

Configuración Automática de Algoritmos

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- “Beatriz Galindo” Senior Distinguished Researcher, 2020–2022



UNIVERSIDAD
DE MÁLAGA

- Editor-in-Chief of GECCO 2019



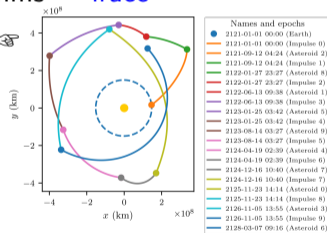
☞ GECCO 2025 es en Málaga!

- (co-)Editor-in-Chief of ACM Transactions on Evolutionary Learning and Optimization (ACM TELO)



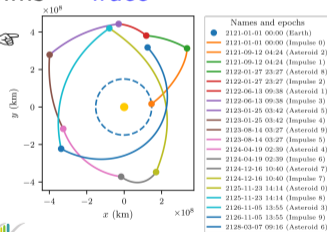
My research is about ...

- Benchmarking and Empirical Analysis of Optimization Algorithms
 - 👉 Reproducibility in Evolutionary Computation [López-Ibáñez, Branke & Paquete, 2021]
- Multi-objective optimization 👉 **EAF package** 👉 **moocore package**
- Interactive optimization (human-in-the-loop)
 - 👉 Machine Decision Makers [López-Ibáñez & Knowles, 2015]
- Automatic configuration, selection and design of algorithms 👉 **irace**
- Expensive optimization ... , Asteroid Routing Problem 👉



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- Expensive optimization ... , Asteroid Routing Problem 👉
- Applications, applications, applications!
 - Optimization in steel manufacturing
 - School bus routing for SEND students
 - Supply chain design for Personalised Medicine
 - Bayesian Optimisation with dynamic constraints
 - Intervowen Optimisation



Mario collects phone orders for 30 minutes.

Mario wants to schedule deliveries to get back to the pizzeria as fast as possible.

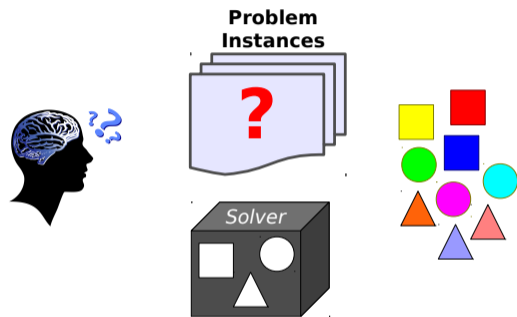


- Scheduling deliveries is an *optimization problem*
- A different *problem instance* arises every 30 minutes
- Limited time for solving, say *one minute* (online)
- Limited time to implement an optimization algorithm, say *one week* (offline)

Traditional design of optimization algorithms

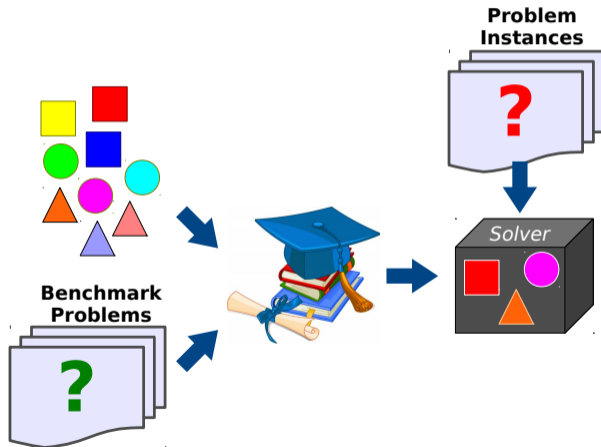


Traditional design of optimization algorithms



Traditional design of optimization algorithms

Human expert + intuition + trial-and-error/statistics



Modern high-performance optimizers involve a large number of design choices and (hyper)-parameter settings

- Exact solvers
 - Design choices: alternative models, pre-processing, variable selection, value selection, branching rules ...
 - + numerical parameters
 - IBM CPLEX: 63 parameters that control the optimization

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- Exact solvers
 - Design choices: alternative models, pre-processing, variable selection, value selection, branching rules ...
 - + numerical parameters
 - IBM CPLEX: 63 parameters that control the optimization
- (Meta)-heuristic solvers
 - Design choices: solution representation, operators, neighborhoods, pre-processing, strategies, ... + numerical parameters
 - Many are *hidden*

Modern high-performance **optimizers** software involve a large number of design choices and (hyper)-parameter settings

Domain	Software	Parameters	
ML	WEKA	768	[Kotthoff et al., 2016]
	Auto-sklearn	110	[Feurer et al., 2015]
Code optimization	GCC	172 flags + 195 numerical	[Pérez Cáceres et al., 2017b]
Databases	Cassandra	23	[Silva-Muñoz et al., 2021]

Modern high-performance **optimizers** software involve a large number of design choices and (hyper)-parameter settings



Design choices and parameters everywhere

- *Categorical* parameters

`localsearch` \in { tabu search, SA, ILS }

- *Ordinal* parameters

`neighborhoods` \in { small, medium, large }

- *Numerical* parameters (integer and real-valued)

population sizes, acceptance temperature, hidden constants, ...

- *Conditional* parameters are only active for specific values of other parameters:

temperature only enabled if `localsearch == "SA"`

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*Configuring an algorithm means
setting its categorical, ordinal and numerical parameters*

Challenges

Challenges

- ✗ Many alternative design choices and parameter settings
- ✗ Nonlinear interactions among algorithm components and/or parameters
- ✗ Algorithms are stochastic
- ✗ Problem instances used for design (benchmark instances) are not identical to the ones found in the real-world
- ✗ Performance assessment is difficult (statistical analysis)

Traditional approaches

Traditional approaches

- Trial-and-error design guided by expertise/intuition
 - ✗ prone to over-generalizations,
 - ✗ limited exploration of design alternatives,
 - ✗ human biases
- Guided by theoretical studies
 - ✗ often based on over-simplifications,
 - ✗ specific assumptions,
 - ✗ few parameters

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Can we make this approach more principled and automatic?

The algorithm configuration problem

- 1 Find the best algorithm configuration
given a set of *training problem instances*
- 2 Repeatedly use this algorithm configuration to solve
unseen problem instances

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A problem with many names:

offline parameter *tuning*,
automatic algorithm configuration,
hyper-parameter optimization,
hyper-heuristics, genetic programming,
meta-optimisation, programming by optimisation [Hoos, 2012], ...

Offline configuration vs. Online control

Offline tuning / Algorithm configuration

- Learn best configuration before *solving* the real problem instance
- Configuration done on training problem instances
- Performance measured over test (\neq training) instances

Offline configuration vs. Online control

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Online tuning / Parameter control / Reactive search

- Learn best configuration *while* solving each instance
- No training phase but more expensive *while* solving
- Very popular in continuous optimization
- Ultimate goal: parameter-free algorithms

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All online methods have parameters that are configured offline

AC is a mixed-integer stochastic black-box optimization problem

Mixed-decision variables

- discrete (categorical, ordinal and integer) and real-valued
- conditional parameters, box-constraints and other constraints

Stochasticity

- of the target algorithm
- of the problem instances

Black-box

evaluation requires running a configuration on an instance

Typical tuning goals

- maximize solution quality within given time
- minimize run-time to decision / optimal solution

