



Exploratory Landscape Analysis

Pascal Kerschke and Mike Preuss

Tutorial at GECCO 2019, July 2019 in Prague, Czech Republic

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<https://doi.org/10.1145/3319619.3323389>



Introduction

Instructors

Pascal Kerschke is postdoctoral researcher at the group of *Information Systems and Statistics* at the University of Münster, Germany. He has received degrees in *Data Analysis & Management* (B.Sc., 2010) and *Data Sciences* (M.Sc., 2013) from the TU Dortmund University, Germany, and a PhD in *Information Systems* (2017) from the University of Münster.

His current research interests are algorithm selection, as well as *Exploratory Landscape Analysis* for single- and multi-objective optimization problems.



Mike Preuss is Assistant Professor at Leiden University, The Netherlands, and member of the ERCIS network. Previously, he was with the group of *Information Systems and Statistics* at the University of Münster, Germany. In 2013, he received his PhD at TU Dortmund University, Germany.

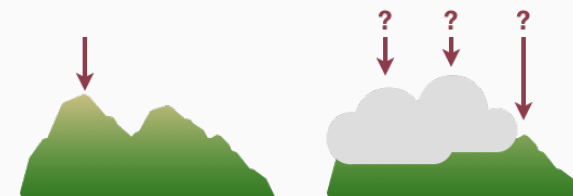
His research interests focus on the field of evolutionary algorithms for real-valued problems, namely on multimodal and multi-objective optimization. He is also active in computational intelligence methods for computer games.



Introduction

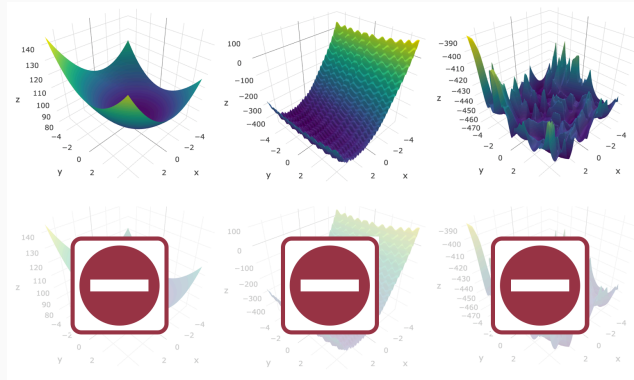
Context:

- *Black-Box Optimization*: find the optimum of a given problem without actually knowing its entire landscape



Introduction

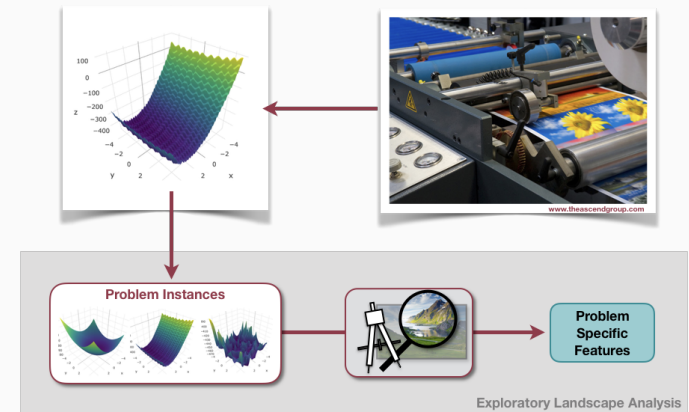
- lack of real-world problems
 ~ use benchmark problems and handle them as black-box



Introduction

Idea of ELA

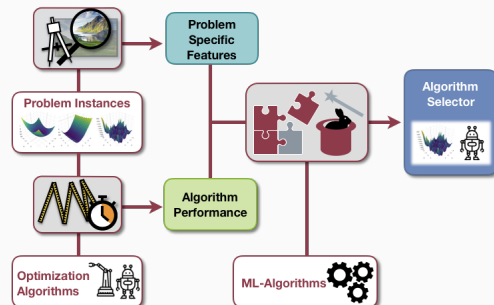
- extract information from (black-box) optimization problems in an automated fashion



Introduction

How is ELA helpful when optimizing a given problem?

- *Algorithm Selection Problem*: find the individually best suited algorithm for an unseen optimization problem



[36] Rice, J. R. (1976). *The Algorithm Selection Problem*. In *Advances in Computers* (pp. 65-118).

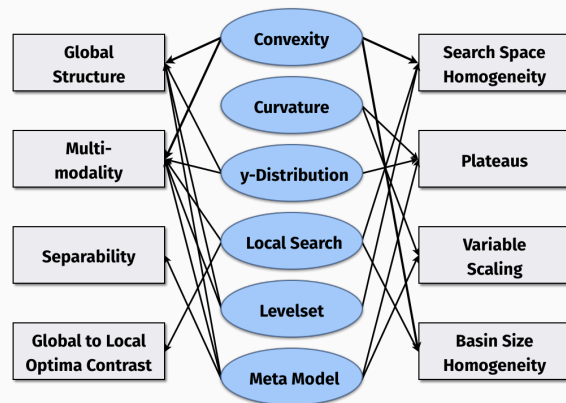
[17] Kerschke, P., Hoos, H. H., Neumann, F. & Trautmann, H. (2019). *Automated Algorithm Selection: Survey and Perspectives*. In *Evolutionary Computation*, Vol. 27, Number 1 (pp. 3-45).

Introduction

Exploratory Landscape Analysis (ELA):

- we aim at finding the “best” algorithm
- also improve understanding of problems, as well as algorithm/problem dependency
- basic idea (exploratory!): we start with **very simple features without clear purpose**
- match existing high-level features (expert knowledge) with our ELA features
- currently: mostly continuous (black-box) (global) optimization, but also in other domains (e.g., TSP)

Introduction



[29] Mersmann, O., Preuss, M. & Trautmann, H. (2010). *Benchmarking Evolutionary Algorithms: Towards Exploratory Landscape Analysis*. In Proceedings of PPSN XI (pp. 71 - 80).

