Prof. Dr. Pascal Kerschke
TU Dresden, “Friedrich List” Faculty of Transport and Traffic Sciences, Big Data Analytics in Transportation, and Center for Scalable Data Analytics and Artificial Intelligence (ScaDS.AI) Dresden/Leipzig

Automated Algorithm Selection

Summer School on Automatic Algorithm Design 2023 // Thursday, June 15, 2023, in Lille, France

Thanks to the Contributions of Many Smart Minds ☺

















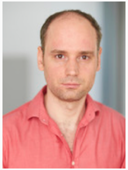






Academic Background

- TU Dortmund University, Dortmund, Germany
    - 2007 – 2010: B.Sc. *Data Analysis and Management*
    - 2010 – 2013: M.Sc. *Data Science*
- University of Münster, Münster, Germany
    - 2013 – 2017: Ph.D. in *Information Systems* (Supervisor: Heike Trautmann)
    - 2017 – 2021: PostDoc at *Data Science: Statistics & Optimization* (head: Heike Trautmann)
- TU Dresden, Dresden, Germany
    - since 2021: Professor for *Big Data Analytics in Transportation*

Where is Dresden?

Travel Times (Train):

- ca. 2h to Berlin
- ca. 2.5h to Prague
- ca. 4h to Frankfurt
- ca. 4h to Hamburg
- ca. 5h to Munich
- ca. 6h to Dortmund
- ca. 9h to Bruxelles
- ca. 10h to Paris
- ca. 11h to Lille

My Wonderful Team ☺

Felix Rauschert

Lennart Schäpermeier

Konstantin Dietrich

Sandy Wolf

Markus Leyser

Jonathan Heins

Felix Hoch

Our Research

Research Interests:

- Automated Algorithm Selection
- Benchmarking
- Data Science
- Exploratory Landscape Analysis
- Optimization:
    - Single-Objective Continuous Optimization
    - Multi-Objective Continuous Optimization
    - Routing Problems (TSP, VRP)
- Machine Learning (AutoML, IML/XAI; Unsupervised, Supervised, and Reinforcement Learning)
- Visualization of Optimization Problems

Research Networks:

- Benchmarking Network
- COSEAL (Configuration and Selection of Algorithms)
- CLAIRE (Confideration of Laboratories for Artificial Intelligence Research in Europe)
- Center for Scalable Data Analytics and Artificial Intelligence (ScaDS.AI) Dresden/Leipzig
- Boysen-TU Dresden-Research Training Group

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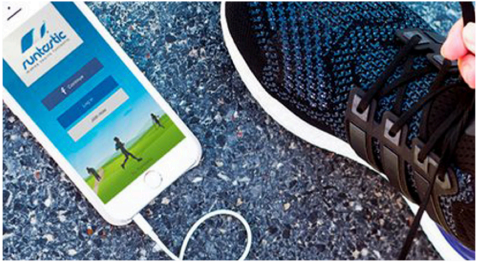
Agenda

- Introduction
  - Optimization
  - Traveling Salesperson Problem
  - Automated Algorithm Selection
- Building Blocks of Automated Algorithm Selection
- Status Quo of Automated Algorithm Selection
  - Traveling Salesperson Problem
  - Single-Objective Continuous Optimization
- Benefits and Perspectives

Introduction

www.dailymail.co.uk


www.autobild.de



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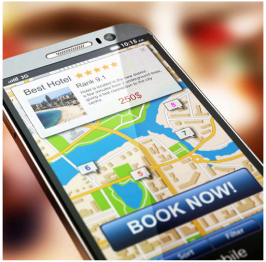
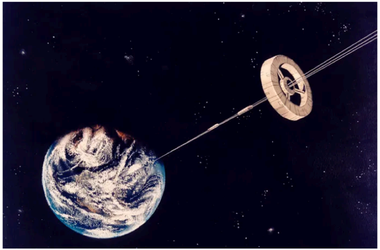


www.aktiv-online.de

internetofbusiness.com



www.spacelegalissues.com

www.newsmax.com

www.autonomousvehicleinternational.com

Introduction

Optimization

Optimization

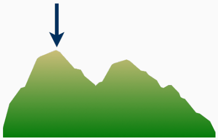
- ideally, such problems can be expressed as a mathematical function $f : \mathcal{X} \to \mathbb{R}$
- full knowledge enables analytical investigations of the underlying model

input → $\boxed{\textbf{model}}$ → **output**

- in such a case, one is interested in x_{opt} such that (w.l.o.g.)

$$x_{opt} = \arg\max_{x \in \mathcal{X}} f(x)$$

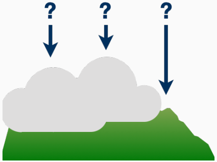
- optimization is quite simple



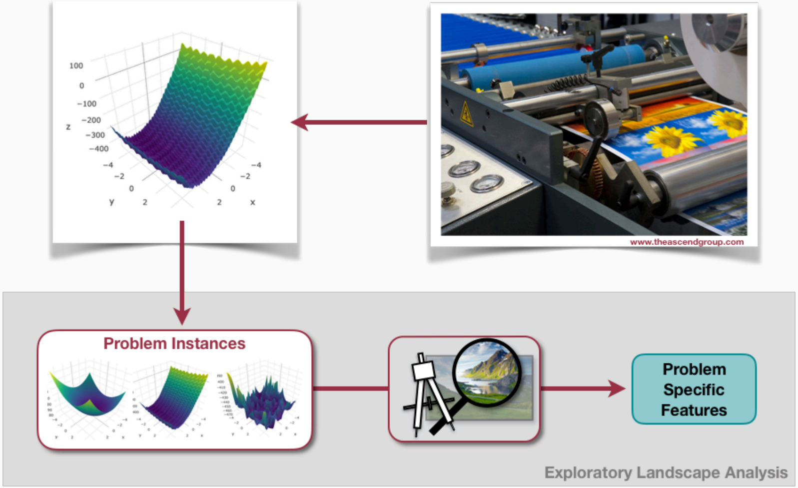
Black-Box Optimization

- unfortunately, in most real-world cases, such mathematical function are unknown
- underlying models become *black-box models*

- x_{opt} has to be determined by sophisticated algorithms that do not need knowledge about the model
- optimization becomes much more challenging



- extract information from (black-box) optimization problems in an automated fashion



Feature-Based Problem Characterization

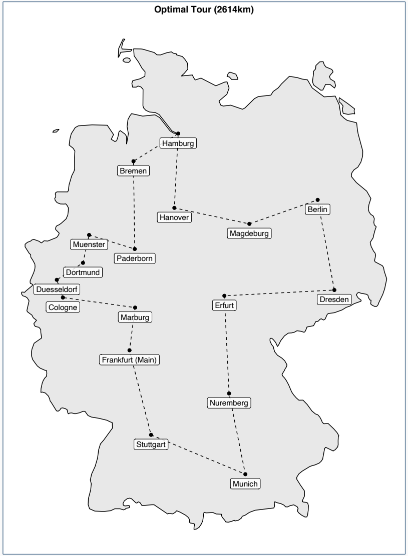
- features are simple (numerical) statistics that “describe” a problem’s structure
- computed based on
  1. continuous problems:
     a “small” sample of n evaluated points $x_{i1}, \dots, x_{id}, i = 1, \dots, n$
     (including their corresponding fitness value y_i)
  2. graph-based problems (e.g., TSP):
     characteristics of a graph (amount of nodes, edge lengths, etc.)
- features help to improve understanding of
  - problems (match features to high-level properties)
  - algorithm-to-problem dependencies
- nowadays, “ELA” is frequently used as synonym for feature-based characterization of continuous single-objective (black-box) optimization problems