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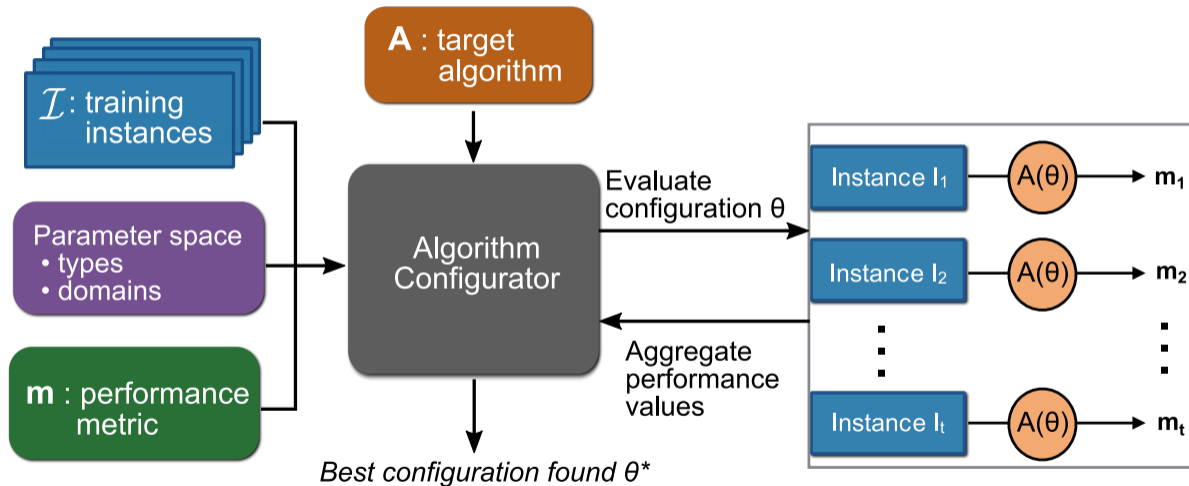
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AC requires specialized methods !

(Offline) Automatic Algorithm Configuration



Racing is a method for the *selection of the best* among a given set of algorithm configurations

- ✓ Reduce effort evaluating low performance configurations
- ✓ Focus effort on selecting the best configurations

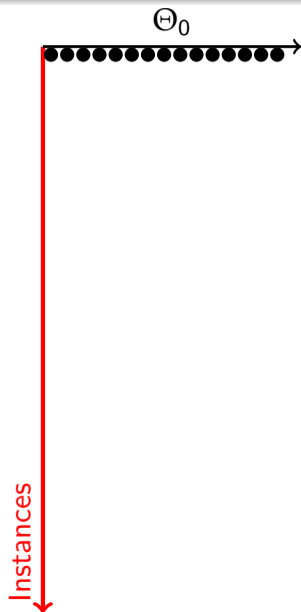


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- start with a set of initial candidates



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- **discard inferior candidates**
as sufficient evidence is gathered against them



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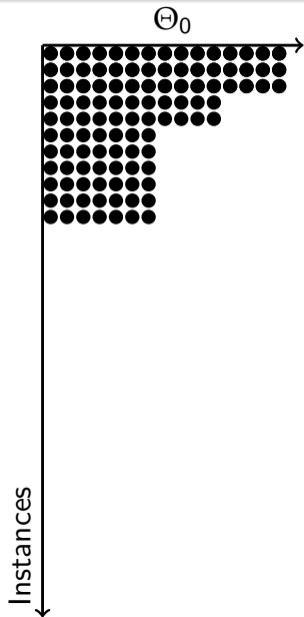
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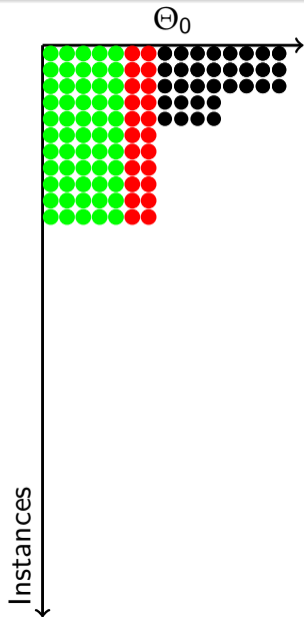
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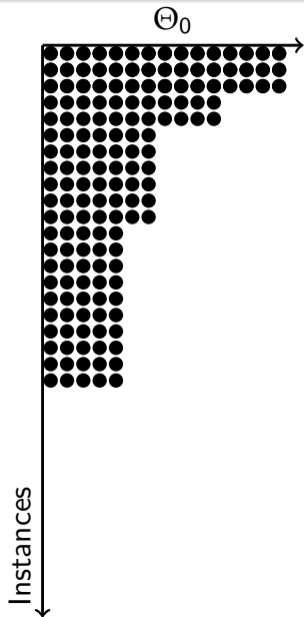
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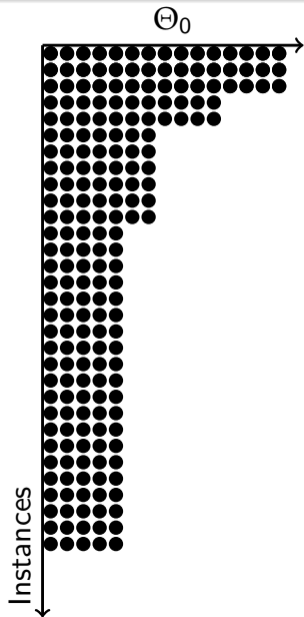
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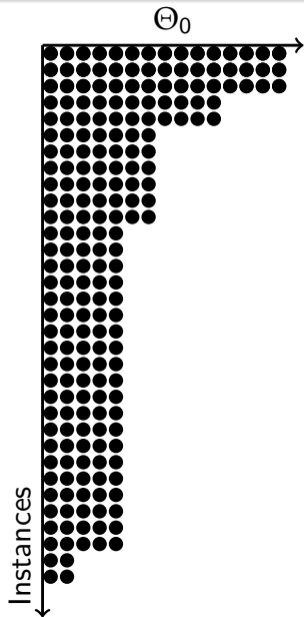
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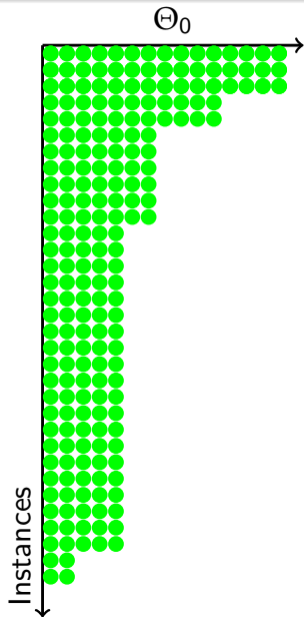
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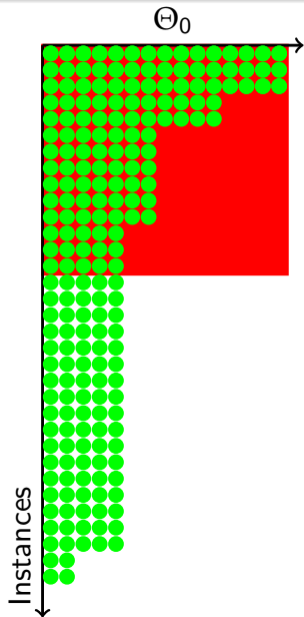
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- ...repeat until a winner is selected
or until computation time expires



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How to discard?

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Statistical tests!

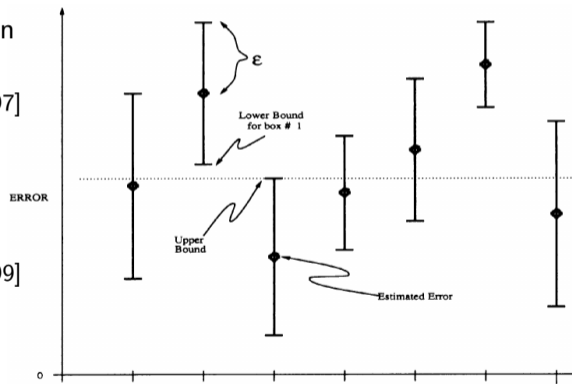
- Paired t-test with/ *without* p-value correction (against the best)

[Maron & Moore, 1997]

- *F-Race*: Friedman two-way analysis of variance by ranks + Friedman post-hoc test

[Conover, 1999]

- *Bayesian*: Bayesian nonparametric statistics [Benavoli et al., 2015]



Taken from Maron & Moore [1997]

Racing (F-race, t-race, ...) is a method for the *selection of the best* among a given set of algorithm configurations

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How to define this set of configurations?

