Algorithm Configuration Survival Guide Part 1

SPECIES Summer School 2023

Leslie Pérez Cáceres

leslie.perez@pucv.cl

Outline

1. Algorithm configuration: know the terrain

2. Configurators & irace: know your resources

3. Configuration examples: know the possibilities

Algorithm configuration

Know the terrain



Optimization Algorithms

They are great!

Especially when they solve problems...
... efficiently

Unfortunately, this is not easy to achieve



Algorithm design

Optimization algorithms can be powerful and flexible tools

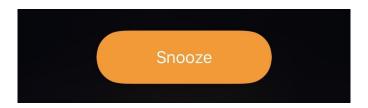




Parameters

Parameters are design choices ...

... postponed until execution time



Parameters

Flexible algorithms often expose many parameters

Algorithm performance is strongly dependent on parameter settings

Algorithm configuration task

The task of finding parameter settings of a **target algorithm** that exhibit **best empirical performance** on a given distribution of **problem instances**.

Algorithm configuration problem

Given a budget B, find a configuration θ^*

$$\theta^* = argmin_{\theta \in \Theta} F(\theta, I)$$

 $F(\theta, I) \rightarrow \text{configuration objective}$

 $\Theta \rightarrow$ parameter space

 $I \rightarrow \text{problem}$ instance set from space P_I

Algorithm configuration problem

Configuration objective:

$$F(\theta, I) = \bigwedge_{i=1}^{|I|} Q(\theta, I_i, b)$$

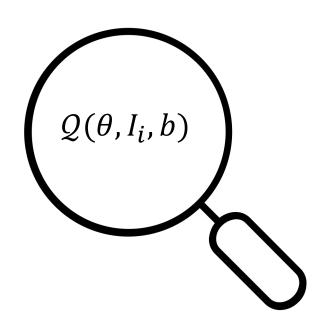
 $Q \rightarrow performance measure$

b → *termination criterion*

Sources of variability in performance

In most cases, we can only estimate performance

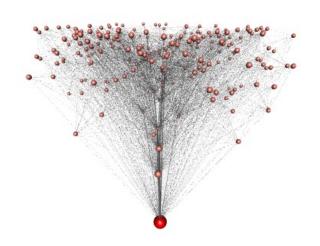
- Parameters values
- Resources: computational budget
- Instances

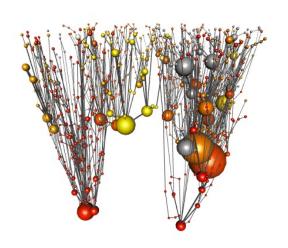


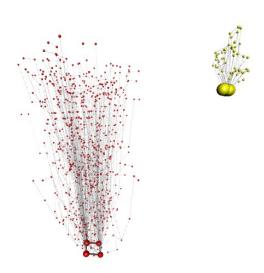
About instances

Instances can define very different landscapes

http://lonmaps.com/gallery/





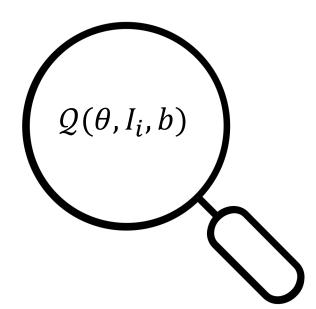


Exploration / exploitation balance for good performance

Sources of variability in performance

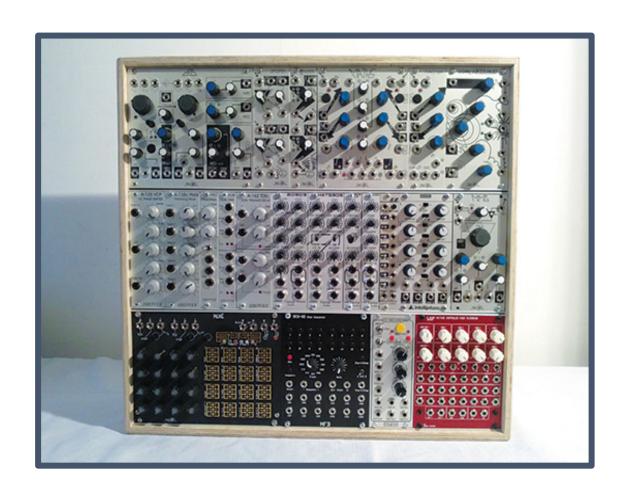
In most cases, we can only estimate performance

- Parameters values
- Resources: computation budget
- Instances



- Platform: platforms, executables, memory, processing loads....
- Stochasticity

Find the best configuration



How to approach the problem?