Introduction

Traveling Salesperson Problem

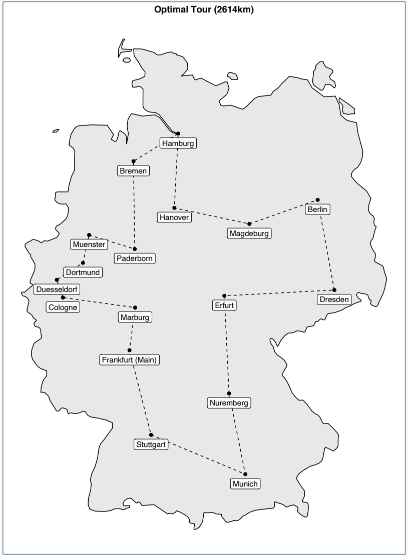
Traveling Salesperson Problem

- classical NP-hard optimization problem
- studied for decades
- important for various applications:
  - transportation logistics
  - circuit board fabrication
  - etc.
- given:
  - a set of cities
  - edges connecting the cities
- goal:
  - find the shortest round trip such that every city is visited exactly once



Optimizing Traveling Salesperson Problems

- optimization algorithms distinguished into
  - exact algorithms
  - inexact heuristics
- exact algorithms:
  - guarantee optimality of found solutions
  - oftentimes expensive / slow
  - state of the art: Concorde [3]
- inexact heuristics
  - usually much faster
  - solution quality (i.e., length of found tours) is very often (at least close to) optimal
  - state of the art are restart variants [11] of:
    - Lin-Kernighan Heuristic (LKH) [18]
    - Genetic Algorithm using Edge Assembly Crossover (EAX) [37]



Introduction

Automated Algorithm Selection

Motivation of Automated Algorithm Selection

- *No Free Lunch Theorem* [51]:
  "better" optimization algorithm depends on problem structure
- similar to choice of preferred vehicle
- don't just rely on "gut-feeling"
- use additional information / data and automated techniques
- *Automated Algorithm Selection*:
  - introduced by John Rice in 1976 [43]
  - combines problem knowledge and (performance) data
  - relies on techniques from (automated) machine learning


https://taz.de/


https://www.wn.de/


https://www.mein-schwarzwald.de/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Automated Algorithm Selection – Survey Articles

[48] Kate A. Smith-Miles (2009).

Cross-Disciplinary Perspectives on Meta-Learning for Algorithm Selection. ACM Computing Surveys, 41:1-25.

- meta-learning perspective
- covers developments from perspective of AI and operations research communities

[26] Lars Kotthoff (2014).

Algorithm Selection for Combinatorial Search Problems: A Survey. AI Magazine, 35(3):48-60.

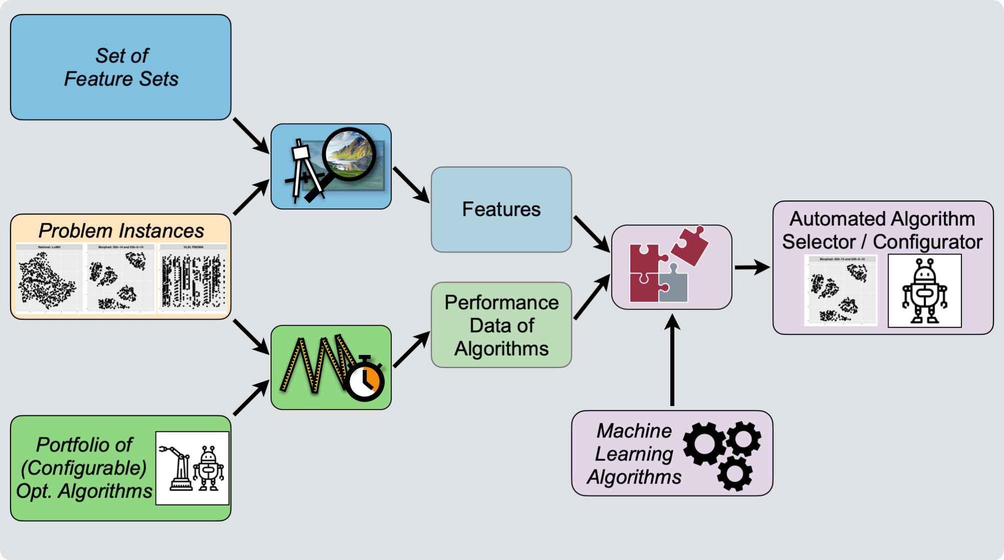
- focus on discrete problems
- explains several aspects of algorithm selection (e.g., online vs. offline selection, static vs. dynamic portfolios, consideration of costs, different prediction types)

[25] Pascal Kerschke, Holger Hoos,
Frank Neumann & Heike Trautmann (2019).
Automated Algorithm Selection:
Survey and Perspectives.
Evolutionary Computation, 27(1):3-45, MIT Press.

- most recent survey
- focus on feature-based per-instance algorithm selection (PIAS)
- connection to related problems (algorithm configuration, schedules, etc.)
- dedicated section on perspectives for future research



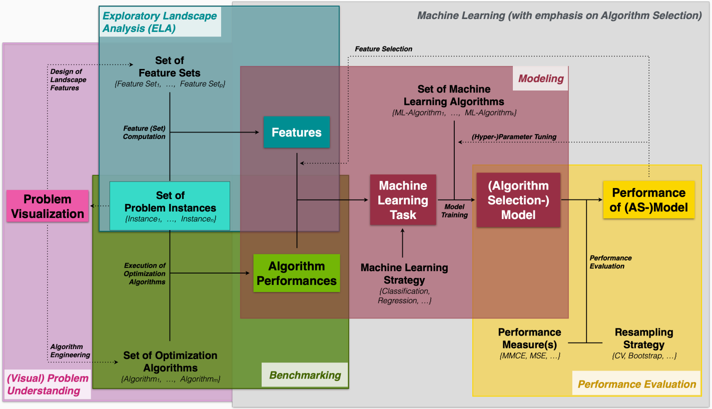

General Idea of Automated Algorithm Selection



Building Blocks of Automated Algorithm Selection

Building Blocks of Automated Algorithm Selection

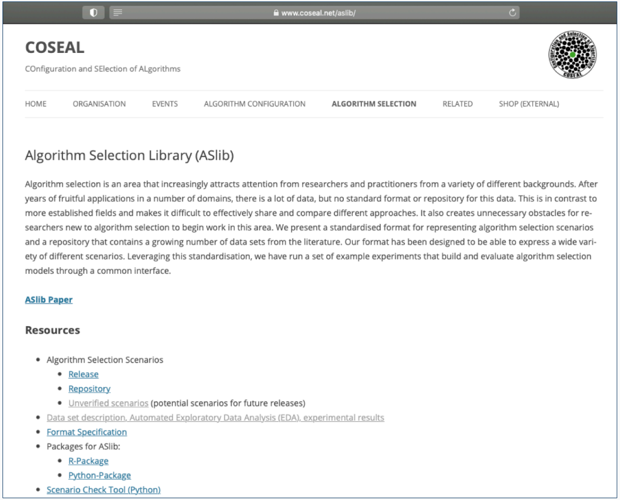
- a good AS model relies on various components [25]:
  - representative problem instances
  - good understanding of problem characteristics
  - cheap and informative features
  - portfolio of competitive and complementary algorithms
  - powerful machine learning algorithms



  - suitable performance measure (w.r.t. optimization algorithm and AS model)
- frequently confronted with various forms of big data

Algorithm Selection Library

- data of numerous AS scenarios can be found in the Algorithm Selection Library (ASLib [6]):
  - initiated by members of the COSEAL network (`coseal.net`)
  - unified format specifications
  - currently contains ≈30 scenarios
  - offers interfaces to python and R
  - overview per scenario
  - validation tool



www.coseal.net/aslib/

COSEAL

COnfiguration and SElection of ALgorithms

HOME ORGANISATION EVENTS ALGORITHM CONFIGURATION **ALGORITHM SELECTION** RELATED SHOP (EXTERNAL)

Algorithm Selection Library (ASlib)

Algorithm selection is an area that increasingly attracts attention from researchers and practitioners from a variety of different backgrounds. After years of fruitful applications in a number of domains, there is a lot of data, but no standard format or repository for this data. This is in contrast to more established fields and makes it difficult to effectively share and compare different approaches. It also creates unnecessary obstacles for researchers new to algorithm selection to begin work in this area. We present a standardised format for representing algorithm selection scenarios and a repository that contains a growing number of data sets from the literature. Our format has been designed to be able to express a wide variety of different scenarios. Leveraging this standardisation, we have run a set of example experiments that build and evaluate algorithm selection models through a common interface.