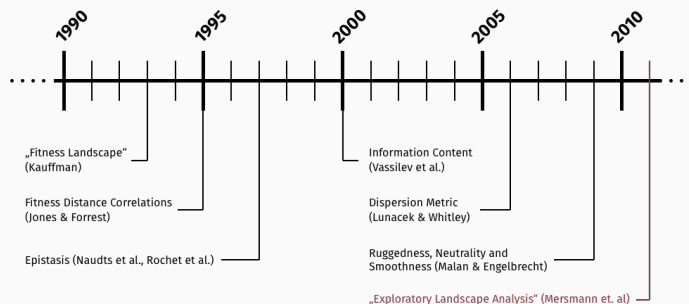
[28] Mersmann, O., Bischl, B., Trautmann, H., Preuss, M., Weihs, C. & Rudolph, G. (2011). *Exploratory Landscape Analysis*. In Proceedings of GECCO 2011 (pp. 829 - 836).

Introduction

- we do not know functional relationships when designing features
- but we can match them to high-level characteristics (multimodality, funnel structure, etc.) of optimization problems
- this enables recognizing important problem properties quickly
- based on initial design of samples x_{i1}, \dots, x_{id} and their corresponding fitness value y_i , $i = 1, \dots, n$
- given an evaluated initial design (initial population?), most ELA features are for free
- there are already several different feature sets

Introduction

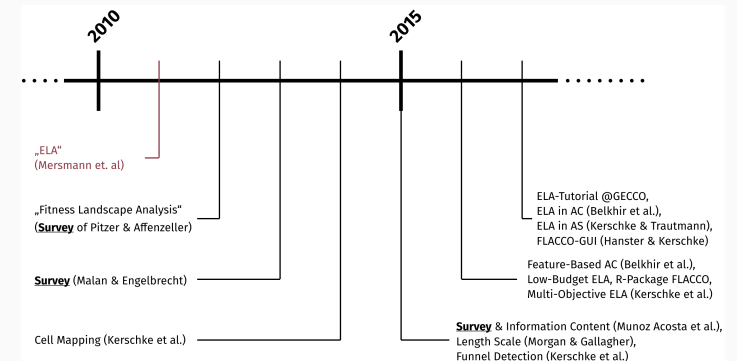
History of Landscape Analysis – Before ELA:



Further details are given in [13, 12, 33, 37, 40, 25, 26, 28]

Introduction

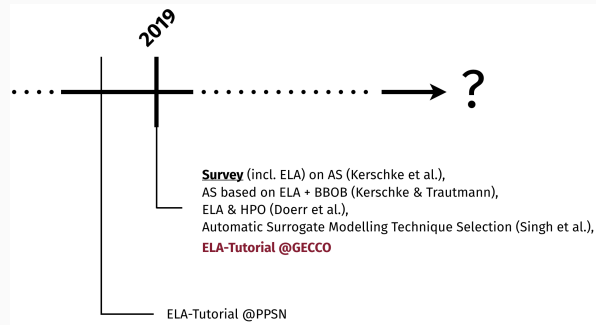
History of Landscape Analysis – Since ELA:



Further details are given in [28, 34, 27, 19, 31, 32, 30, 20, 2, 21, 22, 15, 18, 10, 23, 3]

Introduction

History of Landscape Analysis – Most Recent Developments:



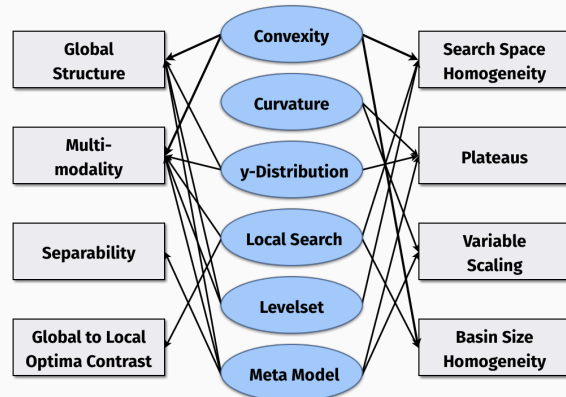
Further details are given in [23, 17, 7, 39]

Single-Objective ELA Features

Single-Objective ELA Features

Classical ELA Features

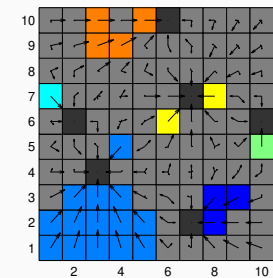
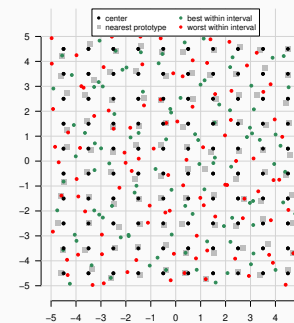
[29] Mersmann, O., Preuss, M. & Trautmann, H. (2010). *Benchmarking Evolutionary Algorithms: Towards Exploratory Landscape Analysis*. In Proceedings of PPSN XI (pp. 71 - 80).



Single-Objective ELA Features

General Cell Mapping Features

[19] Kerschke, P., Preuss, M., Hernández, C., Schütze, O., Sun, J.-Q., Grimme, C., Rudolph, G., Bischl, B. & Trautmann, H. (2014). *Cell Mapping Techniques for Exploratory Landscape Analysis*. In Proceedings of EVOLVE 2014 (pp. 115 - 131).