Offline tuning: set an adequate parameter settings before execution

• Online tuning: set and adjust parameter settings during execution

Manual algorithm configuration

Based on knowledge

- Rule of thumbs
- Default settings
- Literature studies

Trial and error

• Systematic or not ...



- Requires expertise
- Makes a lot assumptions
- Based on simplifications
- No exploration



- Time consuming
- Tedious process

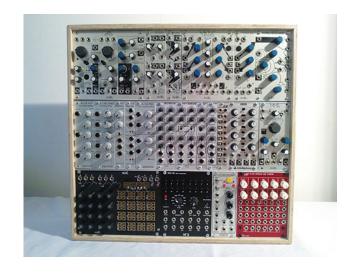


- Prone to bias
- Limited exploration



Manual algorithm configuration

Pros and cons





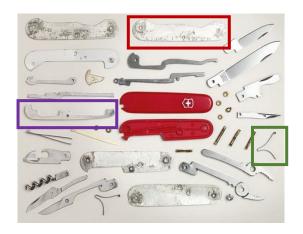
- Allows to obtain knowledge
- Good when limited resources



- Does not promote flexibility
- Avoids to focus on creativity

Automatic Algorithm Configuration

Automatically searching for **high-performing** parameter settings **before the execution** of an algorithm.



Apply specialized tools: configurators

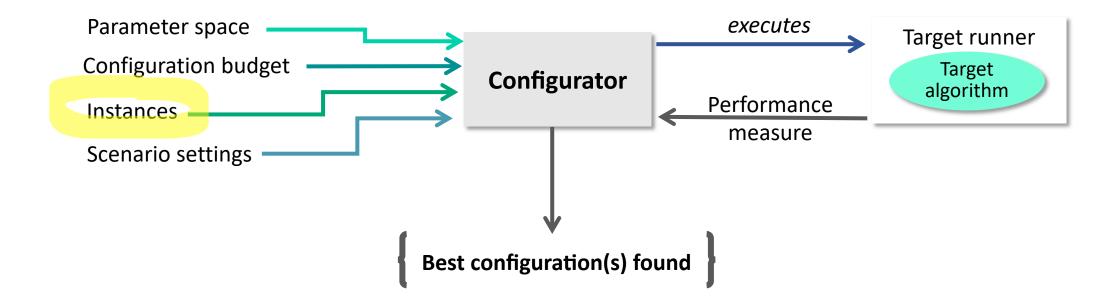
Effectively use available computational resources

Configurators & irace

Know your resources



Algorithm Configurators



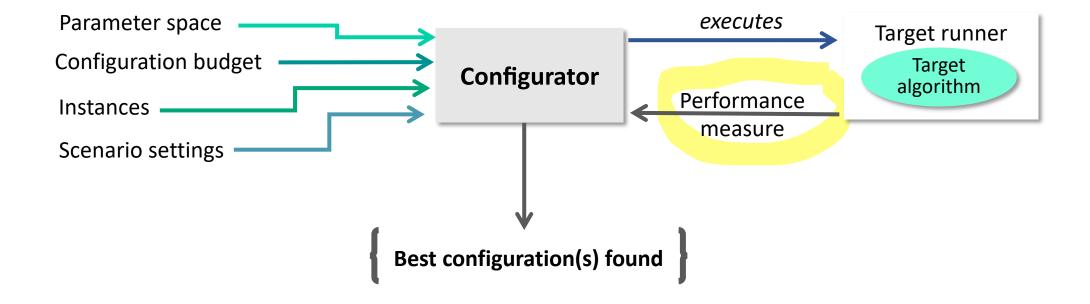
About the instances

Instances must be representative of the ones the algorithm willl encounter in production

Training set: to perform the search for good configurations

Test set: to evaluate configurations (assess overtuning)