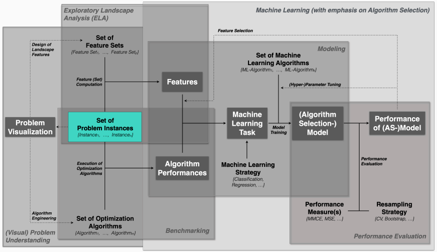
ASlib Paper

Resources

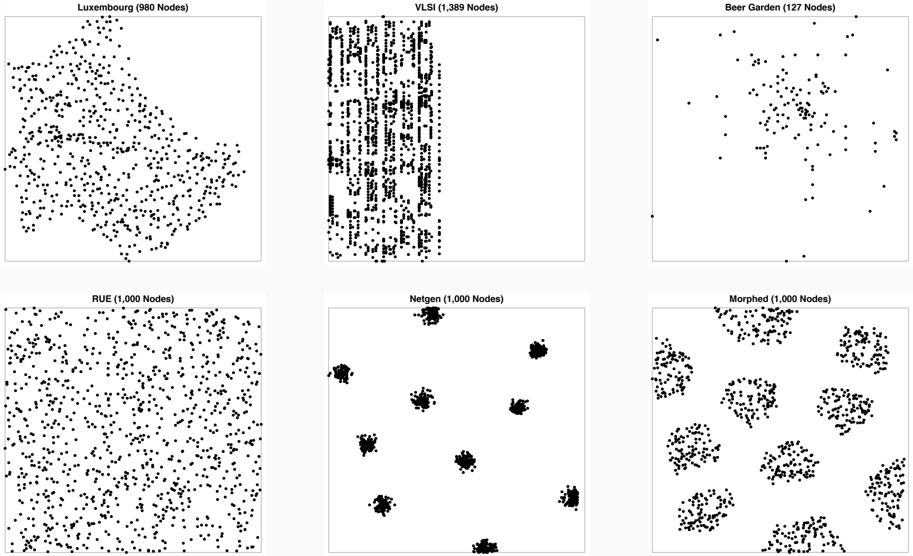
- Algorithm Selection Scenarios
  - Release
  - Repository
  - Unverified scenarios (potential scenarios for future releases)
- Data set description, Automated Exploratory Data Analysis (EDA), experimental results
- Format Specification
- Packages for ASlib:
  - R-Package
  - Python-Package
- Scenario Check Tool (Python)

Building Blocks of AAS – Instances

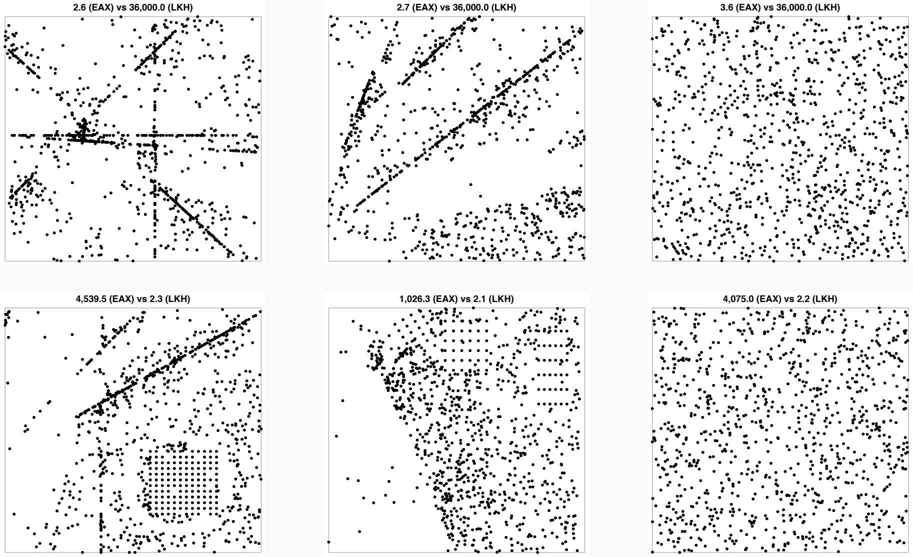
- problem instances of an optimization benchmark
  - possess various “landscape” characteristics, which could potentially be obstacles for certain algorithms
  - are capable of revealing strengths and weaknesses of optimization algorithms
  - provide a playground for simple as well as complex algorithms
  - are representative for real-world problems
- their representation affects the choice of optimization algorithms, features, etc.



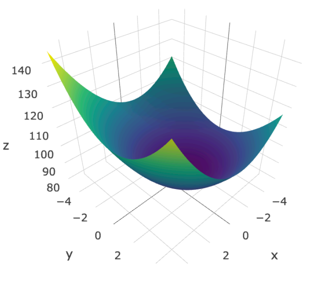
Building Blocks of AAS – Instances: TSP I

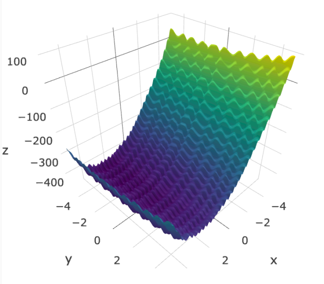


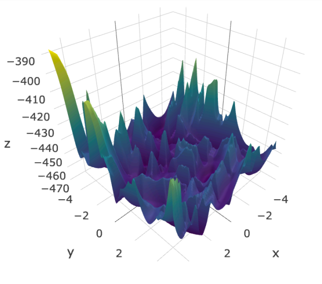
Building Blocks of AAS – Instances: TSP II

