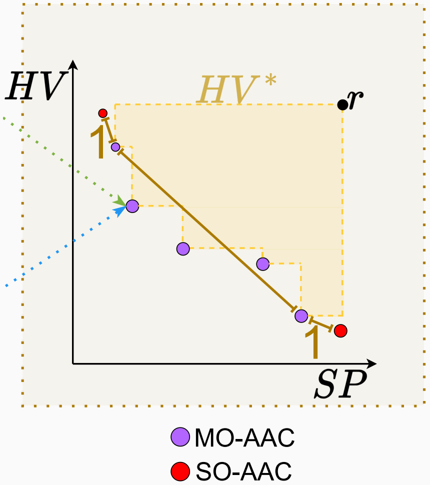
- 7 EMOAs
  - NSGA-II, Omni-Optimizer, SMS-EMOA, MOEA/D, HIGA-MO, MOLE, MOGSA
- 33 test instances
  - ZDT (5), MMF (19), DTLZ (5) , BiObj-BBOB (3)
- 10-fold cross-validation (CV)
- 10 configuration runs per CV-fold
- 25 validation runs per instance



Overview Experiments / Research Questions

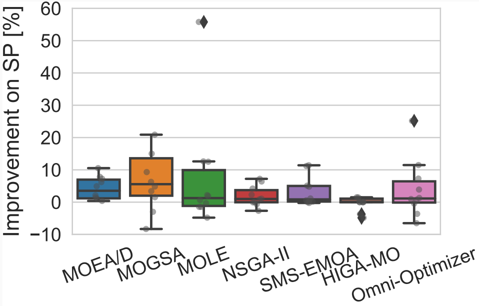


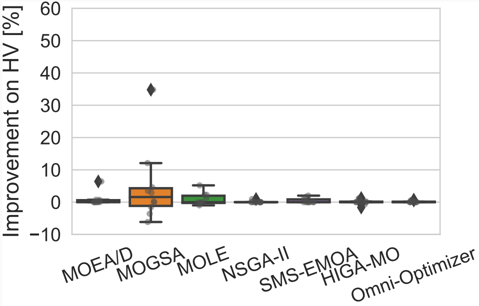
1. How competitive are EMOAs configured with (MO-)AAC?



1. How competitive are EMOAs configured with (MO-)AAC?

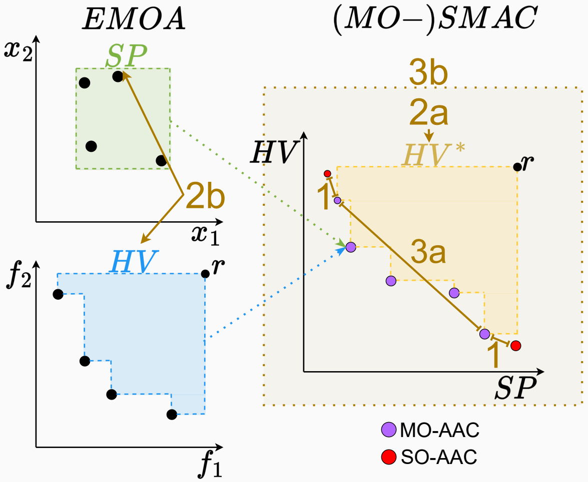
After MO configuration, we compare the two extreme non-dominated solutions to the SO configurations of SP and HV





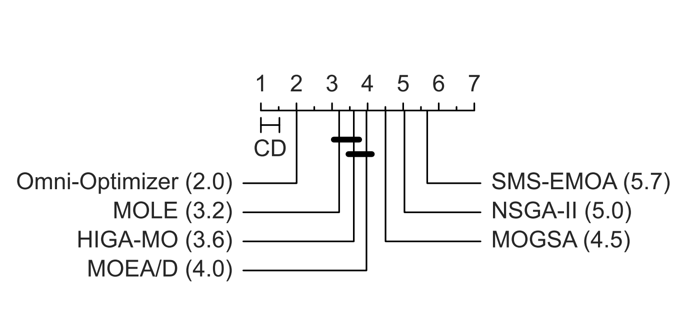
- MO-SMAC finds better configurations for SP compared to SMAC-SP
- SMAC and MO-SMAC find comparable configurations for HV

2a. How configurable are EMOAs?

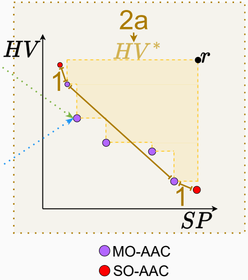


2a. How configurable are EMOAs?