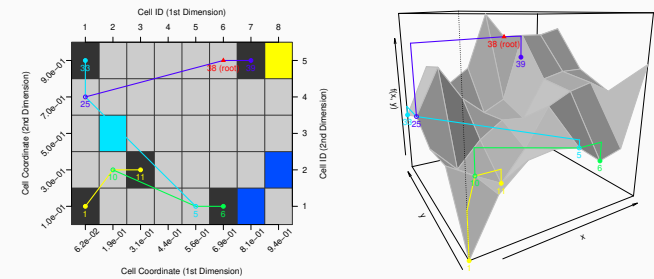


Single-Objective ELA Features

Barrier Tree Features

[11] Hernández, C., Schütze, O., Emmerich, M. T. M., & Xiong, F. R. (2014). *Barrier Tree for Continuous Landscapes by Means of Generalized Cell Mapping*. In Proceedings of EVOLVE 2014.

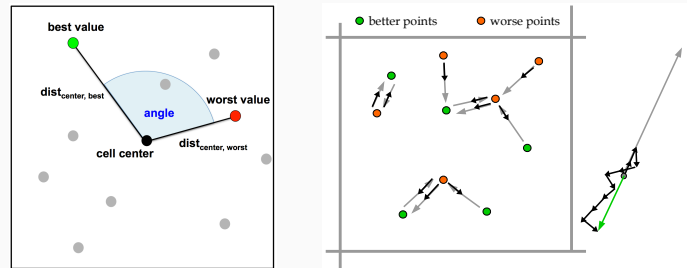
[8] Flamm, C., Hofacker, I. L., Stadler, P. F. & Wolfinger, M. T. (2002). *Barrier Trees of Degenerate Landscapes*. In International Journal of Research in Physical Chemistry and Chemical Physics (pp. 155 - 173).



Single-Objective ELA Features

Cell Mapping Features

[19] Kerschke, P., Preuss, M., Hernández, C., Schütze, O., Sun, J.-Q., Grimme, C., Rudolph, G., Bischl, B. & Trautmann, H. (2014). *Cell Mapping Techniques for Exploratory Landscape Analysis*. In Proceedings of EVOLVE 2014 (pp. 115 - 131).

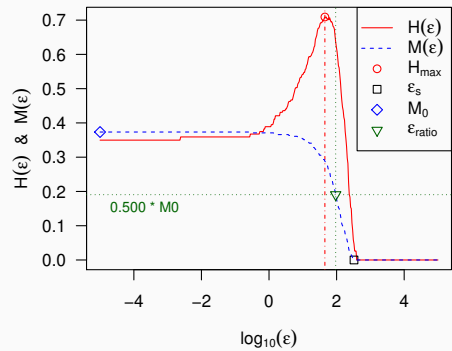


Single-Objective ELA Features

Information Content Features

[31] Muñoz, M. A., Kirley, M., Halgamuge, S. K. (2015). *Exploratory Landscape Analysis of Continuous Space Optimization Problems using Information Content*. In IEEE Transactions on Evolutionary Computation (pp. 74 - 87).

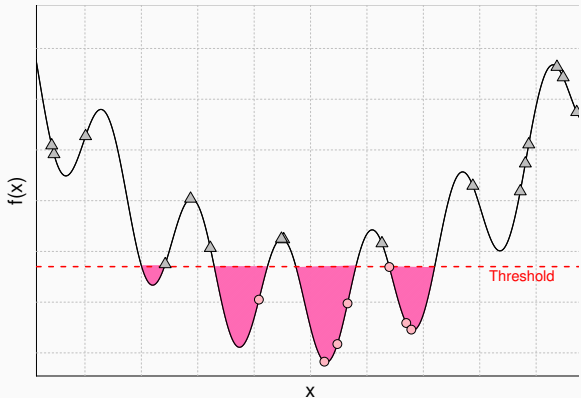
[40] Vassilev, V. K., Fogarty, T. C. & Miller, J. F. (2000). *Information Characteristics and the Structure of Landscapes*. In Evolutionary Computation, Vol. 8, Number 1 (pp. 31 - 60).



Single-Objective ELA Features

Dispersion Features

[25] Lunacek, M. & Whitley, D. (2006). *The Dispersion Metric and the CMA Evolution Strategy*. In Proceedings of GECCO 2006 (pp. 477 - 484).



Single-Objective ELA Features

Hill Climbing Features

[1] Abell, T., Malitsky, Y. & Tierney, K. (2013). *Features for Exploiting Black-Box Optimization Problem Structure*. In Proceedings of LION 2013 (pp. 30 - 36).

Ruggedness Features

[27] Malan, K. M. & Engelbrecht, A. P. (2013). *Ruggedness, Funnels and Gradients in Fitness Landscapes and the Effect on PSO Performance*. In Proceedings of CEC 2013 (pp. 963 - 970).

Nearest Better Clustering Features

[20] Kerschke, P., Preuss, M., Wessing, S. & Trautmann H. (2015). *Detecting Funnel Structures by Means of Exploratory Landscape Analysis*. In Proceedings of GECCO 2015 (pp. 265 - 272).

Length Scale Features

[30] Morgan, R. & Gallagher M. (2015). *Analyzing and Characterising Optimization Problems Using Length Scale*. In Soft Computing (pp. 1 - 18).

Bag of Local Landscape Features

[38] Shirakawa, S. & Nagao, T. (2016). *Bag of Local Landscape Features for Fitness Landscape Analysis*. In Soft Computing, 20(10) (pp. 3787 - 3802).