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How to define this set of configurations?

- Full factorial
- Random sampling
- Iterative update of a probabilistic sampling model
(\approx Estimation of Distribution Algorithm)
 \Rightarrow *Iterated F-Race (I/F-Race)* [Balaprakash et al., 2007]

Iterated Racing

- ① **Sampling** new configurations according to a probability distribution
- ② **Selecting** the best configurations from the newly sampled ones by means of racing
- ③ **Updating** the probability distribution in order to bias the sampling towards the best configurations

I/F-race: Balaprakash, Birattari & Stützle [2007],
Birattari, Yuan, Balaprakash & Stützle [2010]

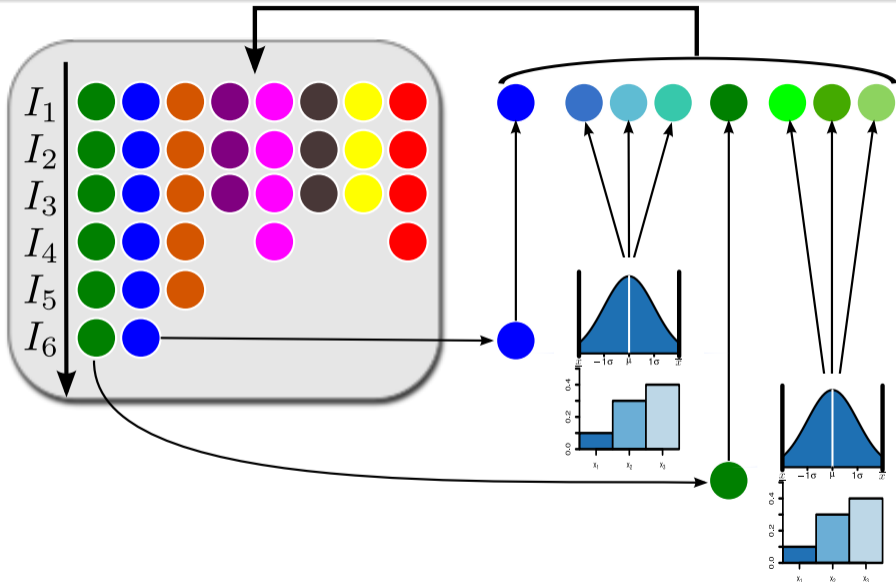
irace (v1): López-Ibáñez, Dubois-Lacoste, Stützle & Birattari [2011]

elitist irace (v2): López-Ibáñez, Dubois-Lacoste, Pérez Cáceres, Stützle & Birattari [2016]

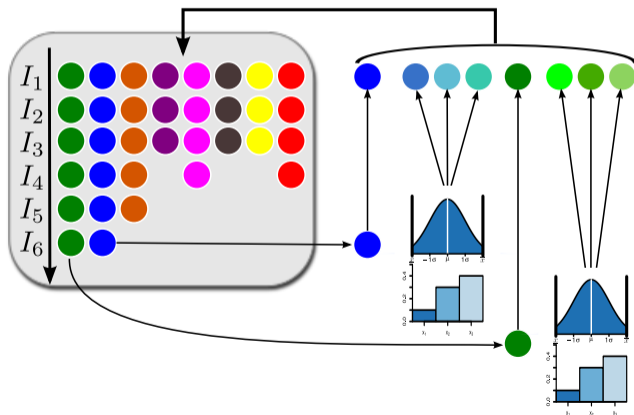
elitist irace + adaptive capping (v3):

Pérez Cáceres, López-Ibáñez, Hoos & Stützle [2017a]

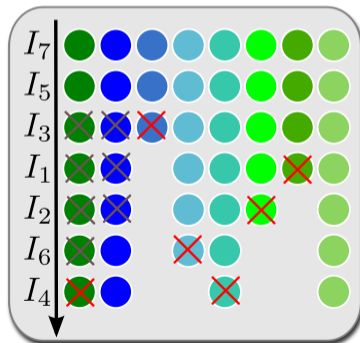
Iterated Racing



- ✗ Each new iteration (race) forgets the results of the previous one
 \Rightarrow Iterated F-race may “lose” the best-so-far configuration



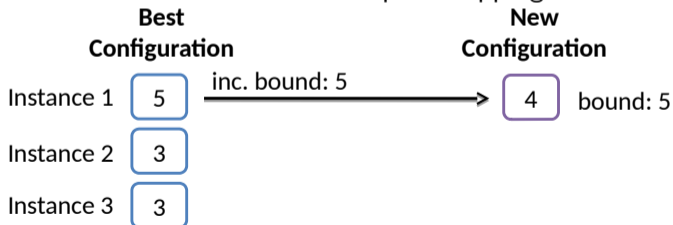
- ✗ Each new iteration (race) forgets the results of the previous one
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- ✓ Protect the best configurations (*elites*) from being discarded unless all their results are considered



- Extension of irace to better handle run-time minimization
- Configuration θ_1 evaluated on I_1 *dominates* θ_2 evaluated on I_2 if

$$I_2 \subset I_1 \quad \text{and} \quad \sum_{i \in I_2} m(\theta_1, i) \leq \sum_{i \in I_2} m(\theta_2, i)$$

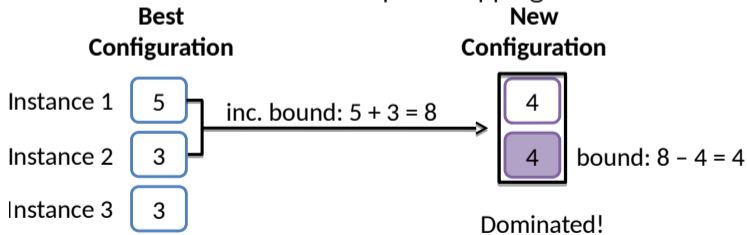
- Adaptive bound: $\kappa_i^{\text{new}} = \sum_{k=1}^i m(\theta_{\text{best}}, k) - \sum_{k=1}^{i-1} m(\theta_{\text{new}}, k)$
- Dominance elimination and adaptive capping:



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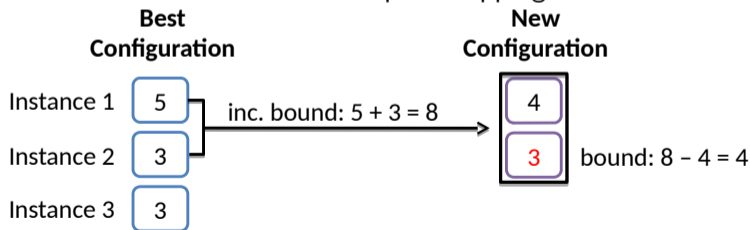
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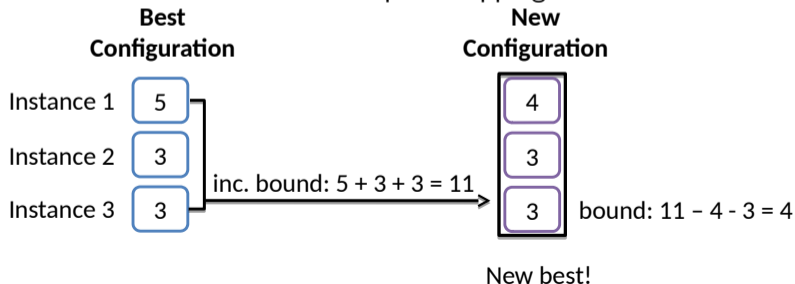
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An overview of applications of irace

- Parameter tuning
 - Exact MIP solvers (CPLEX, SCIP [López-Ibáñez & Stützle, 2014])
 - single-objective optimization metaheuristics
 - multi-objective optimization metaheuristics [López-Ibáñez & Stützle, 2012; Bezerra et al., 2016]
 - semi-interactive tuning [Diaz & López-Ibáñez, 2021]
 - anytime optimization (improve time-quality trade-offs) [López-Ibáñez & Stützle, 2014]
 - command-line flags of GCC compiler [Pérez Cáceres et al., 2017b]
- Automatic algorithm design
 - From a design grammar [Mascia et al., 2014; Martín-Santamaría et al., 2024]
- Machine learning [Lang et al., 2014; Miranda et al., 2014]
 - **mlr** and **mlr3tuning** R packages [Bischl et al., 2013, 2016]
- Design of control software for robots [Francesca et al., 2015]
- Theoretical research [Friedrich et al., 2018; Dang & Doerr, 2019; Hall et al., 2019]

2 098 citations in Google Scholar, 201 000 downloads

The irace Package



Manuel López-Ibáñez, Jérémie Dubois-Lacoste, Leslie Pérez Cáceres,
Thomas Stützle, and Mauro Birattari.