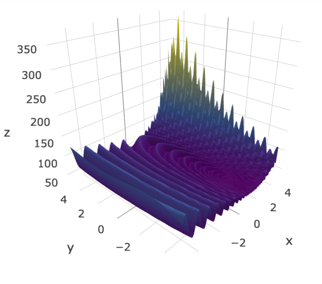


Building Blocks of AAS – Instances: Continuous Optimization



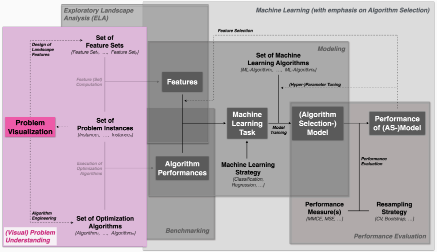




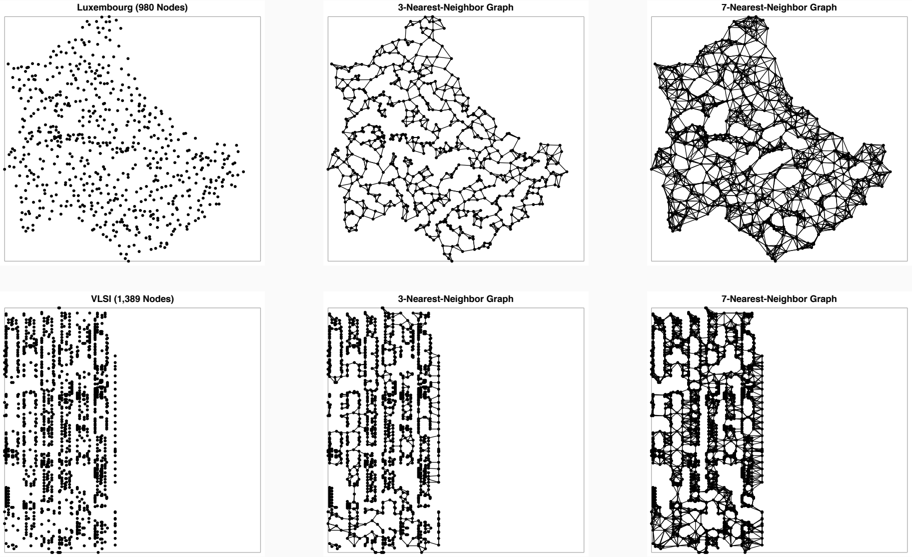


Building Blocks of AAS – Problem Visualization

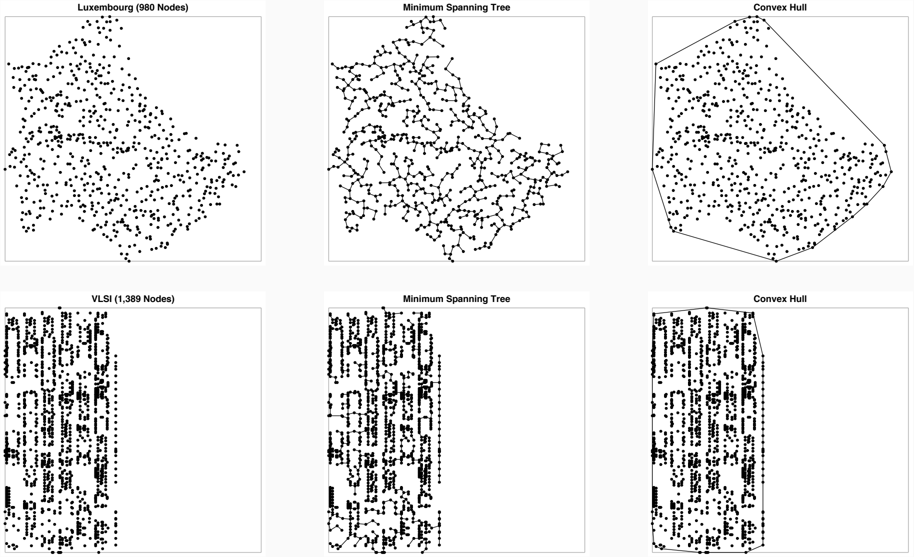
- purpose of problem visualization:
  - get a “feeling” for / better understanding of the domain’s (benchmark) problems
  - look for problem properties, which likely also exist in higher-dimensional (i.e., non-visualizable) versions
  - identify potential pitfalls (“traps”) for optimization algorithms $\rightsquigarrow$ use those findings for improved algorithm engineering



Building Blocks of AAS – Visualization: TSP I

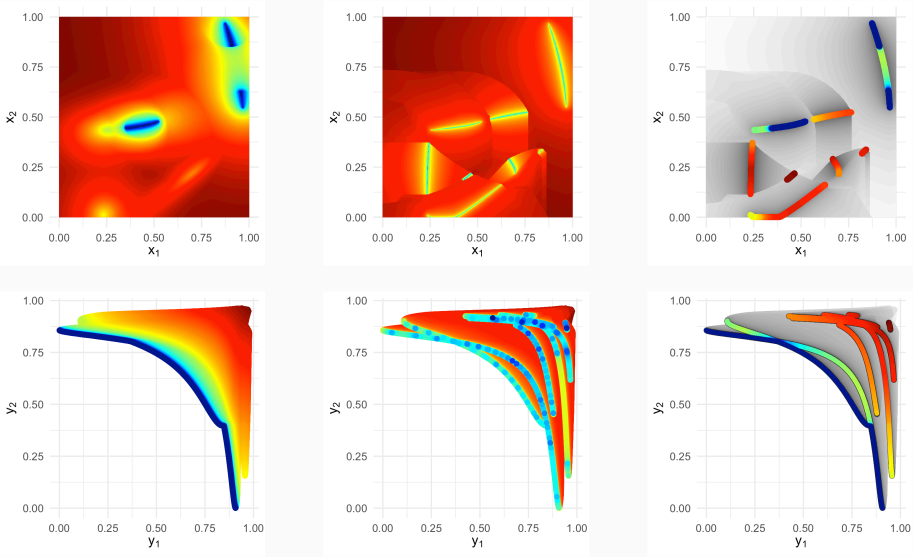


Building Blocks of AAS – Visualization: TSP II



(a) **Ackley**, $pstep = 2\beta$ (b) **Rastrigin**, $pstep = 2\beta$ (c) **Birastrigin**, $pstep = 2\beta$

$\rightsquigarrow$ *Local Optima Networks for Continuous Fitness Landscapes* [1]


1.00
0.75
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0.25
0.00
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x_1
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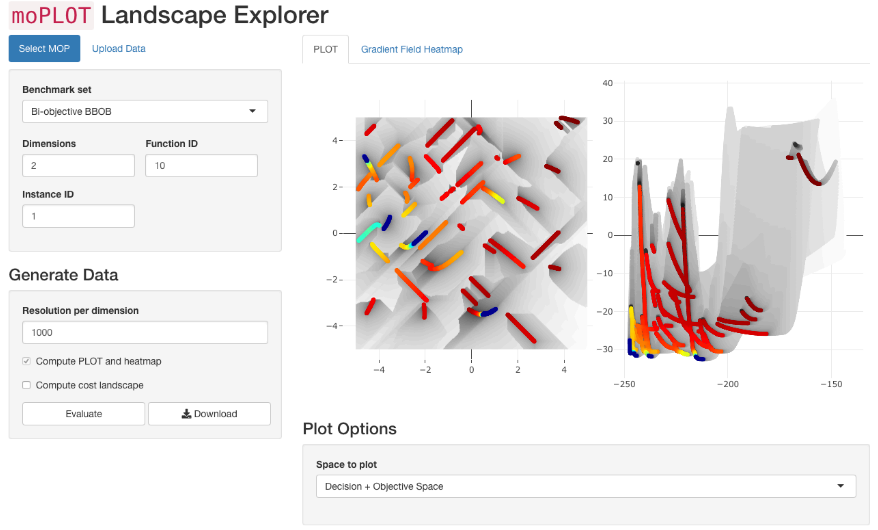
y_2

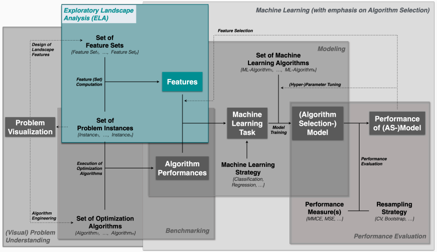
Building Blocks of AAS – Visualization: Multi-Objective Optimization II



⤳ make use of interactive tools such as **moPLOT** [46]

