Automatic Design of Algorithms with iRace for Multi-objective Optimization and Anytime Optimization

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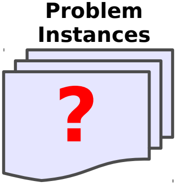
ULB UNIVERSITÉ LIBRE DE BRUXELLES, UNIVERSITÉ D'EUROPE

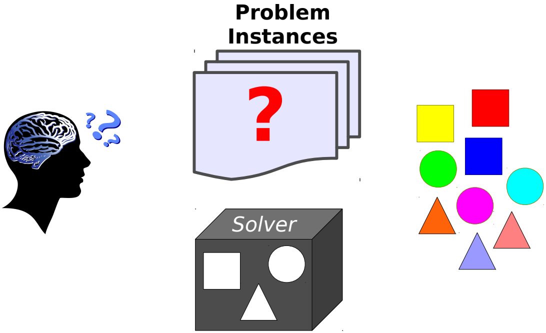
IRIDIA Institut de Recherches Interdisciplinaires et de Développements en Intelligence Artificielle

A non-expert user wants to repeatedly solve a problem

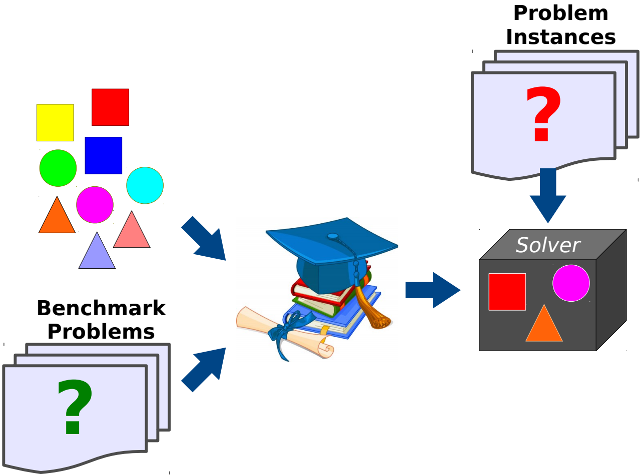


Offline Automatic Design of Algorithms

How to build a solver for this type of problem?

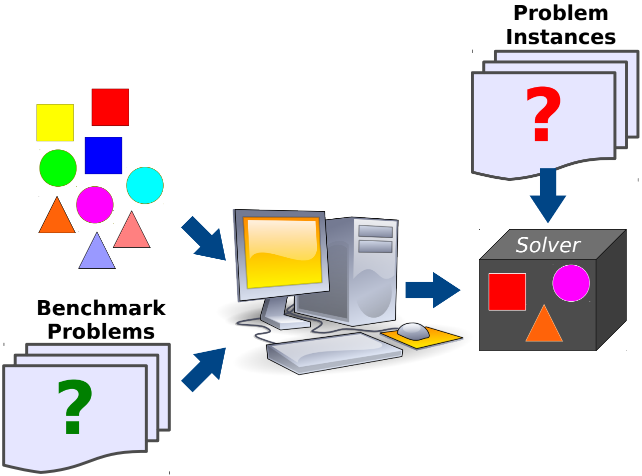


The user could rely on an expert



Offline Automatic Design of Algorithms

Can we replace the expert by an algorithm?



Offline Automatic Design of Algorithms

- ✔ Experts focus on creativity and understanding
- ✔ The machine does the boring experiments and statistics
- ✔ Formalize what is implicitly done in experimental research
- ✔ Avoid human biases

Offline Tuning / Automatic Configuration

- Find the best parameter configuration of a solver from a set of *training instances*
- Repeatedly use this configuration to solve *unseen instances* of the same problem

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Goal: Automatically find a good instantiation of an optimization algorithm from a large space of potential designs for a specific problem.

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Solver	$\Rightarrow$	Flexible algorithmic framework
Parameter space	$\Rightarrow$	Design space of the framework

The algorithm design problem [Birattari, 2009]

Θ : set of potential algorithm designs (possibly infinite)

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Find the best algorithm design θ^* such that:

$$\theta^* = \arg\min_{\theta \in \Theta} c_\theta$$

The algorithm design problem: How to solve it?