We assess the quality of the PF approximation in performance indicator space by the Hypervolume Indicator, i.e. HV*



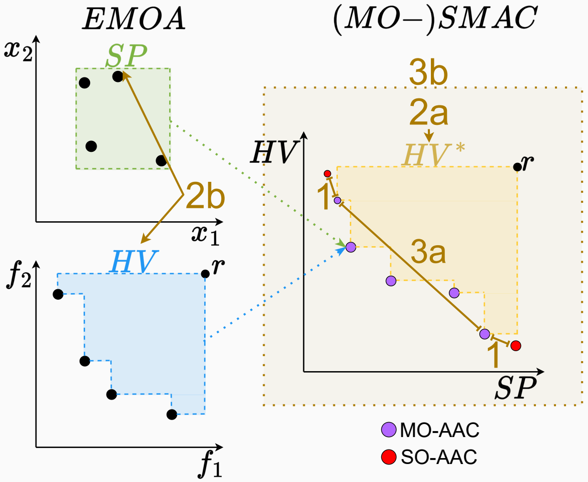
$(MO-)SMAC$



HV*

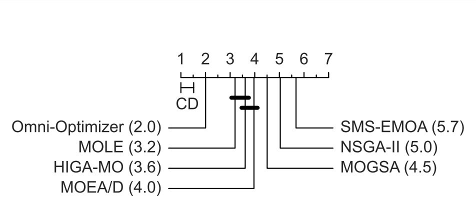
↪ Omni-Optimizer outperforms all other EMOAs

2b. How configurable are EMOAs?

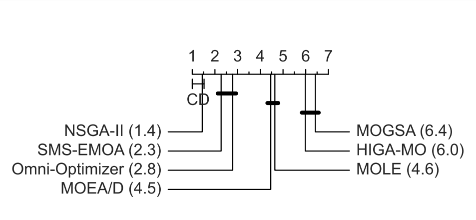


2b. How configurable are EMOAs?

We assess the nondominated configurations generated by MO-SMAC separately regarding SP and HV in original objective space.



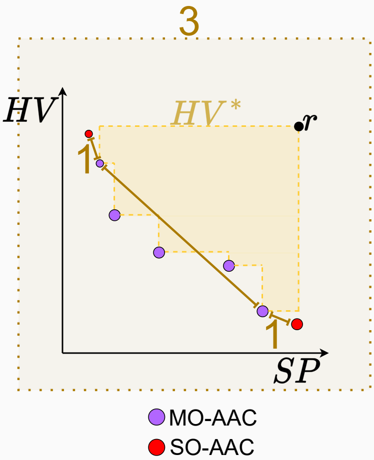
SP



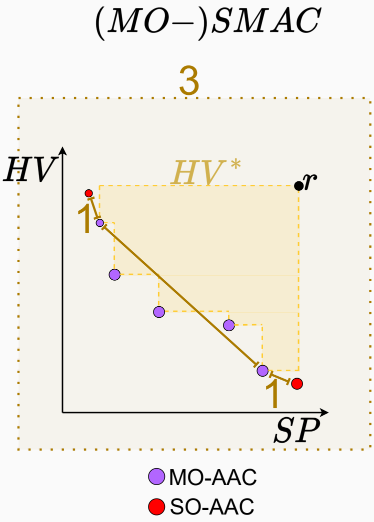
HV

- ↪ Gradient-based EMOAs rank better for SP
- ↪ Omni-Optimizer outperforms all other EMOAs for SP
- ↪ Classical EMOAs rank best for HV

$(MO-)SMAC$



- We will look at the non-dominated (MO-)AAC configurations per algorithm in detail
- We will investigate the trade-off behaviour per EMOA regarding SP and HV



- We will look at the non-dominated (MO-)AAC configurations per algorithm in detail
- We will investigate the trade-off behaviour per EMOA regarding SP and HV
- We will identify 'best trade-off solutions'