(ELA for Single-Objective) Multimodal Optimization

Multimodal Optimization



Multimodal Optimization

- algorithmic ancestry goes back to the 1980s
- yearly competitions and publications steadily produce new methods
- two main algorithmic approaches:
 - parallel, large populations
 - sequential, coordinated restarts
- several components that may be used: archives, clustering methods, methods for obtaining well distributed samples
- ELA could be helpful for selecting components/methods

Multimodal Optimization

- different aims possible
- currently most important (competitions): multiglobal
= find all search space points that are globally optimal
- other options: all optima, well distributed good optima, multiglobal over time, etc.
- interesting: feature values do not change because they do not depend on actual measure, we can reuse feature data
- but we need different algorithms for different goals
- algorithm performances and one sample on the problems enable algorithm selection per criterion

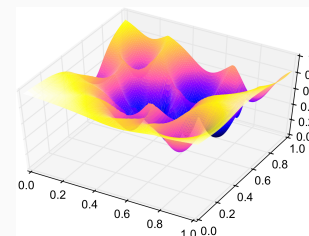
Exemplary Use Cases of ELA

Exemplary Use Cases of ELA: Funnel Detection

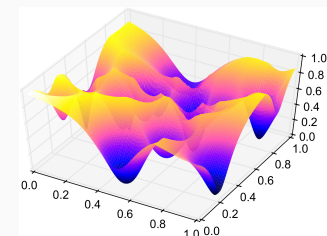
Example 1: **Funnel Detection**

Exemplary Use Cases of ELA: Funnel Detection

- funnel: local optima are located near to each other and pile up to an “upside-down mountain”
- knowledge about underlying global structure, i.e. funnels, helps selecting the right algorithm



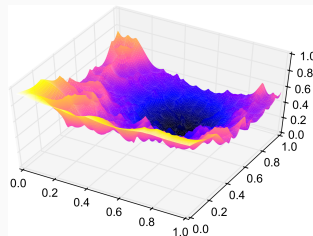
(a) funnel



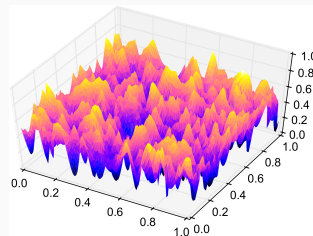
(b) non-funnel (“random”)

Exemplary Use Cases of ELA: Funnel Detection

- different algorithm candidates for either category
- but there is a wide variety within classes funnel and non-funnel



(a) funnel



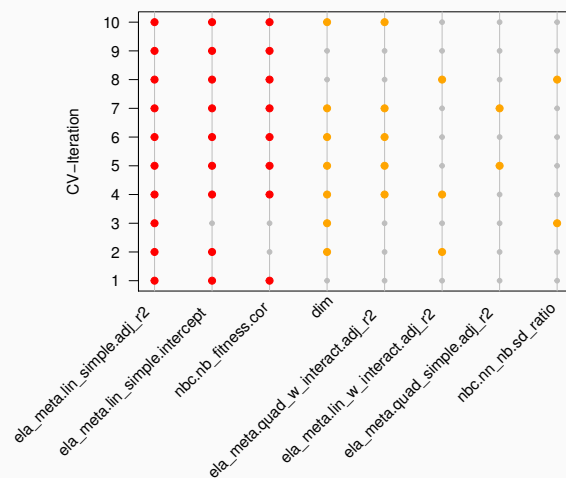
(b) non-funnel ("random")

Exemplary Use Cases of ELA: Funnel Detection

- detailed results in our GECCO paper¹
- used MPM2² to generate a set of 4,000 training instances
- initial designs of size $50 \times d$ observations (small!)
- trained four classifiers (random forest, rpart, kkn and ksvm)
- experimentally driven reduction of the full feature set (300+ features) to 8 features
- validated results on BBOB and subset of problems from CEC-2013 niching competition

1. [21] Kerschke, P., Preuss, M., Wessing, S. & Trautmann H. (2016). Low-Budget Exploratory Landscape Analysis on Multiple Peaks Models. In Proceedings of GECCO 2016 (pp. 229-236)
2. [43, 4] multiple peaks model 2 generator, available in python (optproblems0.9, Wessing, S.) and R (smoof, Bossek, J.)

Exemplary Use Cases of ELA: Funnel Detection

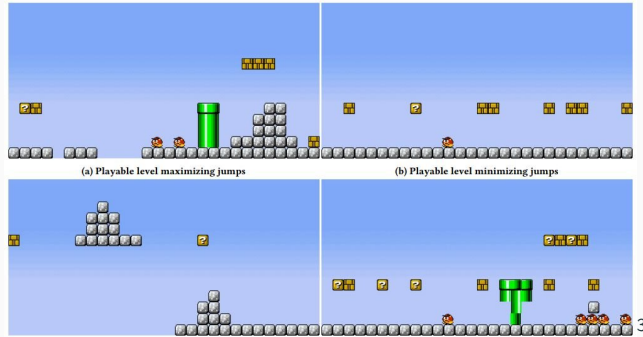


Exemplary Use Cases of ELA: Benchmark Comparison

Example 2: **Benchmark Comparison (BBOB vs. Mario GAN)**

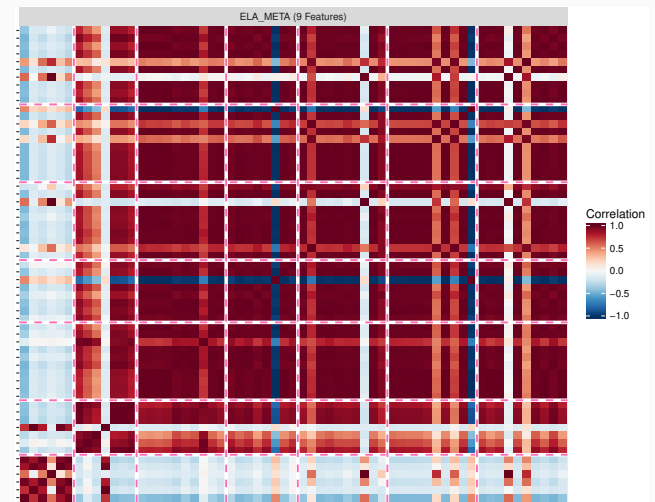
Exemplary Use Cases of ELA: Benchmark Comparison

- using GANs (Generative Adversarial Networks) for generating Super Mario levels
- comparison of underlying optimization problems against BBOB