Traditional approach

1. Expert chooses a number of algorithm designs $\Theta_0 \subset \Theta$
2. Expert chooses a number of benchmark problems $I_0 \subset \mathcal{I}$
3. Estimate c_θ for each $\theta \in \Theta_0$,
   by computing $c(\theta, i)$ for each $i \in I_0$
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Disadvantages

- ✘ Same computational effort spent on good and bad designs
- ✘ Small number of algorithm designs chosen a priori

The racing approach

[Birattari et al., 2002]

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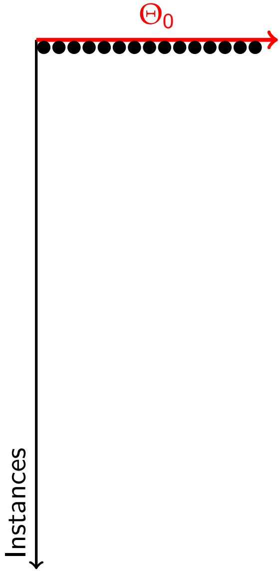

- start with a set of initial candidates

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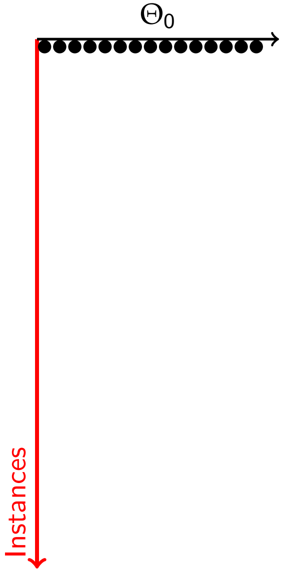

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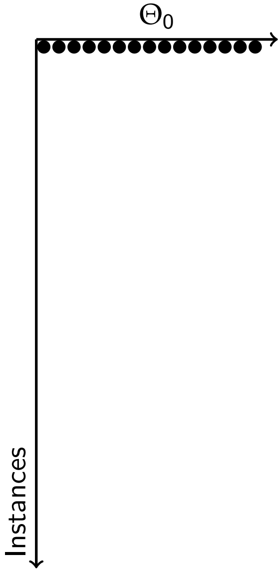

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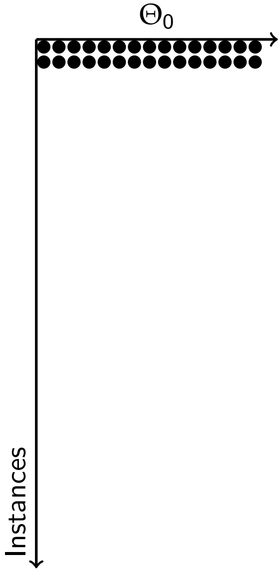

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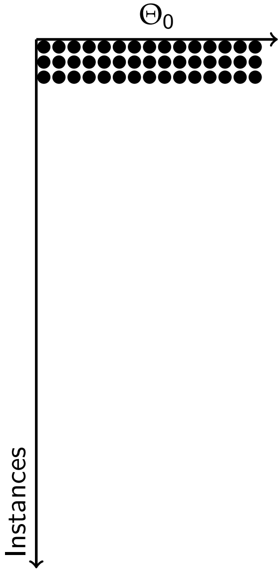

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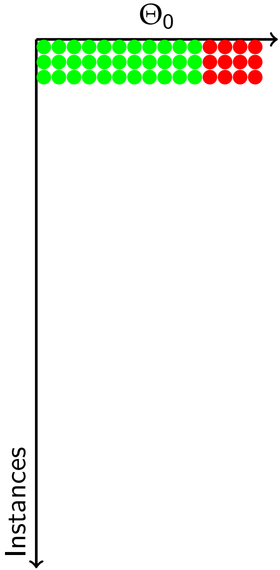

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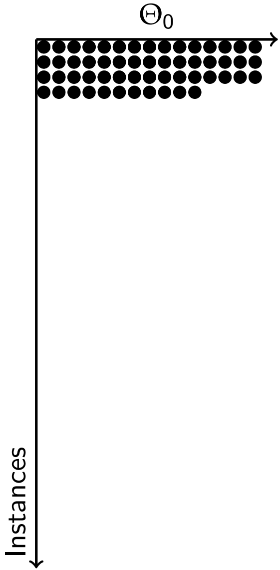
- discard inferior candidates

  as sufficient evidence is gathered against them



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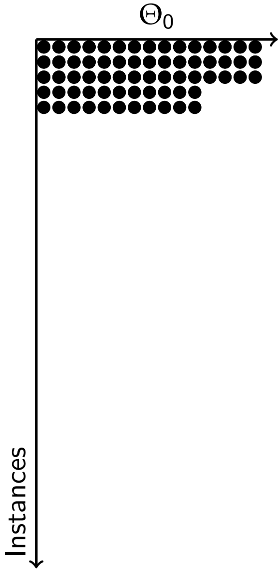