The irace package: Iterated Racing for Automatic Algorithm Configuration.

Operations Research Perspectives, 3:43–58, 2016. doi: [10.1016/j.orp.2016.09.002](https://doi.org/10.1016/j.orp.2016.09.002)

<https://mlopez-ibanez.github.io/irace/>

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- Implementation of Iterated Racing in R

Goal 1: Flexible

Goal 2: Easy to use

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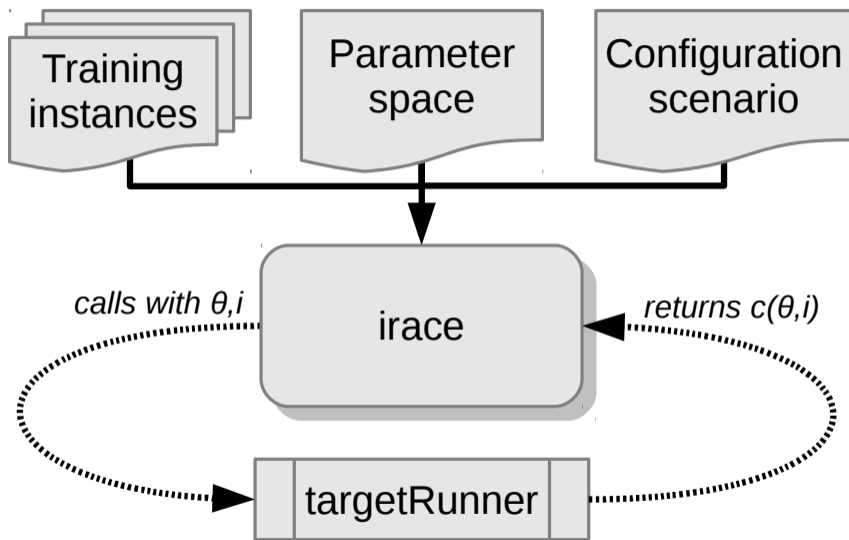
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- Use it through the command-line: (see `irace --help`)

```
irace --max-experiments 1000 --param-file parameters.txt
```

- ✓ No knowledge of R needed

The irace Package



The irace Package: Instances

- TSP instances

```
$ dir Instances/  
3000-01.tsp 3000-02.tsp 3000-03.tsp ...
```

- Continuous functions

```
$ cat instances.txt  
function=1 dimension=100  
function=2 dimension=100  
...
```

- Parameters for an instance generator

```
$ cat instances.txt  
I1 --size 100 --num-clusters 10 --sym yes --seed 1  
I2 --size 100 --num-clusters 5 --sym no --seed 1  
...
```

- Script / R function that generates instances

👉 if you need this, tell us!

The irace Package: Parameter space

- Categorical (**c**), ordinal (**o**), integer (**i**) and real (**r**)
- Subordinate parameters (**| condition**)
- Logarithmic scale (**,log**) (*irace 3.0*)

```
$ cat parameters.txt
```

#	Name	Label/switch	Type	Domain	Condition
	LS	"--localsearch "	c	(SA, TS, II)	
	rate	"--rate="	o	(low, med, high)	
	population	"--pop "	i,log	(1, 100)	
	temp	"--temp "	r	(0.5, 1)	LS == "SA"

- For real parameters, number of decimal places is controlled by option **digits** (**--digits**)

- *maxExperiments* (*maxTime*): maximum number of runs (or overall time) of the target algorithm (tuning budget)
- *testType*: either F-test or t-test

- A script/program that calls the software to be tuned:

```
./target-runner configID instanceID seed instance configuration
```

e.g. :

```
./target-runner 2 1 1234567 3000-01.tsp --localsearch SA ...
```

- An R function

Flexibility: If there is something you cannot tune, let us know!

The irace Package: Other features

- 1 Initial configurations (e.g., default configuration)
- 2 Parallel evaluation:
multiple CPUs, MPI, batch job clusters (SGE, PBS, Torque, Slurm)
- 3 Forbidden configurations (+ rejection):

```
popsize < 5 & LS == "SA"
```
- 4 Recovery file: allows resuming an interrupted irace run
- 5 Test instances
- 6 Repair configurations before being evaluated
- 7 Adaptive capping (for runtime minimization)

The irace Package

Last version 3.5 (23/10/2022) 📖 4.0 very soon !



A detailed user-guide / tutorial:

<https://cran.r-project.org/web/packages/irace/vignettes/irace-package.pdf>



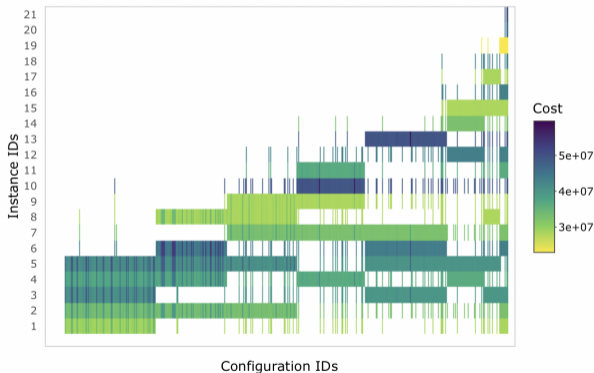
GitHub: <https://github.com/MLopez-Ibanez/irace>



Google group

<https://groups.google.com/d/forum/irace-package>

<https://auto-optimization.github.io/iraceplot/>



- Interactive HTML post-configuration report
- Summary statistics per instance / per configuration / per iteration
- Interactive visualizations
- Ablation report

Automatically Improving the Anytime Behavior of Optimization Algorithms with irace



Manuel López-Ibáñez and Thomas Stützle.

Automatically improving the anytime behaviour of optimisation algorithms.

European Journal of Operational Research, 2014. doi: [10.1016/j.ejor.2013.10.043](https://doi.org/10.1016/j.ejor.2013.10.043).