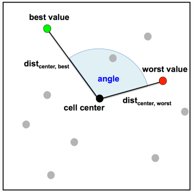
Building Blocks of AAS – Features

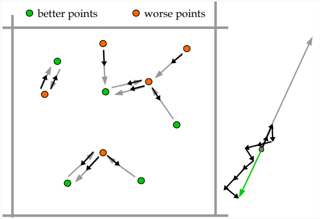
- features (i.e., numeric low-level statistics) capture a problem's essential information
- as informative and cheap as possible
- describe problem properties and/or can be used to discriminate between algorithms
- design of features (but not their practical application) requires domain-knowledge
- for various optimization domains, there exist either precomputed features or tools to compute them
- enables interpretation of algorithm selector's decision making procedure

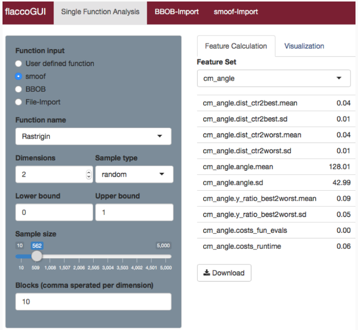


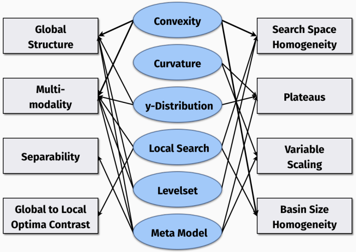
Building Blocks of AAS – Features: Continuous Optimization I

- mainly based on a small sample of (evaluated) points from the problem's landscape
- numerous research groups from all over the world developed hundreds of features
- majority of features available in R-package `flacco` [22], web-application `flaccoGUI` [15], and python-package `pflacco` [41]

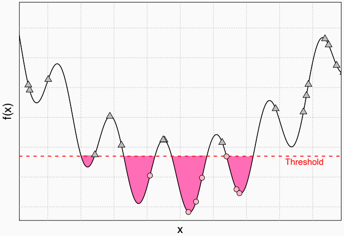




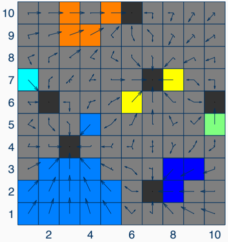




Building Blocks of AAS – Features: Continuous Optimization II



[32]



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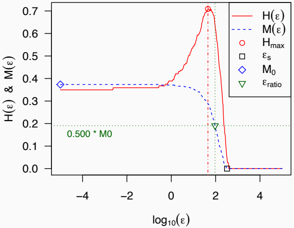

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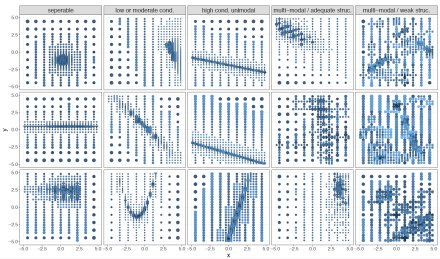

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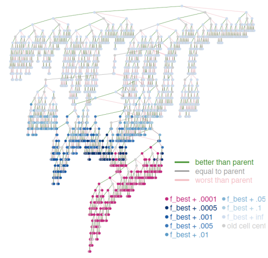
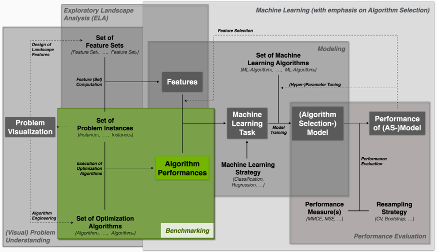
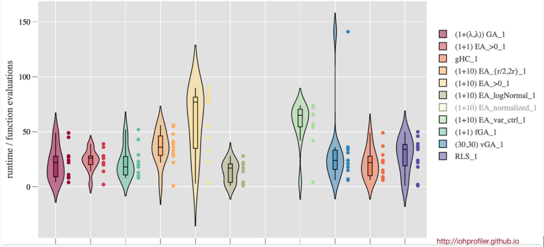


Building Blocks of AAS – Benchmarking

- measures performance of an algorithm (usually runtime or solution quality)
- which algorithms are promising, useless, etc.?
- which problems are easy, challenging, etc.?
- in some domains, large data bases exist [13]
- survey paper on benchmarking optimization algorithms [4]
- investigate how much each algorithm contributes to the portfolio



Building Blocks of AAS – Benchmarking: Tools and Approaches



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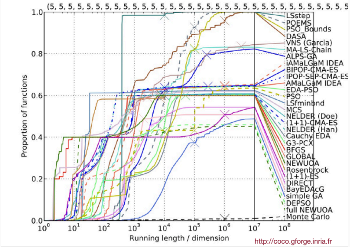

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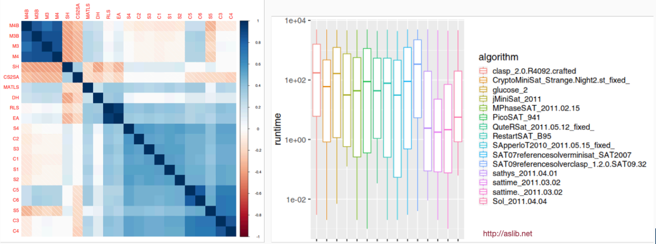

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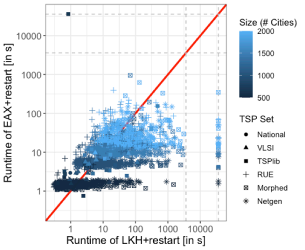
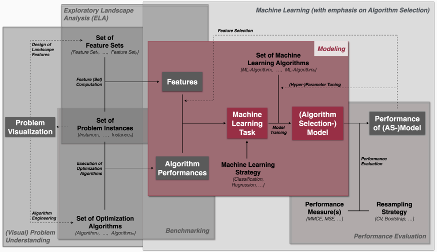


[24]

Building Blocks of AAS – Modeling

- map problem features to algorithm performances
- different approaches:
  - classification: ‘correct’ class is the best algorithm (per instance)
  - regression: model performance per algorithm, and select (per instance) the algorithm with the best predicted performance
  - pairwise regression
  - clustering
  - classifier chains
- quality of the selector highly depends on considered (subset of) features, choice of ML algorithm, its (hyperparameter) configuration



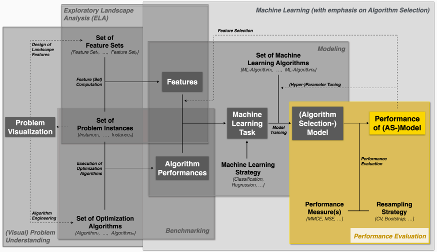
Building Blocks of AAS – Modeling: ML Frameworks

- there exist numerous tools for performing such ML tasks, such as
  - R: **`mlr3`** [28] (https://mlr3.mlr-org.com)
  - python: **`scikit-learn`** [38] (https://scikit-learn.org/stable/)
- algorithm selector attempts to close the gap between a portfolio's SBS (0%) and VBS (100%):
  - *single best solver (SBS)*: best stand-alone algorithm from the portfolio (based on each algorithm's average performance across the whole data set)
  - *virtual best solver (VBS)*: always picking the best algorithm from the portfolio "for free" (oracle-like prediction per instance)
- the SBS and VBS provide the lower and upper limits of the AS performance
- VBS-like performance is unlikely (feature computation is not for free)