Algorithm Configurators



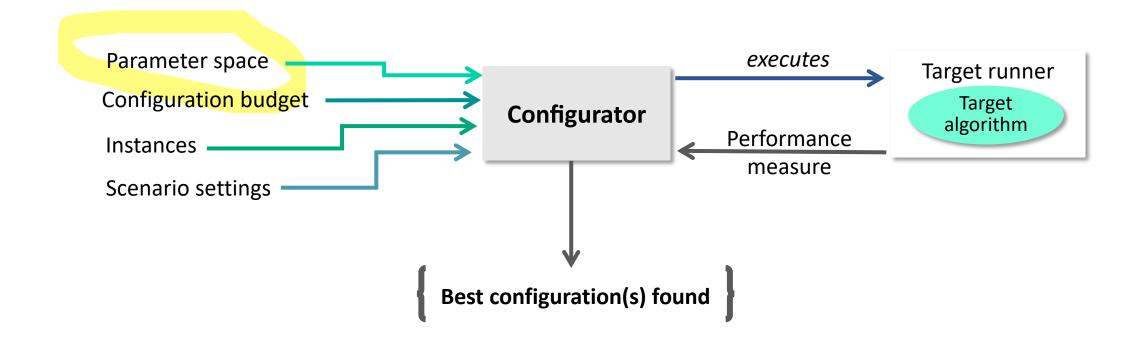
About performance measure

Configuration objective can be:

- Quality-based (solution quality, gap, etc.)
- Resource-based (time to optima, time to x quality, ...)

The performance measure can be penalized for configuration!

Algorithm Configurators



About parameter spaces

Parameter type and domain:

- Categorical
- Ordered
- Numerical:
 - real
 - integer

 algorithm
 Categorical → {AS, MMAS, ACS}

 localsearch
 Ordered → {none, small, medium, large}

alpha Real \rightarrow {0.0, 1.0}

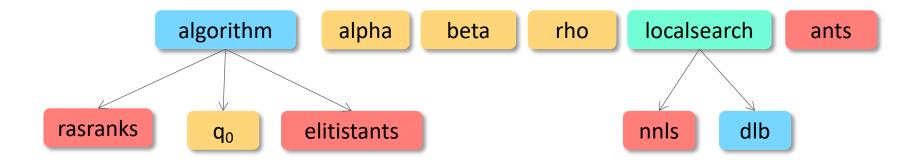
ants Integer \rightarrow {10, 50}

About parameter spaces

Conditionality

Parameters can be activated based on the value of others

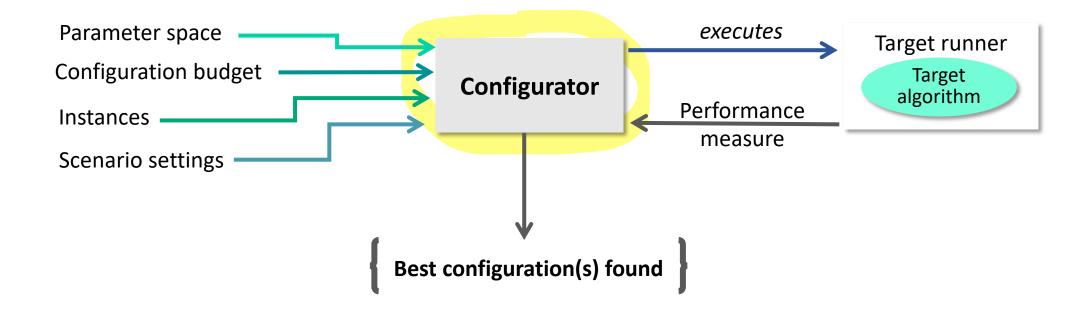
 q_0 is active only if algorithm == "acs"



Algorithm configurators

- * Experimental design: CALIBRA [1]
- * Numerical optimization: MADS [2], CMAES [3], BOBYQA [3]
- * Heuristic optimization: metaGA [4], REVAC [5], ParamILS [6], GGA [7], linear GP[8]
- * Model-based: SPOT [9][10], SMAC [11], GGA++ [12]
- * Sequential statistical testing: F-Race [13], Iterated F-Race [14], irace [15]