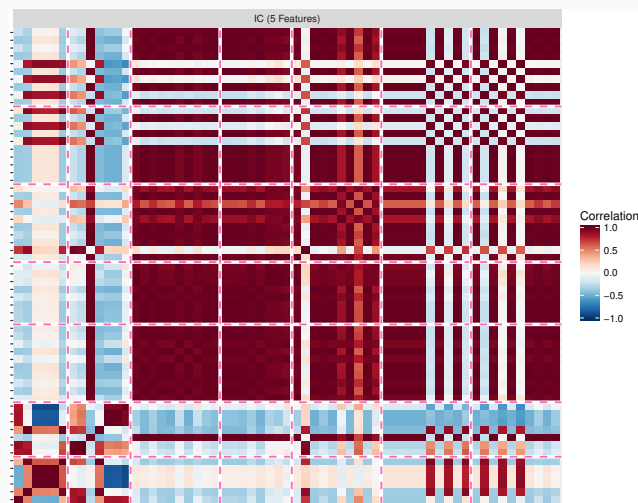


3. [42] Volz, V., Schrum, J., Liu, J., Lucas, S. M., Smith, A., & Risi, S. (2018). *Evolving Mario Levels in the Latent Space of a Deep Convolutional Generative Adversarial Network*. In *Proceedings of GECCO 2018* (pp. 221 - 228).

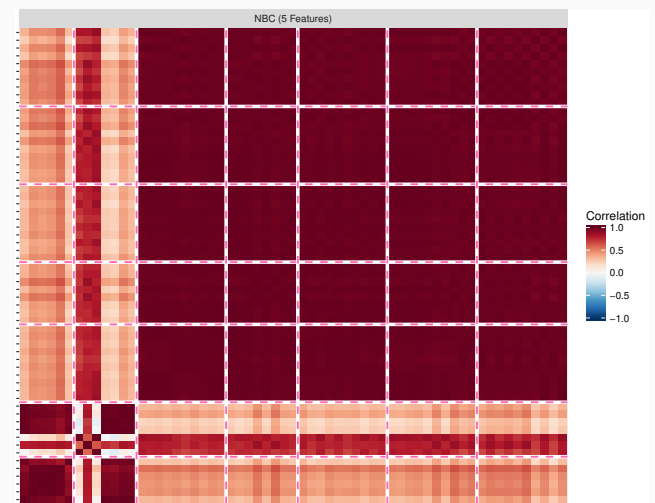
Exemplary Use Cases of ELA: Benchmark Comparison



Exemplary Use Cases of ELA: Benchmark Comparison



Exemplary Use Cases of ELA: Benchmark Comparison

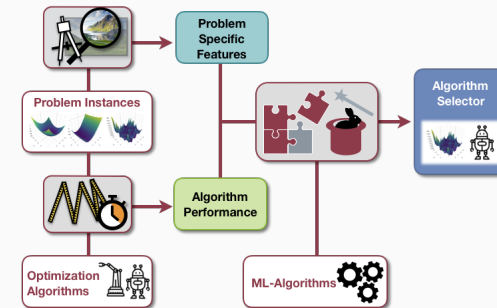


Exemplary Use Cases of ELA: ELA for Algorithm Selection

Example 3: Using ELA for Algorithm Selection

Exemplary Use Cases of ELA: ELA for Algorithm Selection

- *Algorithm Selection Problem*: find the individually best suited algorithm for an unseen optimization problem



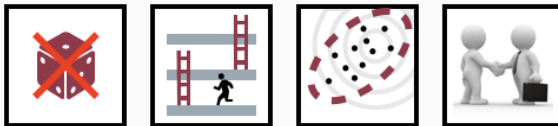
[36] Rice, J. R. (1976). *The Algorithm Selection Problem*. In *Advances in Computers* (pp. 65-118).

[17] Kerschke, P., Hoos, H. H., Neumann, F. & Trautmann, H. (2019). *Automated Algorithm Selection: Survey and Perspectives*. In *Evolutionary Computation*, Vol. 27, Number 1 (pp. 3-45).

Exemplary Use Cases of ELA: ELA for Algorithm Selection

Experimental setup - Part 1:

- COCO⁴: platform storing the performances of (129) optimization algorithms



~ considered 12 solvers from COCO

- 2x deterministic: BSrr, BSqi
- 5x multi-level approaches: MLST, fmincon, fminunc, HMLST, MCS
- 4x CMA-ES variants: CMA-CSA, IPOP400D, HCMA, SMAC-BBOB
- 1x commercial solver: OQNLP

4. [9] Hansen, N., Auger, A., Mersmann, O., Tušar, T. & Brockhoff, D. (2016). *COCO: A Platform for Comparing Continuous Optimizers in a Black-Box Setting*. ArXiv e-print arXiv:1603.08785. Link to COCO: <http://coco.gforge.inria.fr/>

Exemplary Use Cases of ELA: ELA for Algorithm Selection

Experimental setup - Part 2:

- all 24 BBOB problems
- problem dimensionality: $d \in \{2, 3, 5, 10\}$
- accuracy threshold: $\tau = 10^{-2}$
- performance measure: relative ERT (per problem)
- computed ca. 100 ELA features per problem based on initial designs of $50 \times d$ observations
- performed automated feature selection
- tried different machine learning algorithms

Exemplary Use Cases of ELA: ELA for Algorithm Selection

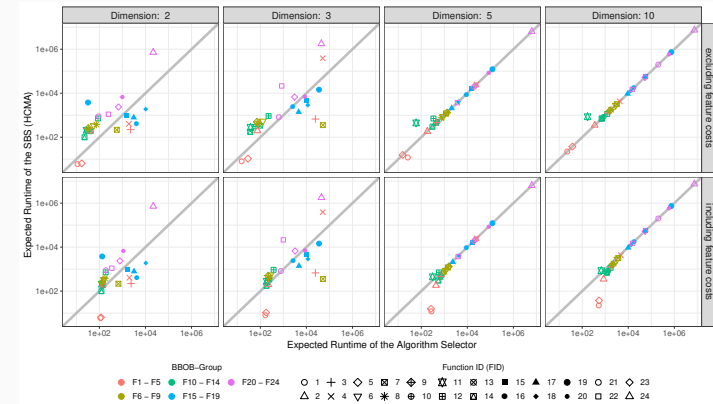
Results - Part 1:

- Single-Best Solver from Portfolio: HCMA (relERT ≈ 30.4)
 \leadsto on average 30x number of function evaluations (in relation to best possible solver per problem)
- Best Algorithm Selector: classification-based SVM (relERT ≈ 14.2)
 \leadsto less than half of the number of function evaluations of HCMA
- always predicts either fmincon, HCMA, HMLS or MLSL
- nine features employed by selector:
 - 1 (cell mapping) angle,
 - 1 levelset,
 - 1 y-distribution,
 - 2 meta-model and
 - 4 NBC features

Results - Part 2:

- detailed results can be found here:

[23] Kerschke, P. & Trautmann, H. (2018). *Automated Algorithm Selection on Continuous Black-Box Problems By Combining Exploratory Landscape Analysis and Machine Learning*. In *Evolutionary Computation*, Vol. 27, Number 1 (pp. 99 - 127)

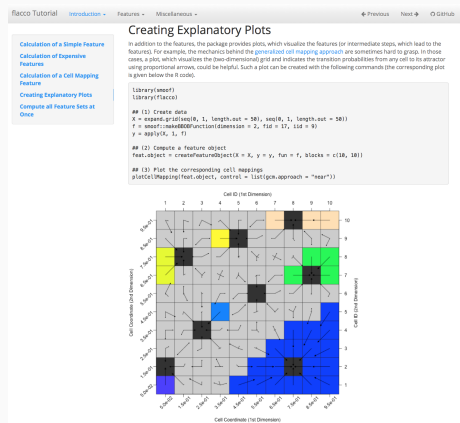


FLACCO + GUI

FLACCO + GUI

- flacco: Feature-Based Landscape Analysis of Continuous and Constraint Optimization Problems
- unified interface for multiple (single-objective) sets of configurable features
- stable release on CRAN / developers version on GitHub
- multiple visualization techniques (partially shown on these slides)
- tracks # of function evaluations and run time - per feature set
- a comprehensive description of FLACCO can be found here^{5,6}

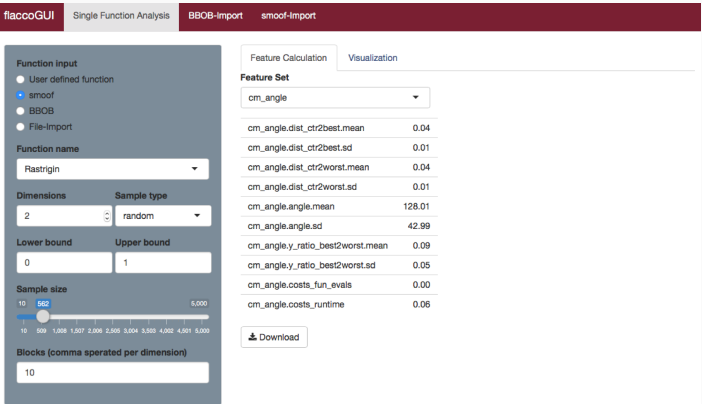
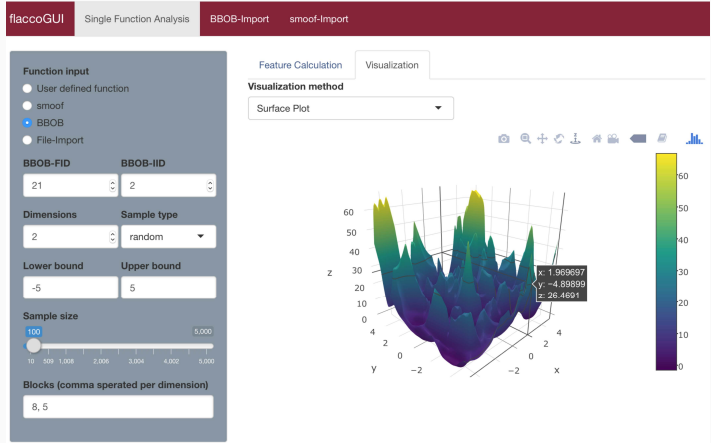
5. [22] Kerschke, P. & Trautmann, H. (2016). *The R-Package FLACCO for Exploratory Landscape Analysis with Applications to Multi-Objective Optimization Problems*. In *Proceedings of CEC 2016*.
 6. [14] Kerschke, P. (2017). *Comprehensive Feature-Based Landscape Analysis of Continuous and Constrained Optimization Problems Using the R-Package flacco*. In *arXiv 1708.05258*
 URL: <https://arxiv.org/abs/1708.05258>.