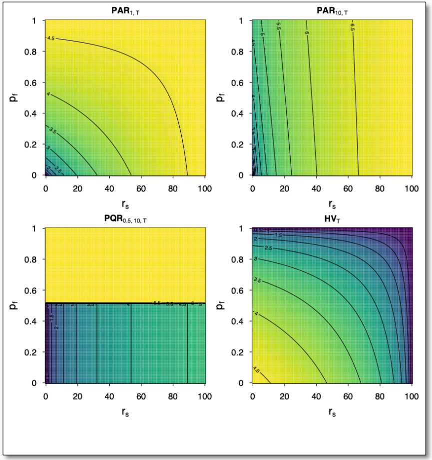
Problem	Algorithm			VBS
	A	B	C	
P1	1	5	2	1
P2	1500	1	1	1
P3	50	150	1	1
...	...	...	...	...
P50	8	1	10	1
∅	34	10	3	1
			SBS	

Building Blocks of AAS – Performance

- avoid overfitting by using a resampling strategy (crossvalidation, bootstrap sampling, holdout, etc.)
- use an appropriate performance measure
  - accuracy (often the default in classification) $\rightsquigarrow$ treats all errors equally
  - oftentimes, the misclassification penalty is a better choice as it can help the selector to focus on the relevant cases (where misclassifications are actually costly)
- pass the selector's performance to the previous (modeling) stage to find a better selector



- one needs one scalar value for each pair of algorithm and problem instance
- need to handle information of repeated runs (to assess algorithm stochasticity)
- need to treat performance of failed runs (e.g., penalized by 10-fold of maximum budget)
- aggregate performance across all runs (per pair of algorithm and problem instance)
- typical measures (depending on the domain):
  - penalized average runtime (e.g., PAR10 or PAR2)
  - penalized quantile runtime (e.g., PQR10)
  - expected runtime



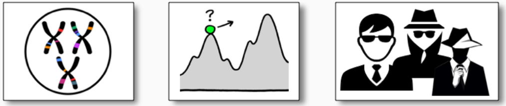
Status Quo of Automated Algorithm Selection

Status Quo of Automated Algorithm Selection

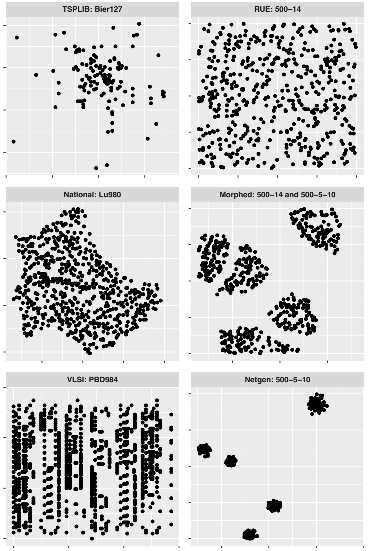
Traveling Salesperson Problem

Automated Algorithm Selection in TSP

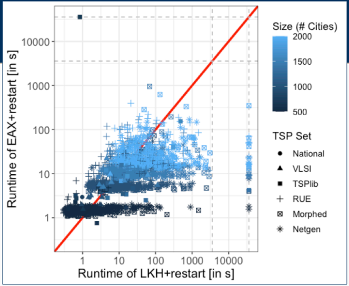
- most comprehensive AS study for TSP [24]
- six TSP sets with 1 845 instances in total:
  - ‘real-world’ TSP sets: TSPLib, National, VLSI
  - artificial TSP sets: RUE, Netgen, Morphed
- five state-of-the-art solvers:
  - EAX [37]
  - LKH [18]
  - restart variants of EAX and LKH [11]
  - MAOS [52]

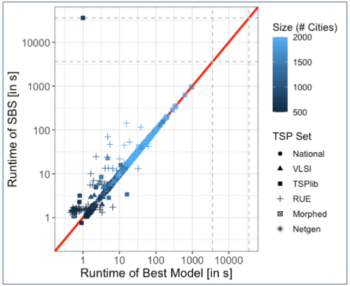


- feature sets (with 400+ features):
  - TSPmeta [35]
  - UBC [20]
  - Pihera [39]



- measured performance via PQR10 scores[1]
- baselines for performance assessment:
  - single-best solver (SBS): 36.30s (here: EAX+restart)
  - virtual best solver (VBS): 10.73s
  - 2nd-best solver (LKH+restart): 565.85s
- trained 14 candidate AS models per feature set
  - decision trees, random forests, SVMs, MARS models
  - classification, regression, paired regression
- considered 4 feature selection strategies per selector
- best found selector:
  - classification-based SVM
  - uses 16 of the 400+ features
  - PQR10-score: 16.75s (closed 75% of SBS-VBS gap)

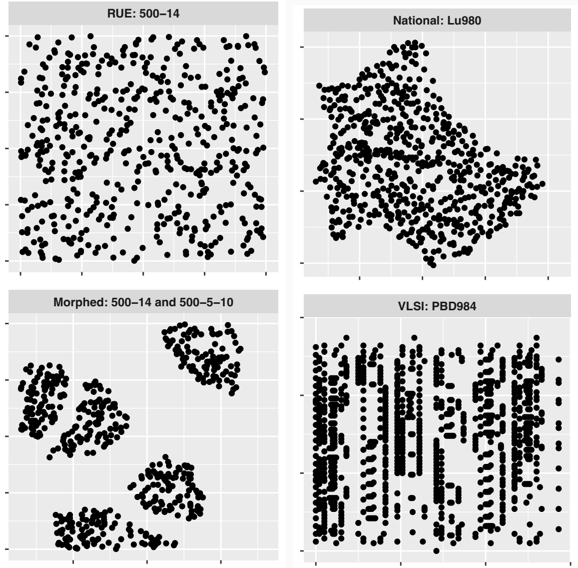




1. $\mathrm{PQR}_{p,f,T}(A,I) = \begin{cases} f \cdot T, & \text{if } \sum_{i=1}^{m} \mathbb{1}\{r_i^{A,I} < T\} < \lfloor m \cdot p + 1 \rfloor \\ q_p(r_1^{A,I}, \dots, r_m^{A,I}), & \text{otherwise} \end{cases}$

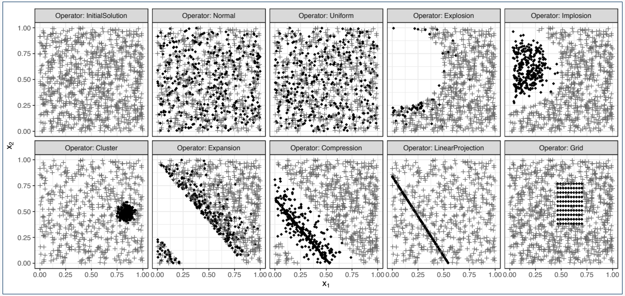
Gap Between Artificial and Real-World Problems

- set of representative and discriminative TSP instances is essential
- limited amount of real-world instances
- instance generators create very artificial problems

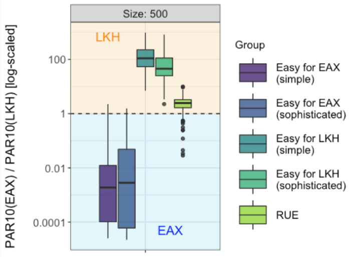


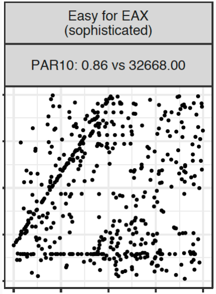
Bridging the Gap

- designed "more realistic" mutation operators [7] capable of creating more structural instances



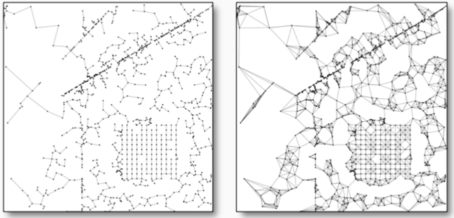
- evolved TSP instances that were tailored to be easy for EAX and challenging for LKH (and vice versa)