Algorithm Configurators



The irace package: Iterated Racing for Automatic Algorithm Configuration. Manuel López-Ibáñez, Jérémie Dubois-Lacoste, Leslie Pérez Cáceres, Thomas Stützle and Mauro Birattari. *Operations Research Perspectives* volume 3, pages 43–58 (2016)

Webpage:

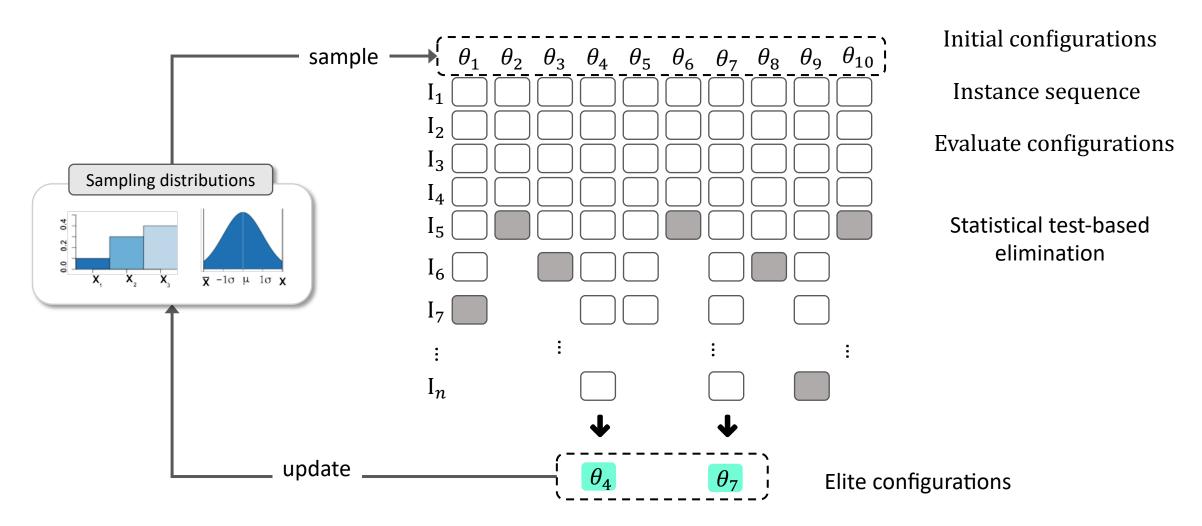
http://iridia.ulb.ac.be/irace/

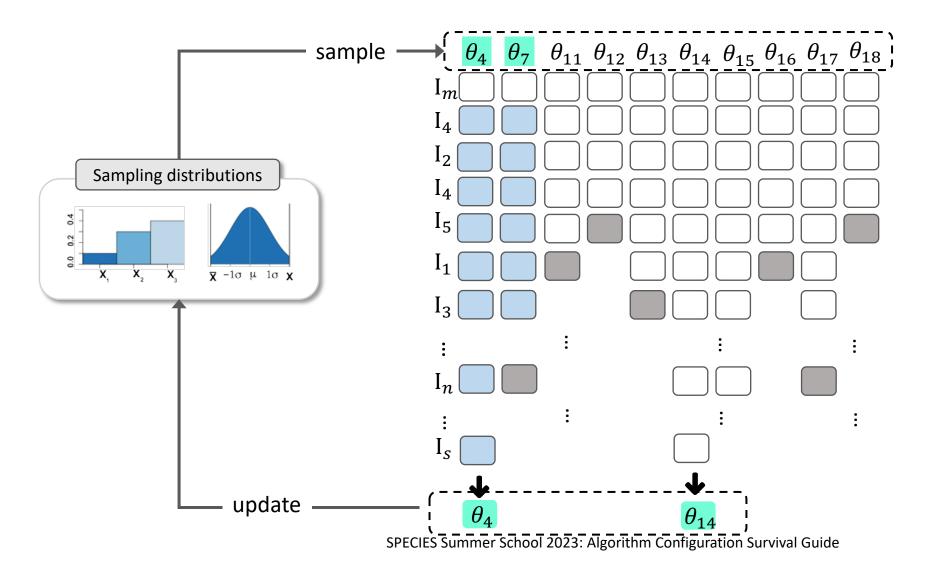
R package:

http://cran.r-project.org/package=irace

Iterated racing + Estimation of distribution

- State of the art configurator
- Implemented in R
 - Multiplatform
 - Flexible
- Parallel evaluation (MPI, multicores, grid engine)
- Several scenario options