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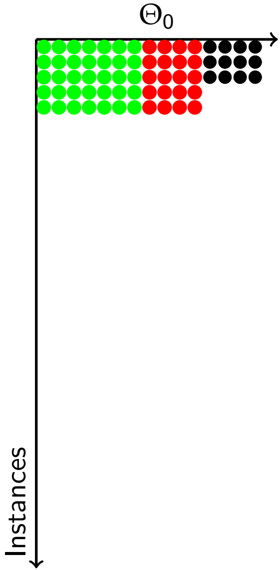

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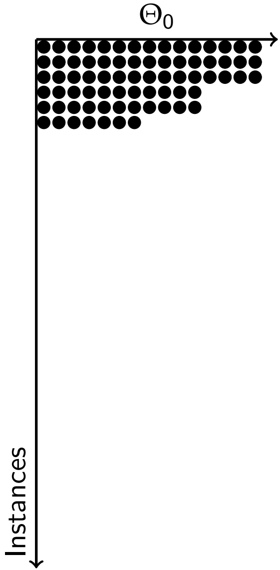

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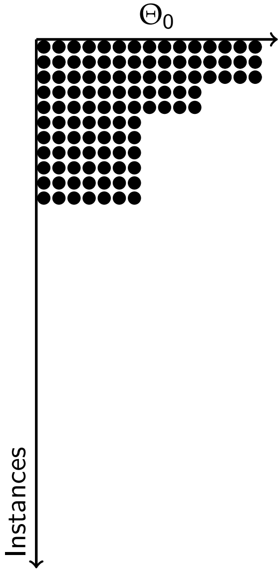

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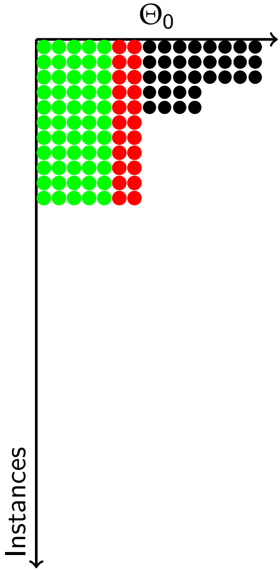

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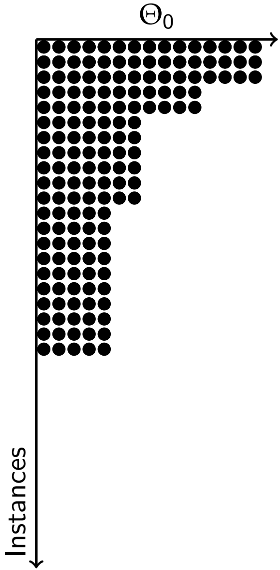

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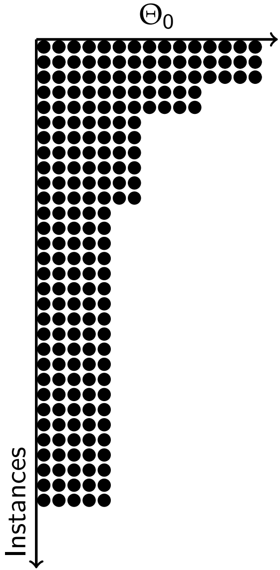

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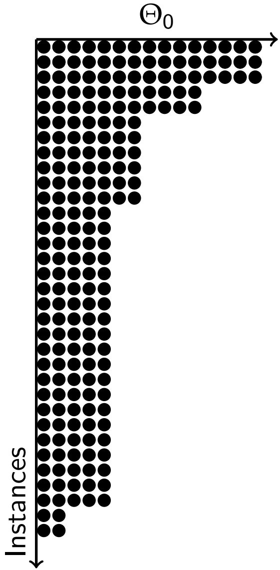

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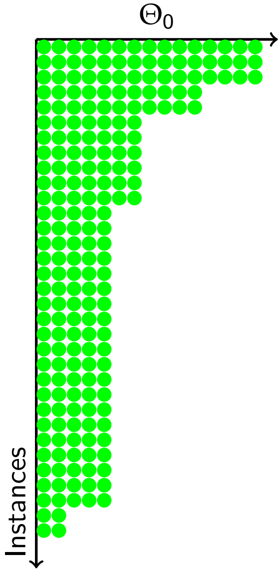
- ... repeat until a winner is selected

  or until computation time expires



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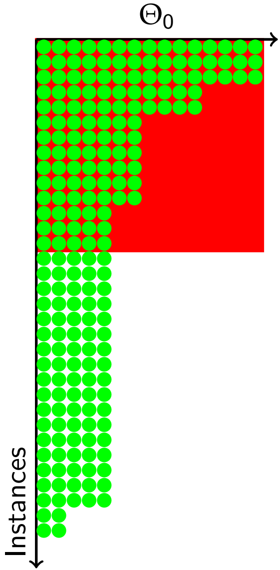

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How to discard?

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Statistical testing!