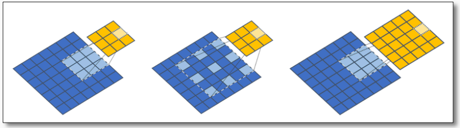




Deep Learning as Feature-Free Alternative

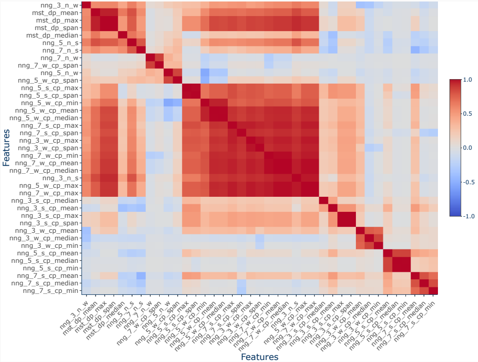
- features need to be cheaply computable, informative and discriminative
- investigated applicability of deep learning as “feature-free” alternative [47]
- images of TSP instances as input
    - scatterplot of cities
    - minimum spanning tree
    - k-nearest neighbor graph (with $k = 5$)
- different convolutional neural networks
- closed SBS-VBS-gap:
    - classical AS approach: 17.9%
    - CNN based on cities: 17.8%
    - CNN based on cities + MST: 21.5%



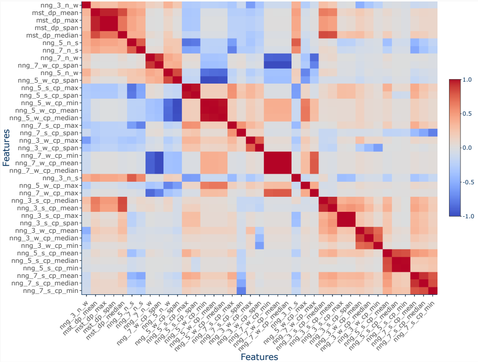


Robustness of TSP Features

- many TSP features are affected by instance size or search space dimensionality
- recent studies examined the potential of normalization [16, 17]



without normalization



with normalization

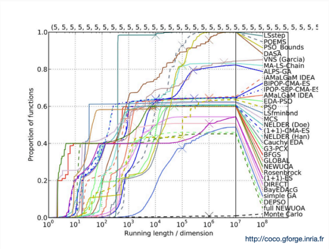
- dashboard at: https://tsp-features.shinyapps.io/normalization-eda/

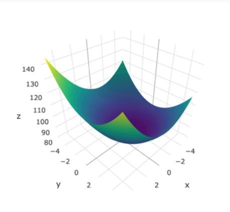
Status Quo of Automated Algorithm Selection

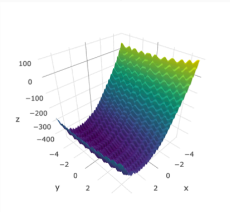
Continuous Black-Box Optimization

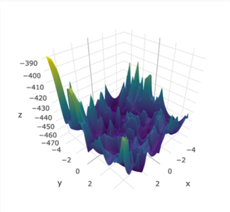
Automated Algorithm Selection in Continuous Black-Box Optimization

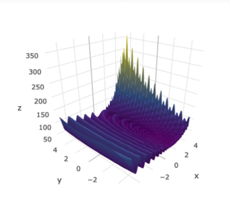
- conducted the up to now most comprehensive AS study for single-objective continuous optimization [21]
- experiments based on a total of 480 instances from the Black-Box Optimization Benchmark (BBOB) [12]
- considered performance data of all 129 optimization algorithms that were available in COCO [14]




Sphere

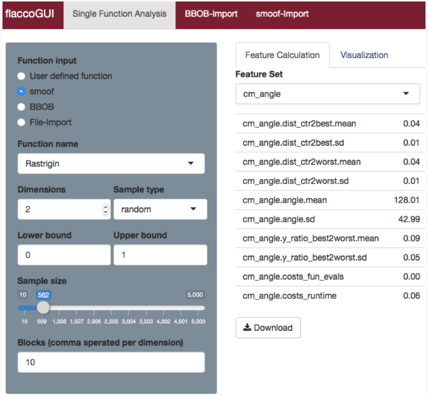

Rastrigin


Gallagher's Gaussian 101-me Peaks


Schaffers F7

Exploratory Landscape Analysis

- *Exploratory Landscape Analysis (ELA)*
  - research area focussing on characterization of continuous optimization problems
  - seminal work [34] has been acknowledged with the *ACM SigEVO Impact Award 2021*
- characterized problems by means of 100+ features using the R-package **`flacco`** [22]
- **`flacco`** is also available for non-R-users:
  - python-package **`pflacco`** [40]
  - platform-independent web application [15] (https://flacco.shinyapps.io/flacco/)



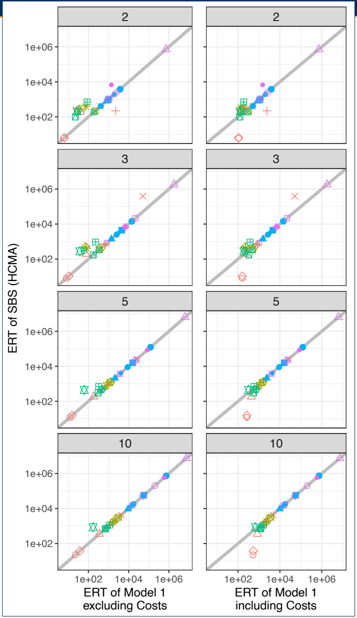
Automated Algorithm Selection in Continuous Black-Box Optimization

- reduced portfolio from 129 to 12 optimizers:



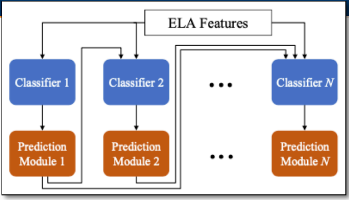

2x deterministic 5x multi-level 4x CMA-ES 1x commercial

- measured performance as PAR10 score of relative expected runtime (relERT)
  $\rightsquigarrow$ virtual best solver (VBS) has to be 1
- hybrid algorithm HCMA [31] is single-best solver with a mean PAR10 score of 30.4
- best found AS model: SVM (using 9 features) with a mean PAR10 score of 14.2



Towards Automated Algorithm Configuration in Continuous Optimization

- feature-based approaches are so far mainly used in AS (but not in AC)
- modularized CMA-ES [49]
  - 9 binary and 2 trinary modules
  - in total, $2^9 \times 3^2 = 4\,608$ configurations possible
  - SBS among all 4 608 configurations was on average 28 times slower than the VBS
- classifier chains in combination with ELA features for landscape-aware AC [42]
  - order of the 11 modules matters
  - 11! (≈40 mio.) classifier chains were investigated
- best classifier chain is competitive
  - relative ERT of 16.02 (40% speed-up over SBS)
  - sometimes even outperformed HCMA