Anytime Algorithm

[Dean & Boddy, 1988]

- May be interrupted at any moment and returns a solution
- Keeps improving its solution until interrupted
- Eventually finds the optimal solution

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Good Anytime Behavior

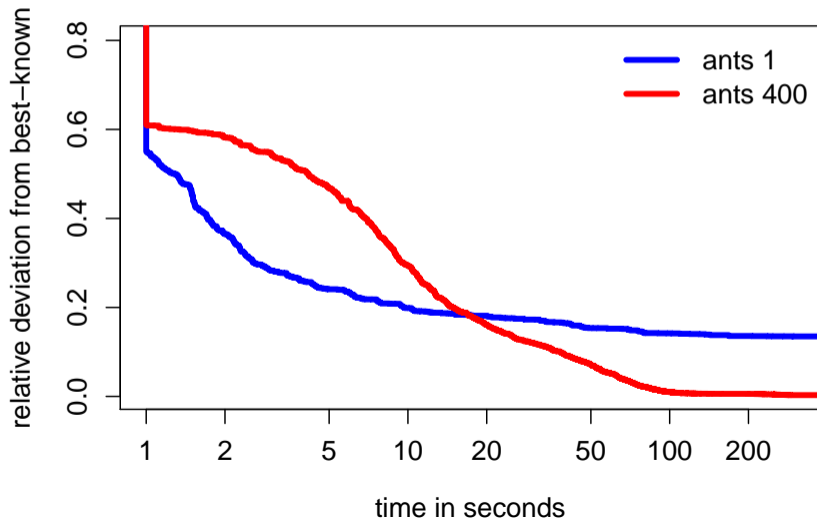
[Zilberstein, 1996]

Algorithms with good “*anytime*” *behavior* produce as high quality result as possible at any moment of their execution.

Automatically Improving the Anytime Behavior

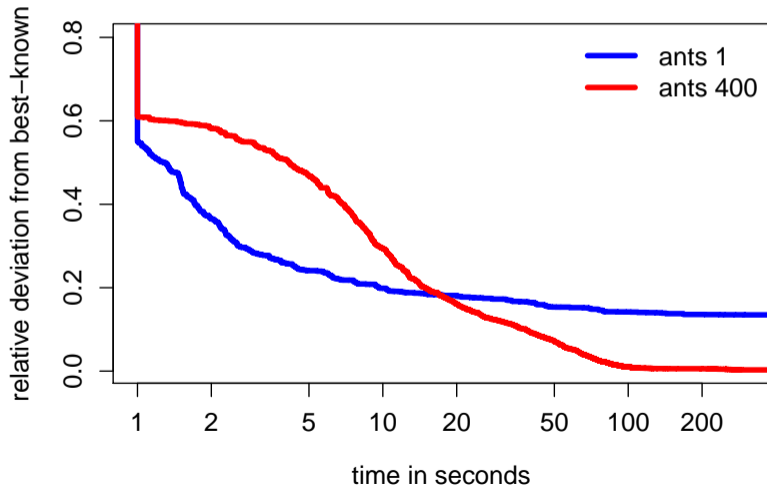
Max-Min Ant System w/o LS

Solution-quality vs. time (SQT) curve / Performance profile



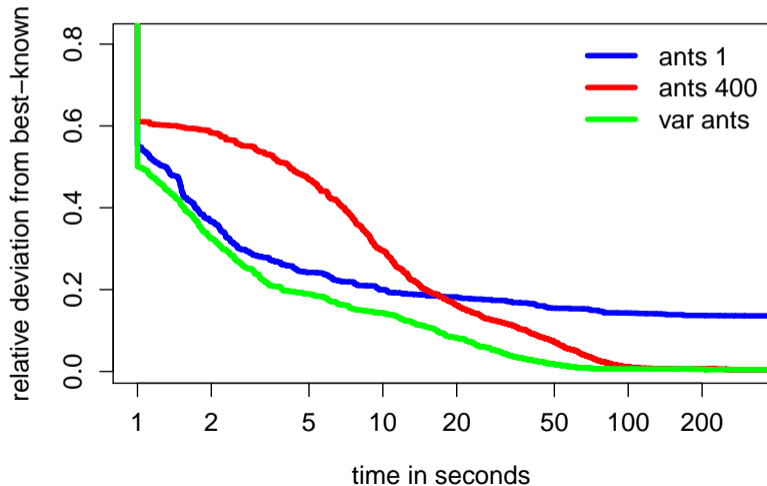
Automatically Improving the Anytime Behavior

Algorithms with good *“anytime” behaviour* produce as high quality result as possible at any moment of their execution [Zilberstein, 1996]



Automatically Improving the Anytime Behavior

Algorithms with good *“anytime” behaviour* produce as high quality result as possible at any moment of their execution [Zilberstein, 1996]



How to improve the anytime behaviour of MMAS?

👉 Online parameter variation:

- Start with 1 ant, add 1 ant every iteration until 400 ants
- Start with $\beta = 10$, switch to $\beta = 2$ after 100 iterations
- ...

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- ...

✗ More parameters!

✗ How to compare SQT curves?

Automatically Improving the Anytime Behavior

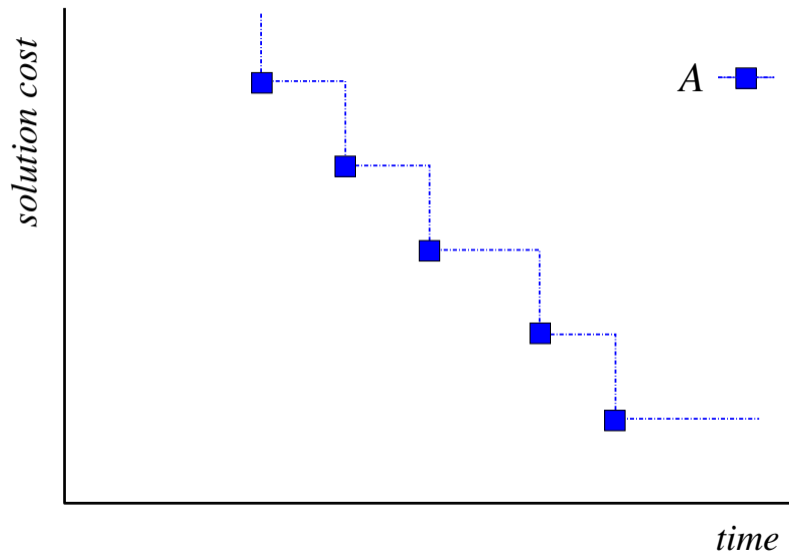
Online parameter control

- ✗ Which parameters to adapt? How? \Rightarrow More parameters!
- ✓ Use irace (offline) to select the best parameter control strategies

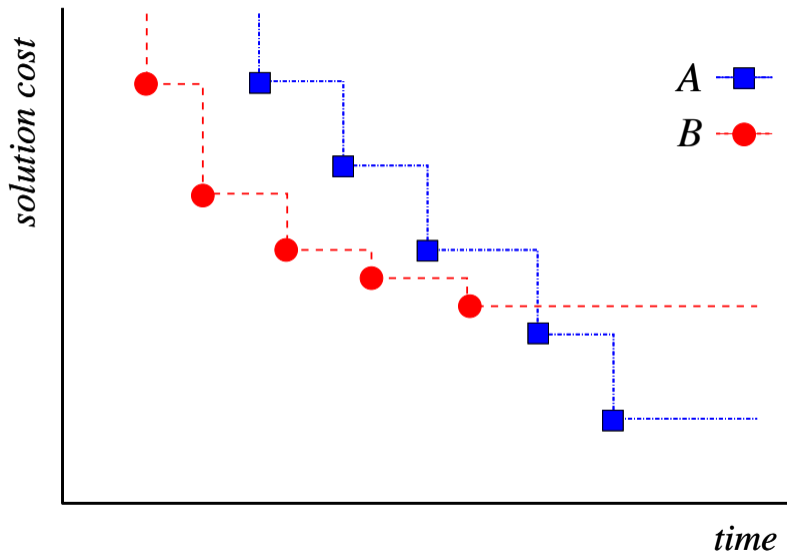
Improve Anytime Behavior

- ✓ More robust to different termination criteria
- ✗ How can irace compare SQT curves?