- *F-Race:* Friedman two-way analysis of variance by ranks + Friedman post-hoc test
- Alternative: paired t-test with/without p-value correction (against the best)

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How to sample algorithm designs?

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How to sample algorithm designs?

- Full factorial
- Random sampling
- Iterative refinement of a sampling model
  ⇒ *Iterated F-Race (I/F-Race)* [Balaprakash et al., 2007]

Iterated F-Race [Balaprakash et al., 2007]

Require:

Training instances: $\{I_1, I_2, \dots\} \sim \mathcal{I}$,
Parameter space: X,
Cost measure: $\mathcal{C}\colon \Theta \times \mathcal{I} \to \mathbb{R}$,
Tuning budget: B

$\Theta_1 \sim \texttt{SampleUniform}(X)$
$\Theta^{\text{elite}} := \texttt{Race}(\Theta_1,\ B_1)$
$i := 2$
while $B_{\text{used}} \leq B$ **do**
    $\Theta^{\text{new}} \sim \texttt{Sample}(X, \Theta^{\text{elite}})$
    $\Theta_i := \Theta^{\text{new}} \cup \Theta^{\text{elite}}$
    $\Theta^{\text{elite}} := \texttt{Race}(\Theta_i,\ B_i)$
    $i := i + 1$
Output: Θ^{elite}

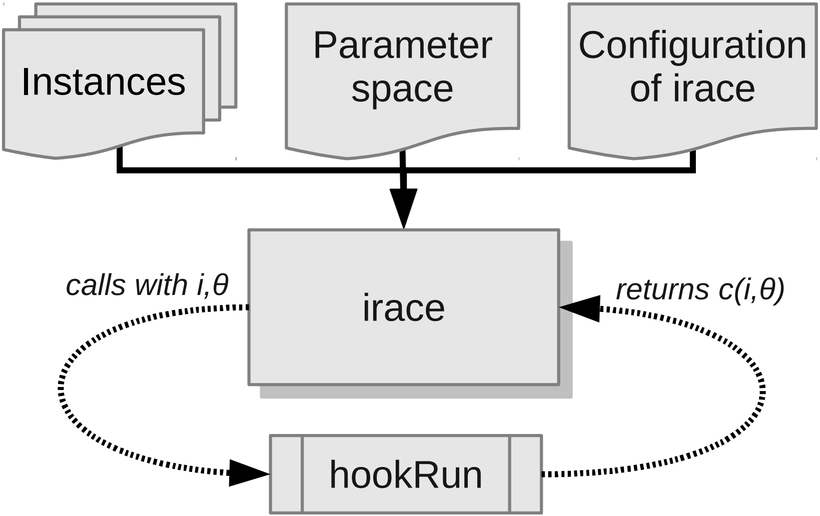
The `irace` Package

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

Manuel López-Ibáñez, Jérémie Dubois-Lacoste, Thomas Stützle, and Mauro Birattari. **The irace package, Iterated Race for Automatic Algorithm Configuration.** *Technical Report TR/IRIDIA/2011-004*, IRIDIA, Université Libre de Bruxelles, Belgium, 2011.

- Implementation of I/F-Race with a few extensions
- R package available at CRAN
- Flexible
- Easy to use
- No knowledge of R needed
- Command-line wrapper: `irace --help`

The irace Package



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- Parameter space:

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LS          c  {SA, best, first}
rate        o  {low, med, high }
population  i  (1, 100)
temp        r  (0.5, 1)          if LS == "SA"
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- Initial configurations may be explicitly provided
- Parallel execution:
  - on a single machine (`multicore` package)
  - using MPI (`Rmpi` package)
  - using a Grid Engine cluster (with `qsub` and `qstat`)

Advance Applications of irace

1. Automatic design of multi-objective optimization algorithms
2. Automatically improving the anytime behavior of algorithms

Multi-objective Optimization

Multiple objective functions: $\vec{f} = (f_1(x), f_2(x), \dots)$

No a priori knowledge $\Rightarrow$ *Pareto-optimality*

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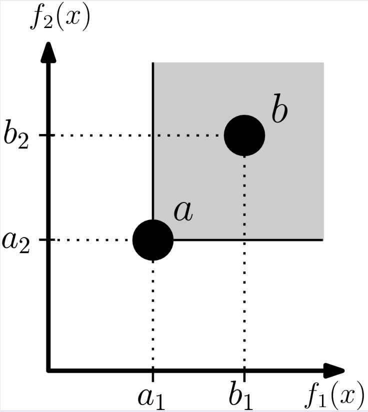
a dominates *b*