The irace package: some features

- Different parameters types
 - categorical, ordinal, real, integer, log real, log integer
- Configuration repair: fix configurations when generated
- Automatic rejection: remove undesirable configurations
- Adaptive capping: for runtime minimization objectives
- Deterministic / stochastic mode

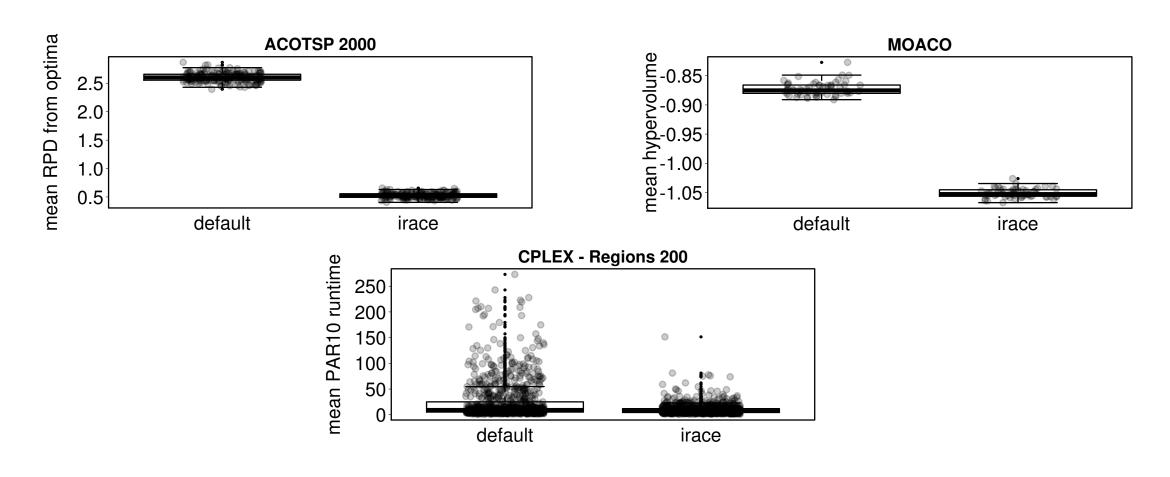
Configuration examples

know the possibilities

Yes, you can!



Default configuration tests



During the design process ...

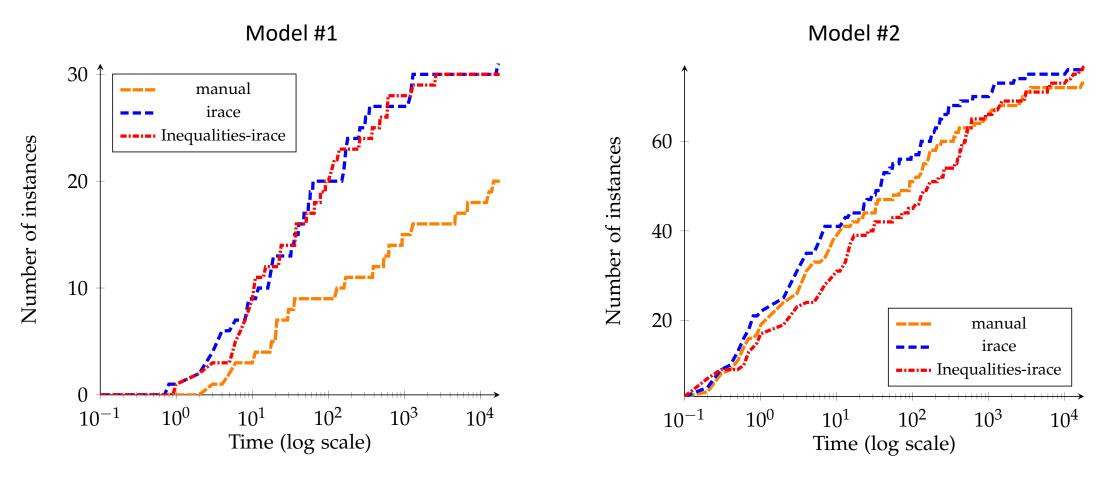
Irace can help to get know our algorithm

Example:

Column generation algorithm and branch-and-cut-and-price algorithm

- Reduced the mean execution time of the column generation algorithm
- Improved performance of the branch-and-cut-and-price algorithm

During the design process ...