		Baseline			CC		COCO	
D	Function	SBS	CMA	IPOP	no	with	HCMA	BRENT
2	01-05	110.12	401.30	106.11	42.09	48.25	0.55	0.27
	06-09	20.65	17.30	3.75	6.56	8.53	2.80	7920.81
	10-14	2.96	3.69	5.09	1.77	3.27	1.53	3065.59
	15-19	6.81	417.56	5.95	21.16	22.11	5.16	2478.98
	20-24	116.69	372.84	106.89	37.88	39.42	76.85	3664.40
	all	52.73	251.92	47.30	22.53	24.97	17.98	3238.73
3	01-05	27.93	161.67	19.96	46.90	48.33	6.46	0.09
	06-09	5.30	296.04	2.88	15.75	16.97	1.80	4284.56
	10-14	2.98	3.54	3.05	1.70	2.99	1.24	3007.97
	15-19	6.65	330.75	7.17	10.40	10.91	4.27	1946.15
	20-24	48.43	245.90	48.41	35.12	35.83	34.61	2846.85
	all	18.80	203.89	16.85	22.23	23.26	10.01	2339.31
5	01-05	51.80	38.33	27.47	4.68	5.76	0.57	0.06
	06-09	5.14	320.47	2.36	2.69	3.37	1.41	3130.59
	10-14	2.23	2.44	2.44	1.61	2.59	0.79	2129.87
	15-19	9.35	223.61	10.75	7.59	7.88	3.04	1445.89
	20-24	44.44	1161.38	180.26	10.89	11.20	8.73	1078.98
	all	23.32	350.44	46.42	5.61	6.28	2.97	1491.52
10	01-05	45.53	12.46	12.47	11.64	12.62	0.05	0.05
	06-09	5.26	454.39	1.79	1.77	2.16	1.01	1967.78
	10-14	1.99	2.51	2.27	2.24	3.00	0.58	1477.10
	15-19	3.88	316.59	15.80	8.56	8.79	2.93	1120.49
	20-24	31.62	434.65	175.75	19.60	19.75	23.51	783.99
	all	18.17	235.36	43.27	9.05	9.56	5.81	1032.47
all	01-05	58.84	153.44	41.50	26.33	28.74	1.91	0.12
	06-09	9.09	272.05	2.69	6.69	7.76	1.75	4325.93
	10-14	2.54	3.04	3.21	1.83	2.96	1.04	2420.13
	15-19	6.67	322.13	9.92	11.93	12.42	3.85	1747.88
	20-24	60.30	553.69	127.83	25.87	26.55	35.93	2093.55
	all	28.26	260.40	38.46	14.86	16.02	9.19	2025.51

Benefits and Perspectives

Cross-Domain Benefits

- achieved substantial performance gains in various optimization domains [25]:
  - Traveling Salesperson Problem [27, 24, 55, 47]
  - Single-Objective Continuous Optimization [5, 21]
  - Propositional Satisfiability (SAT) Problem [53, 54, 33, 29, 30]
  - Traveling Thief Problem [50]
  - Bin-Packing Problem [2]
  - Answer Set Programming (ASP) [19, 29, 30]
  - Quantified Boolean Formula (QBF) Problem [29, 30]
  - AI Planning [44, 45, 8]
  - ...

Automated Algorithm Selection: Survey and Perspectives

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Abstract

It has long been observed that for practically any computational problem that has been intensely studied, different instances are best solved using different algorithms. This is particularly pronounced for computationally hard problems, where in most cases, no single algorithm defines the state of the art; instead, there is a set of algorithms with complementary strengths. This performance complementarity can be exploited in various ways, one of which is based on the idea of selecting, from a set of given algorithms, for each problem instance to be solved the one expected to perform best. The task of automatically selecting an algorithm from a given set is known as the *per-instance algorithm selection problem* and has been intensely studied over the past 15 years, leading to major improvements in the state of the art in solving a growing number of discrete combinatorial problems, including propositional satisfiability and AI planning. Per-instance algorithm selection also shows much promise for boosting performance in solving continuous and mixed discrete/continuous optimisation problems. This survey provides an overview of research in automated algorithm selection, ranging from early and seminal works to recent and promising application areas. Different from earlier work, it covers applications to discrete and continuous problems, and discusses algorithm selection in context with conceptually related approaches, such as algorithm configuration, scheduling, or portfolio selection. Since informative and cheaply computable problem instance features provide the basis for effective per-instance algorithm selection systems, we also provide an overview of such features for discrete and continuous problems. Finally, we provide perspectives on future work in the area and discuss a number of open research challenges.

Keywords

Automated algorithm selection, automated algorithm configuration, combinatorial optimisation, continuous optimisation, machine learning, metalearning, feature-based approaches, exploratory landscape analysis, data streams.

1 Introduction

It has long been observed that for well-studied computational problems for which several high-performance algorithms are available, there is typically no single algorithm

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 Evolutionary Computation 27(1): 3–45

Cross-Domain Benefits

- AAS enables to exploit the potential (of portfolios) of state-of-the-art optimization algorithms [6]
- aims at closing the gap between a portfolio's SBS (0%) and VBS (100%)

	classif/ ksvm (0.48)	classif/ randomForest (0.52)	classif/ rpart (0.42)	regr/ lm (0.48)	regr/ randomForest (0.65)	regr/ rpart (0.34)	cluster/ XMeans (0.22)
SAT11–HAND	0.72*	0.62	0.59	0.48	0.65	0.47	0.12
SAT11–INDU	0.10	0.15*	0.11	0.13	0.01	–0.29	0.01
SAT11–RAND	0.76	0.85	0.86	0.83	0.90*	0.82	0.54
SAT12–ALL	0.63	0.70	0.06	0.43	0.72*	0.32	–0.01
SAT12–HAND	0.60	0.70	0.37	0.51	0.75*	0.45	0.08
SAT12–INDU	0.37	0.44	–0.18	0.24	0.47*	–0.01	–0.16
SAT12–RAND	–0.00	0.10	0.34*	0.28	0.25	–0.50	0.10
SAT15–INDU	0.25	0.22	0.21	0.09	0.49*	0.02	–0.10
QBF–2011	0.67	0.79	0.72	0.71	0.88*	0.70	0.43
QBF–2014	0.46	0.53	0.38	0.35	0.79*	0.52	0.07
MAXSAT12–PMS	0.62	0.65	0.62	0.63	0.90*	0.62	0.60
MAXSAT15–PMS–INDU	0.31	0.37	0.27	0.46	0.64*	0.19	0.45
CSP–2010	0.55	0.67	0.83*	0.66	0.77	0.29	0.23
CSP–MZN–2013	0.82	0.79	0.68	0.83	0.91*	0.77	0.16
PROTEUS–2014	0.73	0.73	0.47	0.77	0.81*	0.71	0.54
ASP–POTASSCO	0.39	0.43	0.47	0.55	0.80*	0.53	0.40
PREMAR–ASTAR–2015	0.23	0.16	0.23	0.16	0.29*	0.16	0.22

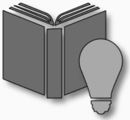
Key Benefits

Profitable Performance

- large speed-up compared to (standalone versions of) state-of-the-art algorithms
- requires less resources / leads to increased profitability

Automated Optimization

- independent of human experts
- high likelihood to select a well-performing algorithm



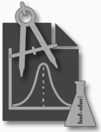
Increased Interpretability

- captures interplay between problem structure and algorithm performance
- key to interpretability of algorithmic search behavior

Research Perspectives

From Text Book to Real-World

- generate more “real-worldish” problem instances
- consider streaming data
- augment data (sensors, weather, traffic, etc.)



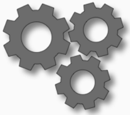
Theoretical Fundamentals of Features

- increase robustness (w.r.t. problem size, scaling, etc.)
- features capable of dealing with stochasticity

Dynamic Algorithm Selection (and Configuration)

- monitor search behavior during the optimization run
- develop features that characterize the search behavior
- switch and configure algorithms dynamically during the run

Research Perspectives



Improve Algorithm Selection Models

- deepen understanding about potential of deep learning
- incorporate automated feature selection strategies

Performance Assessment

- measure the anytime behavior
- multi-objective view (e.g., solution quality vs. runtime)

Apply Concepts to Various TSP-Extensions

- weighted TSP
- Traveling Thief Problem (TTP)
- variants of the Vehicle Routing Problem (VRP)

Thank You!

Any Comments or Questions?!

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