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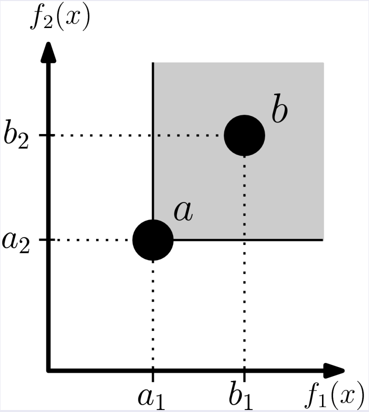
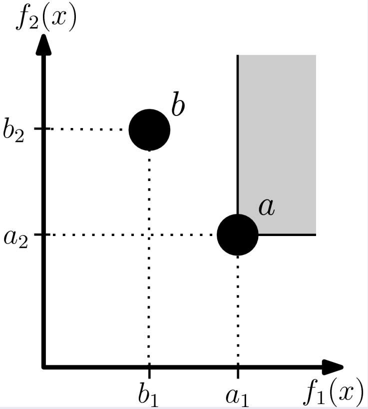
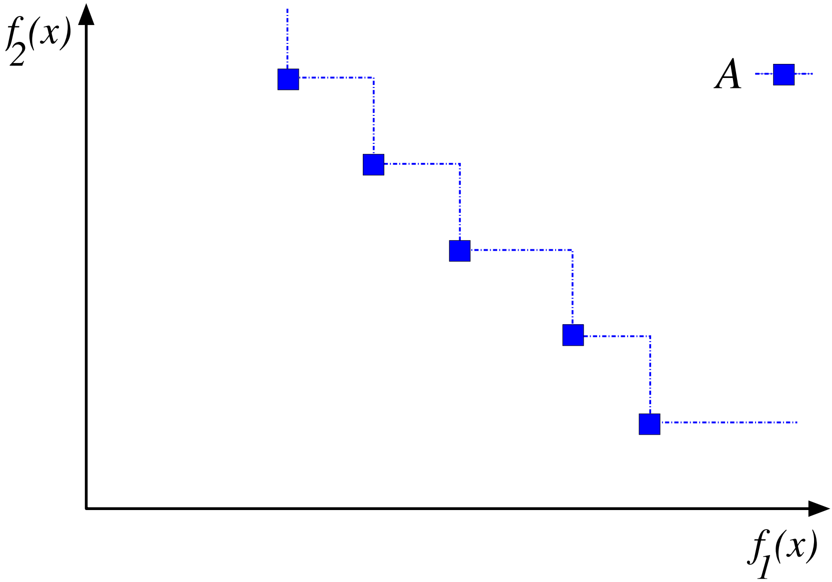


a and *b* nondominated



Multi-objective Optimization



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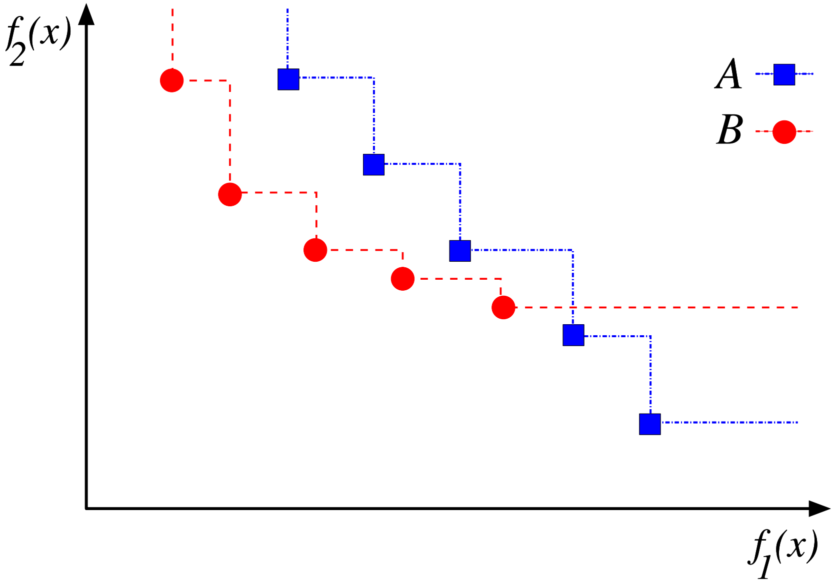