Work performed with Alessia Violin for her Ph.D. Thesis.

When resources change ...

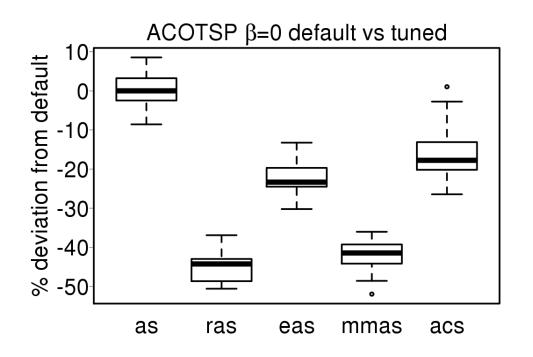
What happens with the performance of default settings?

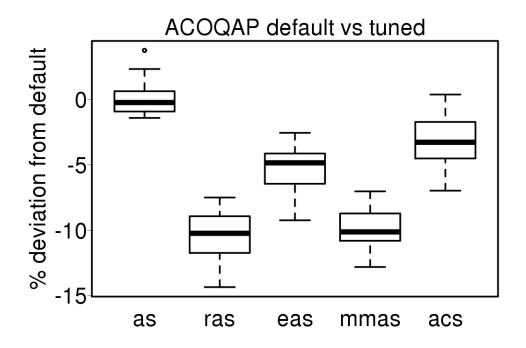
Algorithm: ACOTSP / ACOQAP

Strongly restricted execution budget

Are the current ACO settings still adequate?

When resources change ...





When the platform change ...

What happens with the performance of "default settings"?

Algorithm: GCC

Different platforms

Are GCC optimization settings preferrable?

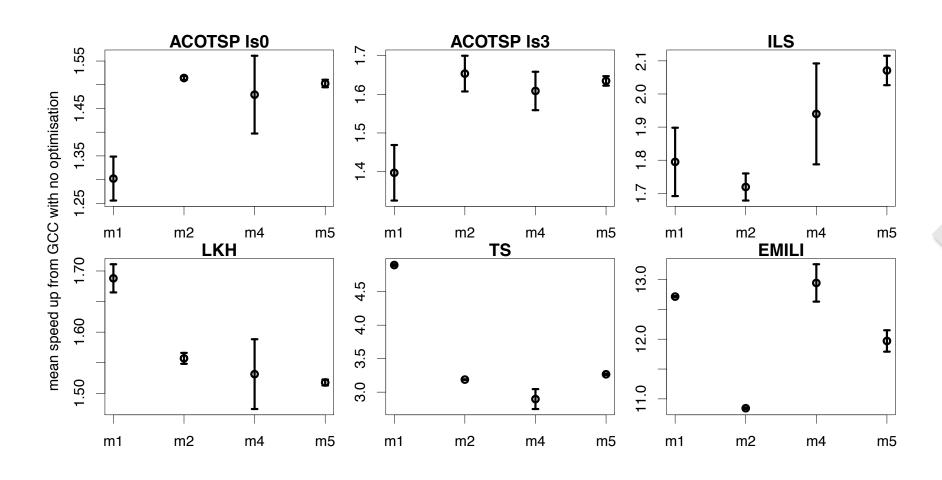
When the platform changes ...

We used irace to configure the optimization options of GCC

- Two parameter spaces
 - 172 categorical parameters
 - 367 mixed parameters
- Experiments: compiling six optimization algorithms (C, C++)
- In 4 different machines

Compared to –O3 settings

When the platform changes ...



Speed up from -O3 in different machines

Take home message

- Parameter settings have often a large effect over performance
 - Configure when evaluating / comparing algorithms
- Any type of configuration is better than no configuration

- Configuration is useful not only for performance
 - But also for getting knowledge about an algorithm
- A configurator can provide assistance in the task of algorithm design

Take home message: perspectives

- Has the potential to enable automated algorithm design
 - Parameter tuning
 - Component selection
 - Algorithmic structure

Why?