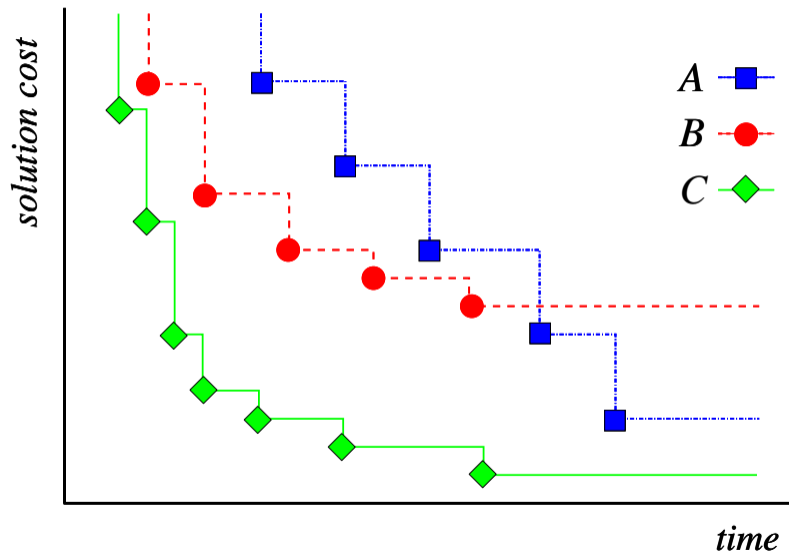
Automatically Improving the Anytime Behavior



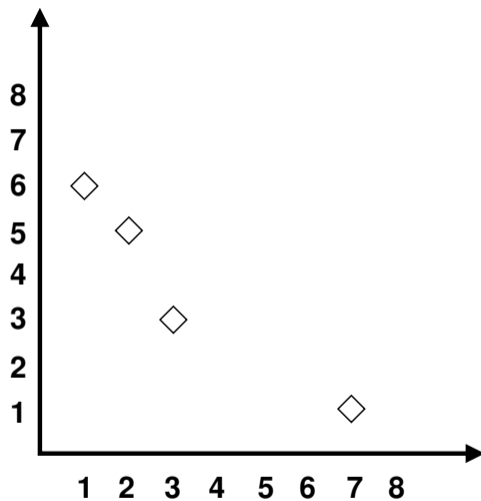
Automatically Improving the Anytime Behavior



Automatically Improving the Anytime Behavior

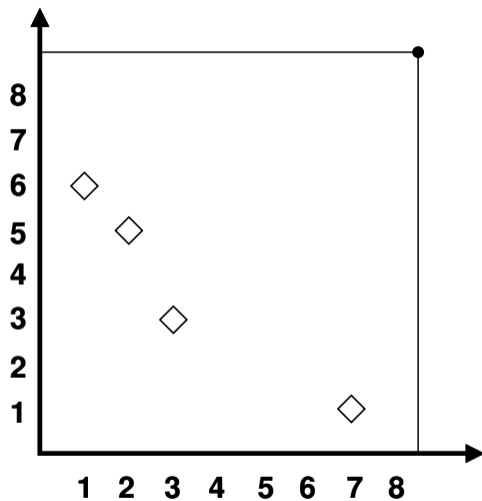


Automatically Improving the Anytime Behavior



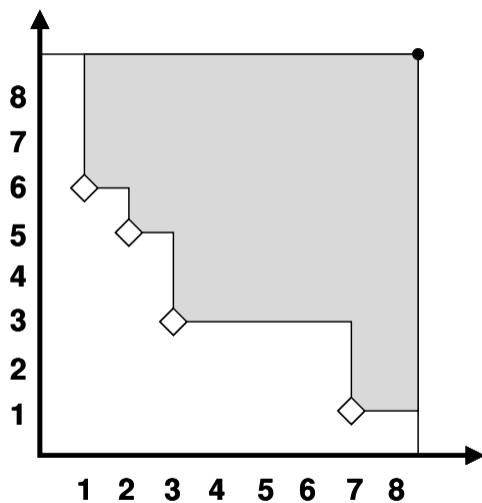
Hypervolume measure \approx Anytime behaviour

Automatically Improving the Anytime Behavior



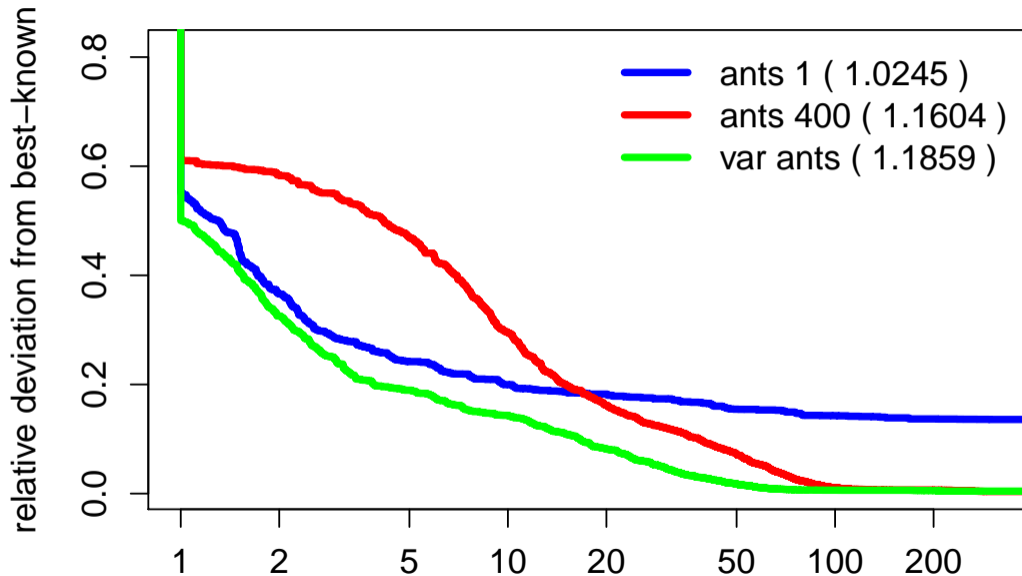
Hypervolume measure \approx Anytime behaviour

Automatically Improving the Anytime Behavior



Hypervolume measure \approx Anytime behaviour

Automatically Improving the Anytime Behavior



Automatically Improving the Anytime Behavior

`irace` + hypervolume = automatically improving the anytime behavior of optimization algorithms

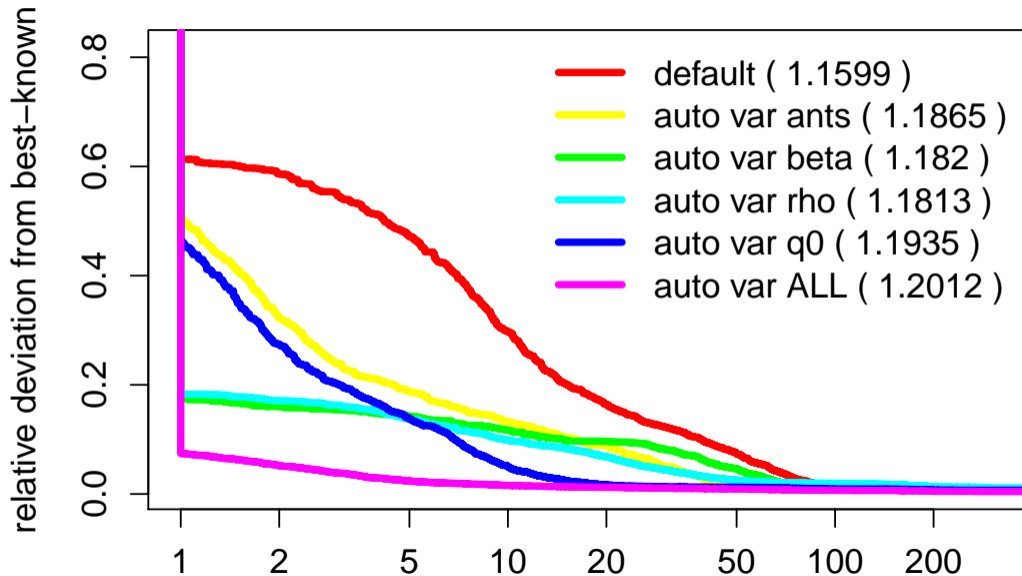
- 1 Run configuration until large stopping time
- 2 Compute hypervolume of SQT curve
- 3 Evaluate anytime behavior according to hypervolume