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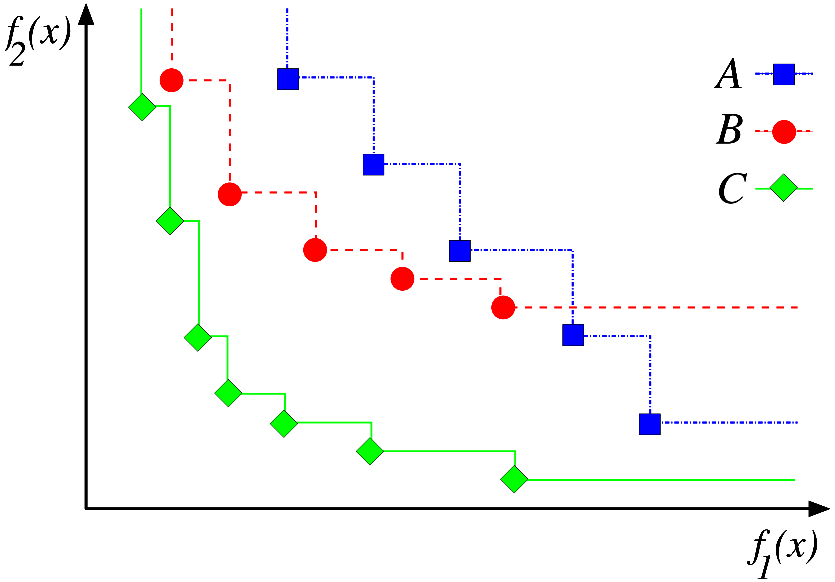
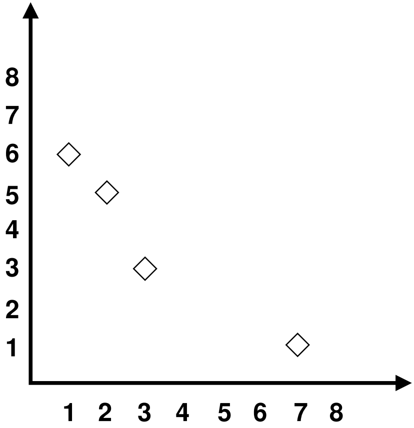


Hypervolume measure



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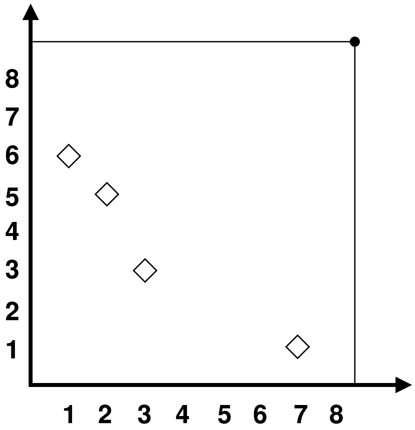

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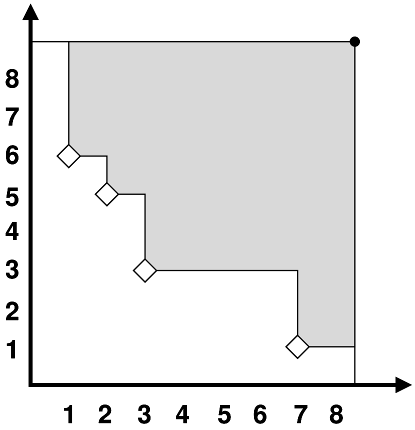

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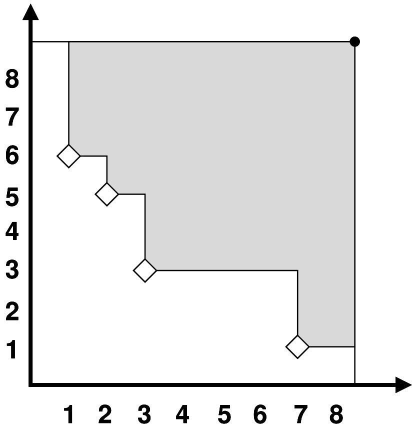

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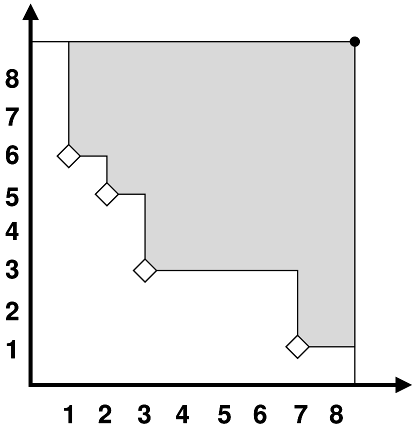