- 1. Free designers of the tedious task of fully configuring and algorithm
- Focus on the creation of new/better algorithmic components and structures

In the next episode of the survival guide ...

We try irace!

Thanks for your attention!

Questions, comments?

References

- [1] B. Adenso-Díaz and M. Laguna. Fine-tuning of algorithms using fractional experimental design and local search. *Operations Research*, 54(1):99–114, 2006.
- [2] C. Audet and D. Orban. Finding optimal algorithmic parameters using derivative-free optimization. *SIAM Journal on Optimization*, 17(3):642–664, 2006.
- [3] Z. Yuan, M. A. Montes de Oca, T. Stützle, and M. Birattari. Continuous optimization algorithms for tuning real and integer algorithm parameters of swarm intelligence algorithms. *Swarm Intelligence*, 6(1):49–75, 2012.
- [4] J. J. Grefenstette. Optimization of control parameters for genetic algorithms. IEEE Transactions on Systems, Man, and Cybernetics, 16(1):122–128, 1986.
- [5] V. Nannen and A. E. Eiben. Relevance estimation and value calibration of evolutionary algorithm parameters. In M. M. Veloso, editor, *Proceedings of the Twentieth International Joint Conference on Artificial Intelligence (IJCAI-07)*, pages 975–980. AAAI Press, Menlo Park, CA, 2007.
- [6] F. Hutter, H. H. Hoos, K. Leyton-Brown, and T. Stützle. ParamILS: an automatic algorithm configuration framework. *Journal of Artificial Intelligence Research*, 36:267–306, October 2009.
- [7] C. Ansótegui, M. Sellmann, and K. Tierney. A gender-based genetic algorithm for the automatic configuration of algorithms. In I. P. Gent, editor, *Principles and Practice of Constraint Programming, CP 2009*, volume 5732 of *LNCS*, pages 142–157. Springer, 2009.

References

- [8] M. Oltean. Evolving evolutionary algorithms using linear genetic programming. Evolutionary Computation, 13(3):387–410, 2005. doi: 10.1162/1063656054794815.
- [9] T. Bartz-Beielstein, C. Lasarczyk, and M. Preuss. Sequential parameter optimization. In *IEEE CEC*, pages 773–780, Piscataway, NJ, September 2005. IEEE Press.
- [10] T. Bartz-Beielstein, C. Lasarczyk, and M. Preuss. The sequential parameter optimization toolbox. In Bartz-Beielstein et al. (2010a), pages 337–360.
- [11] F. Hutter, H. H. Hoos, and K. Leyton-Brown. Sequential model-based optimization for general algorithm configuration. In C. A. Coello Coello, editor, *Learning and Intelligent Optimization*, 5th International Conference, LION 5, volume 6683 of LNCS, pages 507–523. Springer, 2011.
- [12] C. Ansótegui, Y. Malitsky, H. Samulowitz, M. Sellmann, and K. Tierney. Model-based genetic algorithms for algorithm configuration. In Q. Yang and M. Wooldridge, editors, *Proceedings of the Twenty-Fourth International Joint Conference on Artificial Intelligence (IJCAI-15)*, pages 733–739. IJCAI/AAAI Press, Menlo Park, CA, 2015.
- [13] M. Birattari, T. Stützle, L. Paquete, and K. Varrentrapp. A racing algorithm for configuring metaheuristics. In W. B. Langdon et al., editors, *Proceedings of the Genetic and Evolutionary Computation Conference, GECCO 2002*, pages 11–18. Morgan Kaufmann Publishers, San Francisco, CA, 2002.
- [14] P. Balaprakash, M. Birattari, and T. Stützle. Improvement strategies for the F-race algorithm: Sampling design and iterative refinement. In T. Bartz- Beielstein, M. J. Blesa, C. Blum, B. Naujoks, A. Roli, G. Rudolph, and M. Sampels, editors, *Hybrid Metaheuristics*, volume 4771 of *LNCS*, pages 108–122. Springer, 2007.
- [15] M. López-Ibáñez, J. Dubois-Lacoste, L. Pérez Cáceres, T. Stützle, and M. Birattari. The irace package: Iterated racing for automatic algorithm configuration. *Operations Research Perspectives*, 3:43–58, 2016a