Automatically Improving the Anytime Behavior

irace + hypervolume = automatically improving the anytime behavior of optimization algorithms

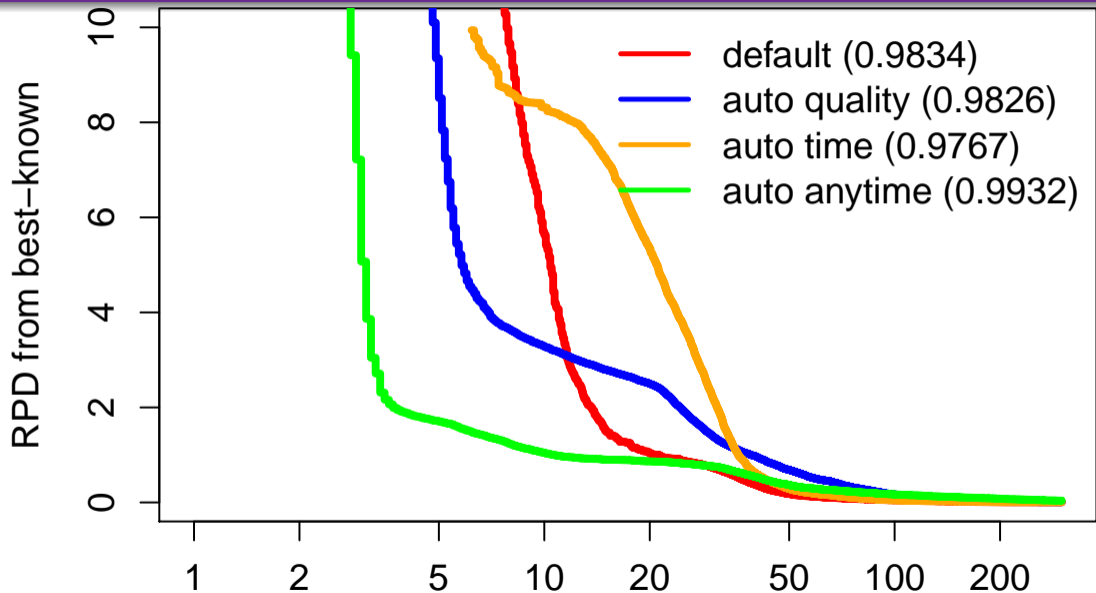
- ① Run configuration until large stopping time
 - ② Compute hypervolume of SQT curve
 - ③ Evaluate anytime behavior according to hypervolume
- Hypervolume (multi-objective) optimization
 - ✓ Objectively defined comparison
 - ✓ Well-known performance measure
 - Automatic configuration using irace
 - ✓ Most effort done by the computer
 - ✓ Best configurations selected by the computer: *Unbiased*

Scenario #1: Experimental comparison



SCIP: an open-source mixed integer programming (MIP) solver
[Achterberg, 2009]

- 200 parameters controlling search, heuristics, thresholds, ...
- Benchmark set: Winner determination problem for combinatorial auctions [Leyton-Brown et al., 2000]
1 000 training + 1 000 testing instances
- Single run timeout: 300 seconds
- irace budget (*maxExperiments*): 5 000 runs



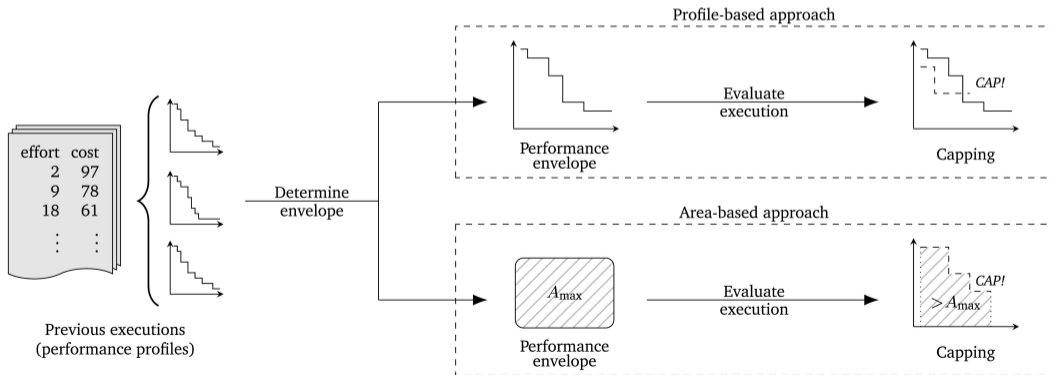
Capping methods for the automatic configuration of optimization algorithms

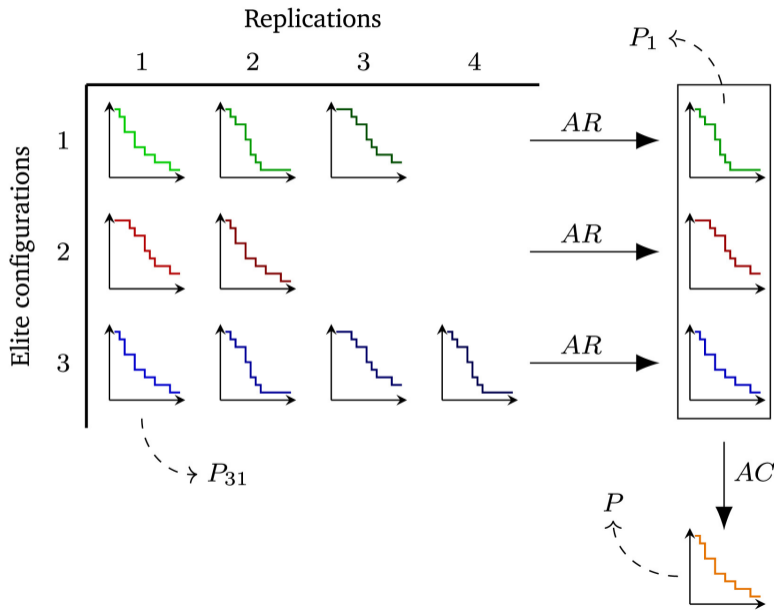


Marcelo De Souza, Marcus Ritt, and Manuel López-Ibáñez.

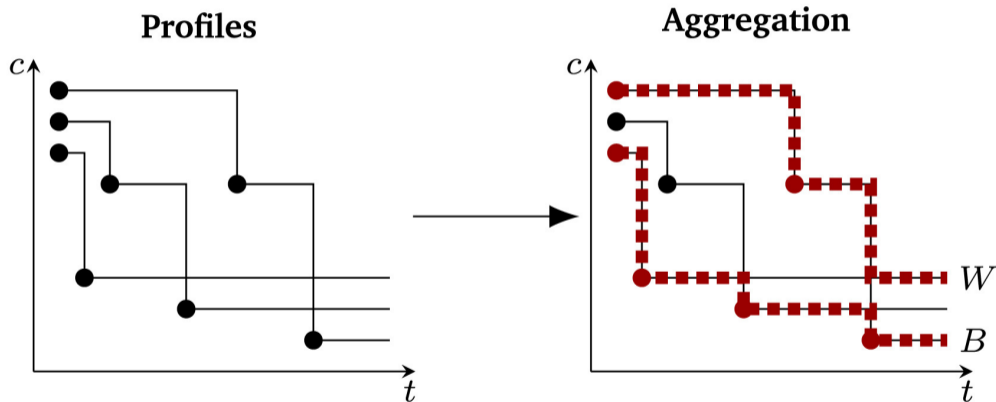
Capping methods for the automatic configuration of optimization algorithms.
Computers & Operations Research, 2022. doi: [10.016/j.cor.2021.105615](https://doi.org/10.016/j.cor.2021.105615).