`irace` + hypervolume = automatic configuration of multi-objective solvers

Automatic Design of MOACO Algorithms

Automatic Design of MOACO Algorithms

- Multiple objective Ant-Q (MOAQ) [Mariano & Morales, 1999] [García-Martínez et al., 2007]
- MACS-VRPTW [Gambardella et al., 1999]
- BicriterionAnt [Iredi et al., 2001]
- SACO [T'Kindt et al., 2002]
- Multiobjective Network ACO [Cardoso et al., 2003]
- Multicriteria Population-based ACO [Guntsch & Middendorf, 2003]
- MACS [Barán & Schaerer, 2003]
- COMPETants [Doerner et al., 2003]
- Pareto ACO [Doerner et al., 2004]
- Multiple Objective ACO Metaheuristic [Gravel et al., 2002]
- MOACO-bQAP [López-Ibáñez et al., 2004]
- MOACO-ALBP [Baykasoglu et al., 2005]
- mACO-$\{1, 2, 3, 4\}$ [Alaya et al., 2007]
- Population-based ACO [Angus, 2007]

M. López-Ibáñez and T. Stützle. The automatic design of multi-objective ant colony optimization algorithms. *IEEE Transactions on Evolutionary Computation*, 2012.

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2. Synthesize knowledge into a configurable MOACO framework able to instantiate existing *and new* MOACO algorithms
3. Use `irace` + hypervolume to find the best MOACO designs

A flexible MOACO framework

- Multi-objective algorithmic design: 10 parameters
- Instantiates 9 MOACO algorithms from the literature
- $> 25\,000$ potential designs
- Underlying ACO settings are also configurable
- Implemented for bi-objective TSP and bi-objective Knapsack

Experiments

Worst	⇓	Best MOACO of literature + fixed ACO settings
		Tuned MOACO design + fixed ACO settings
		Best MOACO of literature + *tuned* ACO settings
		Tuned MOACO design + *tuned* ACO settings
Best		*Tuned* (MOACO design + ACO settings)

Conclusions

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- ✔ `irace` + hypervolume = automatic design of MO algorithms
- ✔ `irace` typically better than humans ...
  ... if given a good design space
- ✔ Another example:

  J. Dubois-Lacoste, M. López-Ibáñez, and T. Stützle. **Automatic configuration of state-of-the-art multi-objective optimizers using the TP+PLS framework**. *GECCO*, 2011.

Automatically Improving the Anytime Behavior of Optimization Algorithms

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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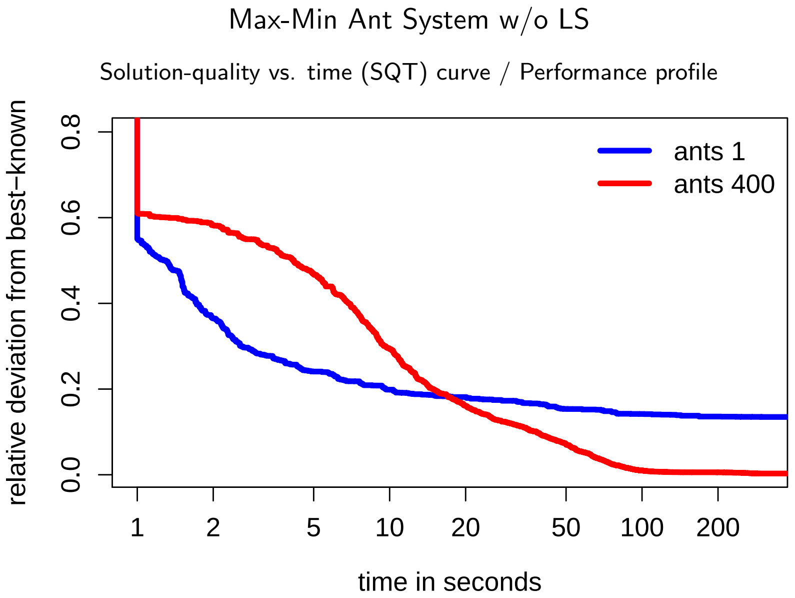
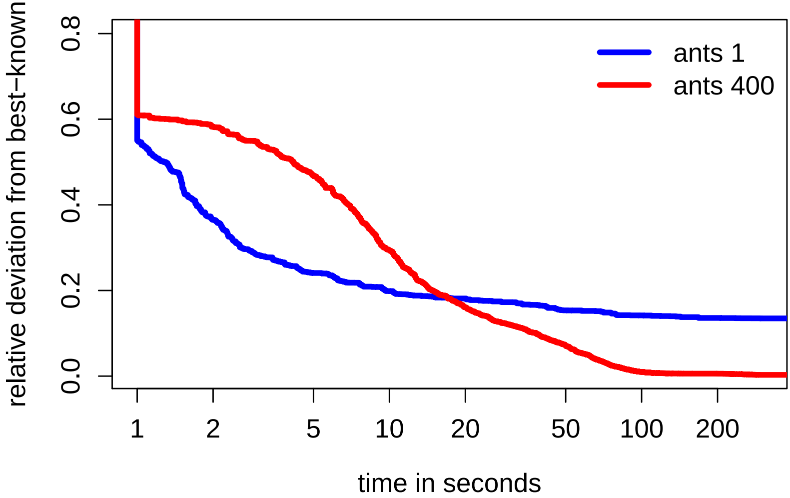
Good Anytime Behavior [Zilberstein, 1996]

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


Max-Min Ant System w/o LS
Solution-quality vs. time (SQT) curve / Performance profile
relative deviation from best−known
0.0
0.2
0.4
0.6
0.8
1
2
5
10
20
50
100
200
time in seconds
ants 1
ants 400

Algorithms with good *"anytime" behaviour* produce as high quality result as possible at any moment of their execution.