7. Tutorial: <http://kerschke.github.io/flacco-tutorial/site/>

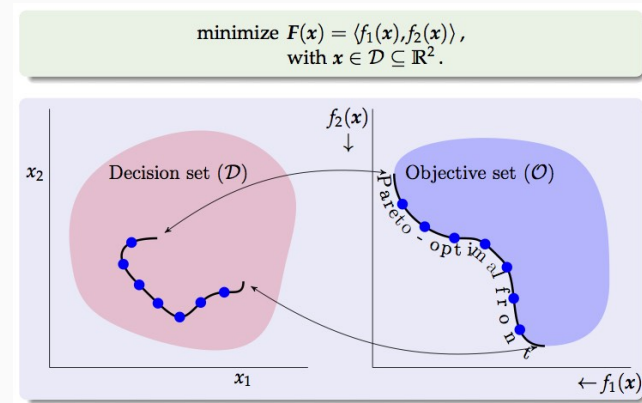
- drawback of flacco:
 - it is an R-package \leadsto only people, who are familiar with (programming in) R benefit of it
- solution:
 - user-friendly GUI⁸ (graphical user interface)
 - platform independent (web-)application: <https://flacco.shinyapps.io/flacco/>
 - the GUI helps people, who
 - (a) are familiar with R, but don't want to bother with the coding
 - (b) are not familiar with R (and just want to perform ELA)
 - (c) don't have access to a computer
 - (d) have access to a computer, but don't have the rights to install R

8. [10] Hanster, C. & Kerschke, P. (2017). *flaccogui: Exploratory Landscape Analysis for Everyone*. In Proceedings of GECCO 2017 Companion (pp. 1215 – 1222).



(ELA for) Multi-Objective Optimization

Multi-Objective Optimization



source: lmarti.github.io

Multi-Objective Optimization

- in single-objective optimization, ELA has shown to be useful for describing the problem landscape based on a small initial design
- currently, there exist almost no landscape features for continuous multi-objective optimization problems
- first approaches for using ELA in the multi-objective setting

Multi-Objective Optimization

- `flacco` originally intended to deal with single-objective optimization problems
- features can also be used to characterize multi-objective problems
- we used DTLZ-⁹ and ZDT-problems¹⁰ (using the R-package `smoof`¹¹)

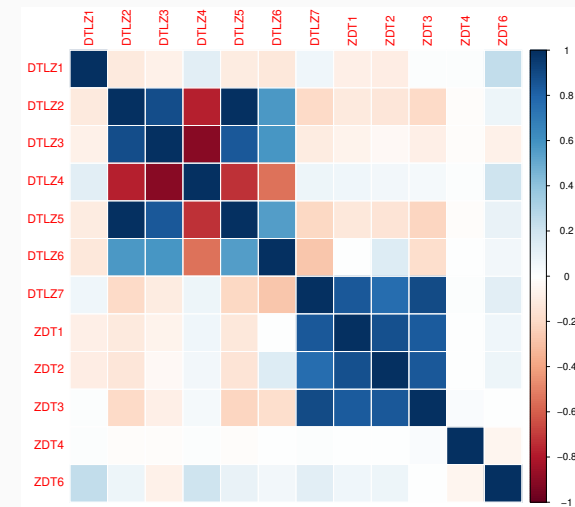
9. [6] Deb, K., Thiele, L., Laumanns, M. & Zitzler, E. (2005). Scalable Test Problems for Evolutionary Multiobjective Optimization. In *Evolutionary Multiobjective Optimization* (pp. 105 - 145)
10. [44] Zitzler, E., Deb, K. & Thiele (2000). Comparison of Multiobjective Evolutionary Algorithms: Empirical Results. In *Evolutionary Computation*, Vol. 8, Number 2 (pp. 173 - 195)
11. [4] Bossek, J. (2017). `smoof`: Single- and Multi-Objective Optimization Test Functions. In *The R Journal*. <https://CRAN.R-project.org/package=smoof>

Multi-Objective Optimization

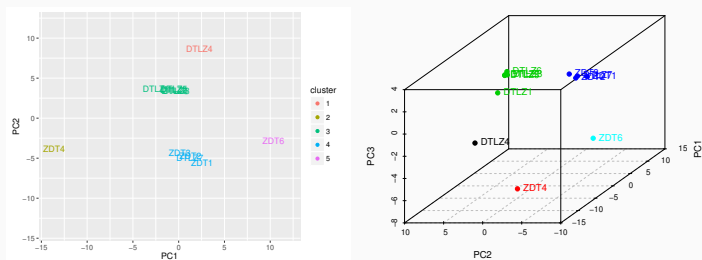
Experimental Setup:

- DTLZ1 to DTLZ7 and ZDT1 to ZDT6 (without ZDT5)
 ~ 120 instances (12 functions with 10 replicates each)
- initial designs: $100 \times d$ samples with $d = 3$
- considered 131 artificially designed “interaction-features”:
 - all 15 feature sets except for GCM and Barrier Trees
 ~ 682 features (341 per objective)
 - aggregated by feature-ratio (objective 1 / objective 2)
 - removed runtimes, as well as all features that contained infinite or non-defined values

Multi-Objective Optimization



Multi-Objective Optimization



Multi-Objective Optimization

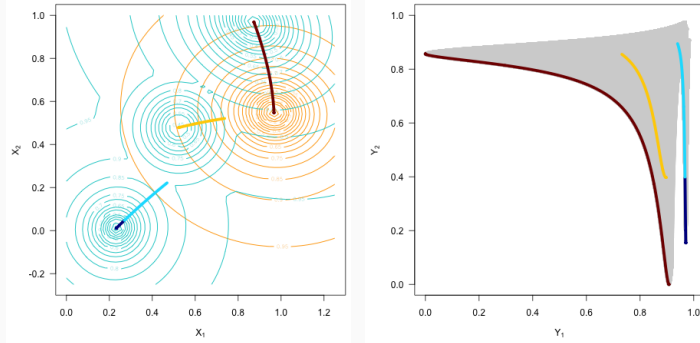
- in single-objective optimization:
 people visualize interaction effects of decision and objective space simultaneously \leadsto line plots, heatmaps, 3D plots, etc.
- in multi-objective optimization:
 visualizing $d \geq 2$ decision variables and $p \geq 2$ objective values (within a single image) is much more complicated
- effect: researchers mainly only focus on the objective space, but neglect the decision space¹²
- conflict: optimization algorithms usually “act” in the decision space (e.g., mutation / recombination within an EA)

12. Exception: Cost landscapes based on Pareto-ranking as defined by Carlos Fonseca.

[5] Fonseca, C. M. M. (1995). *Multi Objective Genetic Algorithms with Application to Control Engineering Problems*. PhD Thesis at the Department of Automatic Control and Systems Engineering, University of Sheffield, Sheffield, UK.