- Adaptive capping only useful for decision algorithms (*time-to-target*)
- In many scenarios, we optimize cost over time until maximum termination time
 - ✗ Running bad configurations until maximum time is *wasteful*
 - ✓ Terminate (*cap*) bad configurations as soon as possible

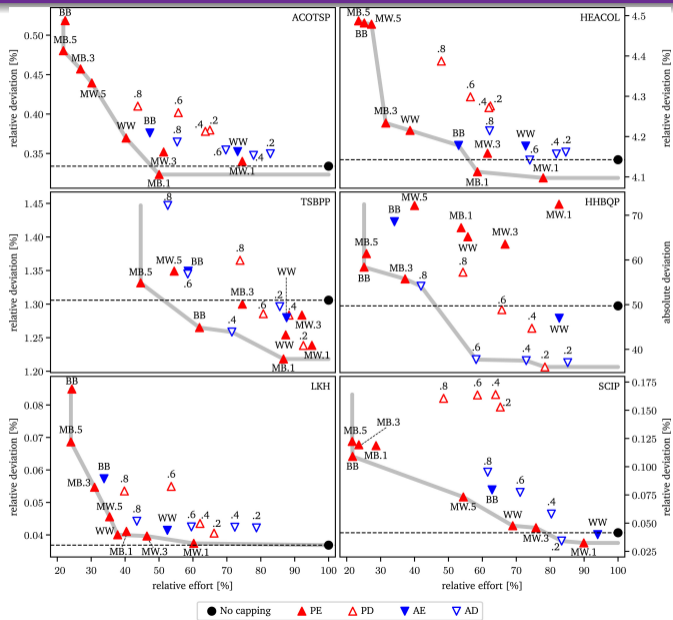




Best and Worst Profile-based Aggregation Methods:



P = profile-based
 A = area-based
 E = elitist
 D = adaptive
 B = best
 W = worst
 M = model



Category	Capping method	Relative effort [%]	Quality loss [%]					
			ACOTSP	HEACOL	TSBPP	HHBQP	LKH	SCIP
Conservative	AD.4	76.1	0.02	0.02	-0.05	-12.24	0.00	0.02
Aggressive	PEMB.1	53.0	-0.01	-0.03	-0.09	17.47	0.00	0.08

- AEBB for scenarios where the configuration budget is time
- Python add-on for irace: <https://github.com/souzamarcelo/capopt>

Why automatic algorithm configuration and design?

- ① More scientific, more principled
- ② The end of the up-the-wall game
- ③ Computing power is exponentially cheaper
- ④ AC tools are becoming better
- ⑤ More interesting, fun and useful

Reason #1: More scientific, more principled

- ✓ Reproducible results
- ✓ Fairer comparisons (best-effort)
- ✓ Avoid / reduce human biases
- ✓ Codify good practices

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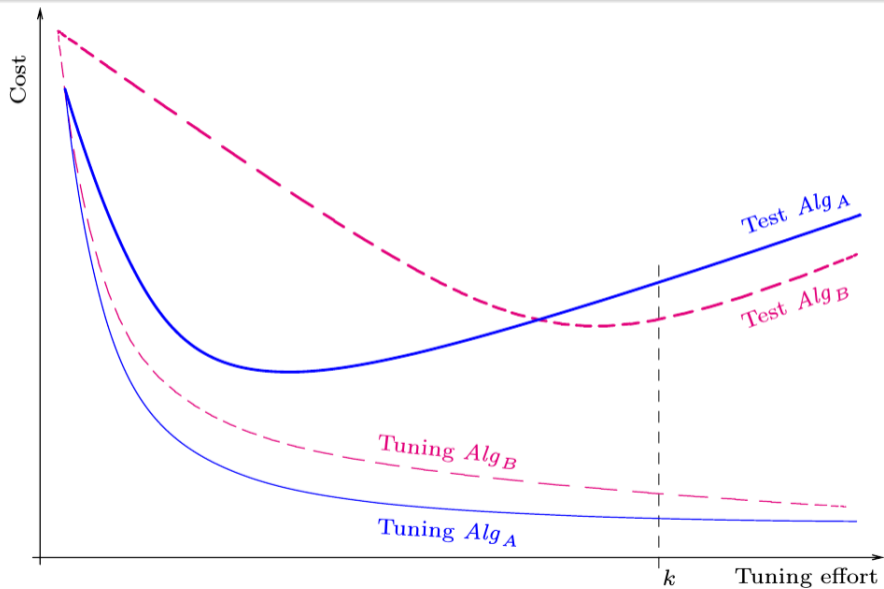
“*For procedures that require parameter tuning, the available data must be partitioned into a training and a test set. Tuning should be performed in the training set only.*”

[Journal of Heuristics: Policies on Heuristic Search Research]

“*The performance of swarm intelligence algorithms [...] is often strongly dependent on the value of the algorithm parameters. Such values should be set using either sound statistical procedures [...] or automatic parameter tuning procedures.*”

[Swarm Intelligence Journal (Springer)]

Over-tuning



(Taken from Birattari [2009])

Reason #2: The End of the Game

“ *The Journal of Heuristics does not endorse the up-the-wall game.* ”
[Journal of Heuristics: Policies on Heuristic Search Research]

“ *True innovation in metaheuristics research therefore does not come from yet another method that performs better than its competitors, certainly if it is not well understood why exactly this method performs well.* [Sörensen, 2015] ”

- Finding a state-of-the-art algorithm is “easy”:

problem modeling + algorithmic components + computing power

- *What* novel components? *Why* they work? *When* they work?

Reason #3: Computing power is exponentially cheaper



Reason #3: Computing power is exponentially cheaper

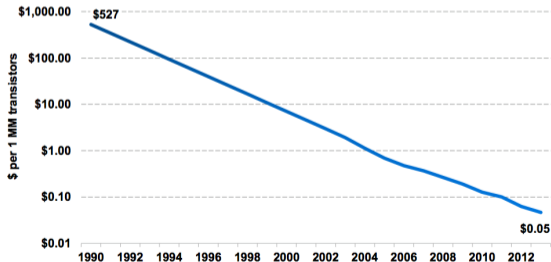
Algorithm Configuration in the Cloud [Geschwender et al., 2014]

Amazon EC2, 8 cores, 7GB memory, \$ 0.58/hour

Compute Costs Declining = 33% Annually, 1990-2013

*Decreasing cost / performance curve enables
computational power @ core of digital infrastructure*

Global Compute Cost Trends



Reason #4: AC tools are becoming better

- Complex parameter spaces: numerical, categorical, ordinal, subordinate (conditional), constraints
- Large parameter spaces (hundreds of parameters)
- Heterogeneous problem instances
- Medium to large configuration budgets (few hundred to many thousands of runs)
- Individual runs may require from seconds to hours
- Multi-core CPUs, MPI, distributed computation clusters

☞ Modern automatic configuration tools (irace, SMAC, ...) are general, flexible, powerful and easy to use

Reason #5: More interesting, fun, and useful

✖ Classical optimization research:

- ① Human-driven design to outperform other algorithmic designs
- ② Analysis of the human-designed algorithm

Reason #5: More interesting, fun, and useful

✗ Classical optimization research:

- ① Human-driven design to outperform other algorithmic designs
- ② Analysis of the human-designed algorithm

✓ Paradigm shift in optimisation research:

*From monolithic algorithms
to flexible frameworks of algorithmic components*

- ① Humans devise *novel* algorithmic components
- ② Data-driven CPU-intensive automatic design
- ③ Analysis of generated data
- ④ Human-driven improvement of components

QUIT LIVING IN THE PAST



Acknowledgments

This tutorial has benefited from collaborations and discussions with my colleagues:

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Zhi Yuan, Marcus Ritt, Marcelo De Souza



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