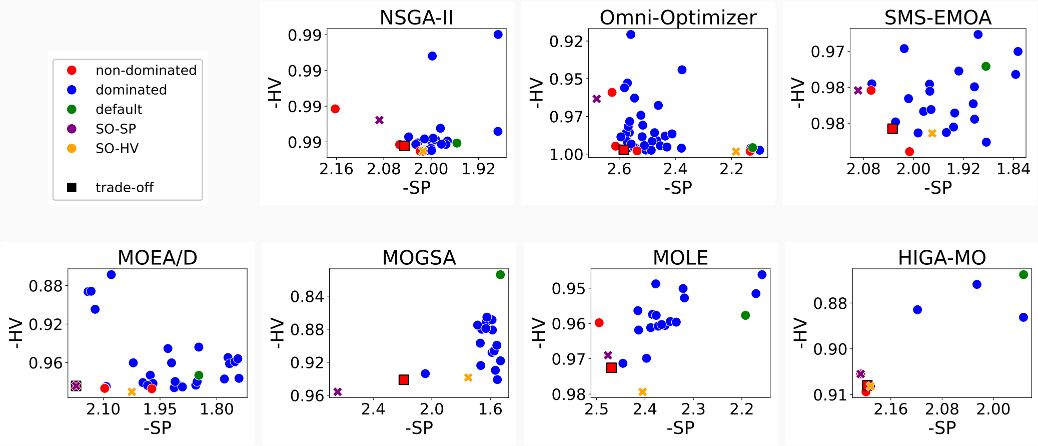
3 How does the trade-off between SP and HV look like?

Algorithm	# configs	unique configs	non-dominated
MOLE	19	19	1
MOGSA	17	17	2
NSGA-II	27	27	4
HIGA-MO	17	17	3
MOEA/D	29	29	3
Omni-Optimizer	42	40	4
SMS-EMOA	23	23	3

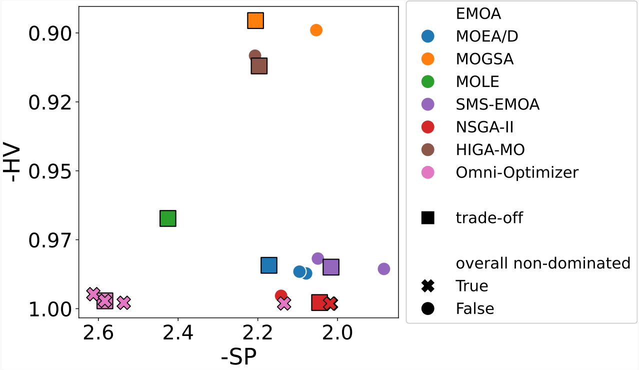
- **In general few non-dominated configurations**
- **Omni-Optimizer has the most configurations**
- Omni-Optimizer and NSGA-II tie on non-dominated configurations
- (MO-) Configuration has a higher impact on SP

3 How does the trade-off between SP and HV look like?

Trade-off behaviour per EMOA regarding SP and HV including best trade-off solutions

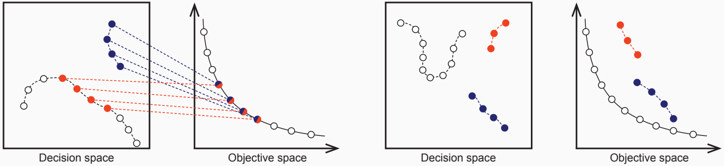


Joint view on EMOA trade-off behaviour: Overall best configurations



- 5 non-dominated overall configurations
- Omni-Optimizer achieved the best overall performance

Summary & Conclusion



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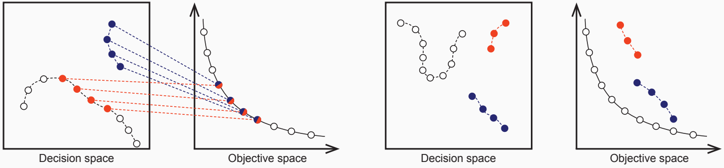

- We showed the huge potential of Multiobjective Automated Algorithm Configuration for EMOAs
- Showed superiority of MO-AAC to SO-AAC
- **Successfully analysed the trade-off between convergence in objective space and diversity in decision space**
- Showed configurability of EMOAs, Omni-Optimizer has overall best performance
- Proposed new default configurations for the considered setting

Future Work

- Widen the scope of the experimental study
- Extend decision (and objective) space
- Use additional benchmark sets, e.g., PeekABoo! [Schäpermeier et. al., '23]

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- Investigate MO-AAC as an optimization problem itself
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- 'Vicious circle' of meta-configuration?
- Configurators can be configured as well

Multimodal Multi-objective Optimization: Bridging the Gap Between Problem Domains and Research Communities

– Workshop at PPSN 2024 –

Please join our workshop at PPSN 2024 !

... organized by

Oliver Schütze, Cinvestav-IPN, Mexico

Lennart Schäpermeier, TU Dresden

Heike Trautmann, Paderborn University

September, 14-18, Hagenberg, Austria

(Workshop Sep. 15)