Multi-Objective Optimization

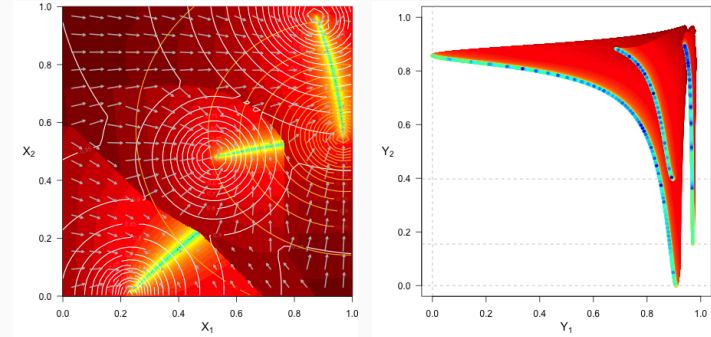
- idea introduced within our paper¹³ from the previous PPSN:
visualize efficient sets, i.e., the set of points from the decision space
whose images are multi-objective local or global optima



13. [24] Kerschke, P., Wang, H., Preuss, M., Grimme, C., Deutz, A., Trautmann, H. & Emmerich, M. (2016). *Towards Analyzing Multimodality of Multiobjective Landscapes*. In Proceedings of PPSN XIV (pp. 962 – 972).

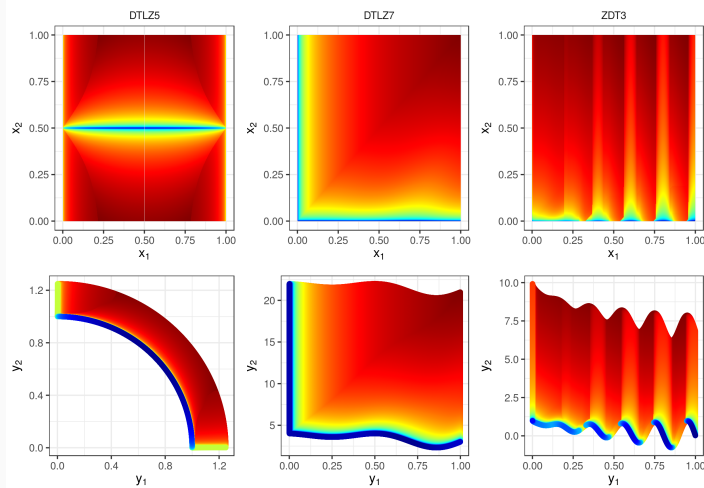
Multi-Objective Optimization

- extended to a visualization of the multi-objective basins of attraction¹⁴

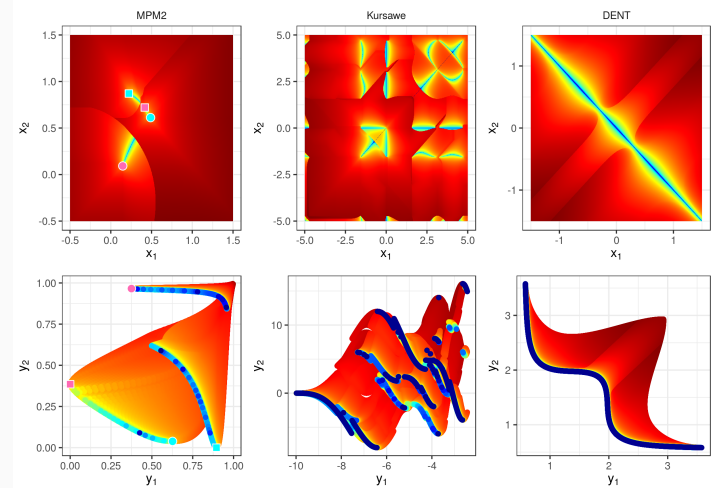


14. [16] Kerschke, P. & Grimme, C. (2017). *An Expedition to Multimodal Multi-Objective Optimization Landscapes*. In Proceedings of EMO 2017 (pp. 329 – 343).

Multi-Objective Optimization



Multi-Objective Optimization



Multi-Objective Optimization

Next Steps w.r.t. ELA for Multi-Objective Optimization:

- analyze numerous multi-objective benchmark problems visually and detect meaningful properties of the landscapes
- develop (simple and) automatically computable features, which *might* capture these properties
- conduct experimental studies to test their applicability
- employ the insights gained from the joined visualization of decision and objective space to either
 - (a) construct better performing algorithms, or
 - (b) use the derived features for training a suitable algorithm selector

Open Issues

Open Issues

- how can we characterize multimodal and/or multi-objective landscapes? \Rightarrow develop new landscape features
- enhance flacco with more ELA features
- how can we find the smallest most informative feature set?
- by how much can we still reduce the size of the initial designs without losing (too much) information?

Open Issues

- (how) can we transfer features from / to different domains? (e.g., funnels also exist in discrete optimization)
- use features to learn more about the algorithms and problems
 1. train well-performing algorithm selection or configuration models based on ELA features
 2. interpret the model's behavior based on the employed features (black-box to white-box)

Open Issues

- how should we extend the existing / established benchmarks?
- GECCO 2019 offers numerous related workshops:
 - Understanding Machine Learning Optimization Problems (UMLOP)
 - Black Box Optimization Benchmarking (BBOB)
 - Game-Benchmark for Evolutionary Algorithms (GBEA)
 - Black Box Discrete Optimization Benchmarking (BB-DOB)
- directions for possible extensions:
 - machine learning problems [35]
 - landscapes of (hyper-)parameter optimization problems [7]
 - problems from domains such as computational games [41]

Thank you!

Comments, Questions and/or Suggestions?

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