Quality vs. Time Trade-off

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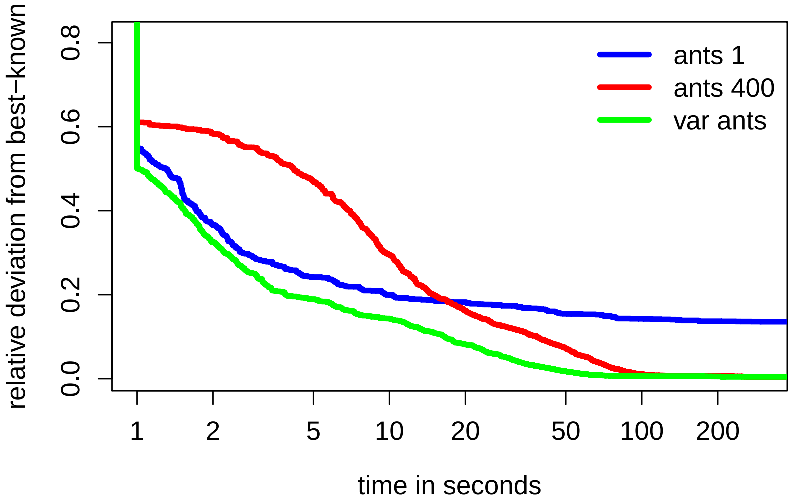

Improving "Anytime" Behaviour

How to improve the anytime behaviour of MMAS?

☞ 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?

Brute-Force Approach

1. Choose *many* different parameter variation strategies
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After one year and a master thesis: [Maur et al., 2010]

- ✔ Strategies for varying *ants*, β, or q_0 that significantly improve the anytime behaviour of MMAS on the TSP.

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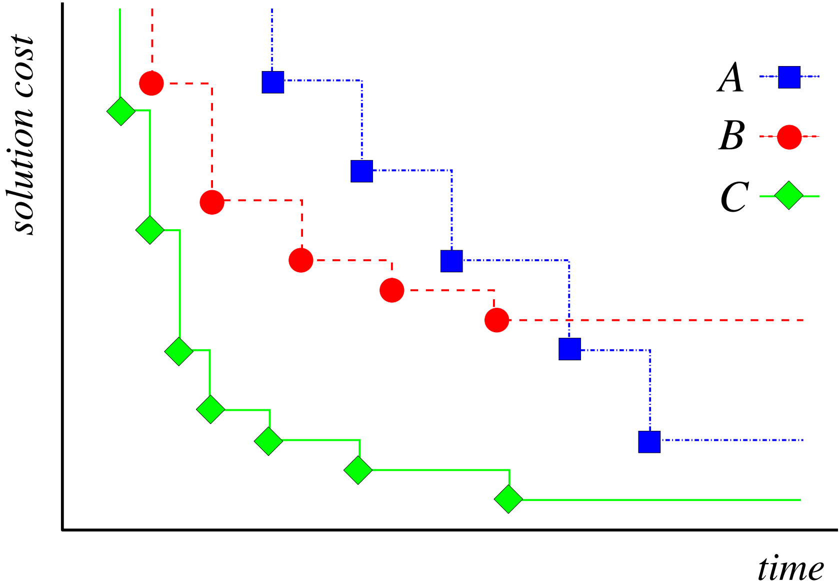
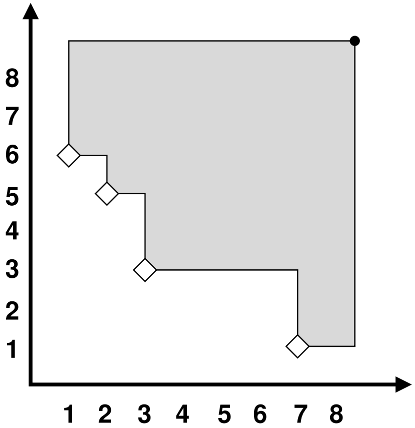
- ✔ Strategies for varying *ants*, β, or q_0 that significantly improve the anytime behaviour of MMAS on the TSP.
- ✘ Extremely time consuming
- ✘ Subjective / Bias

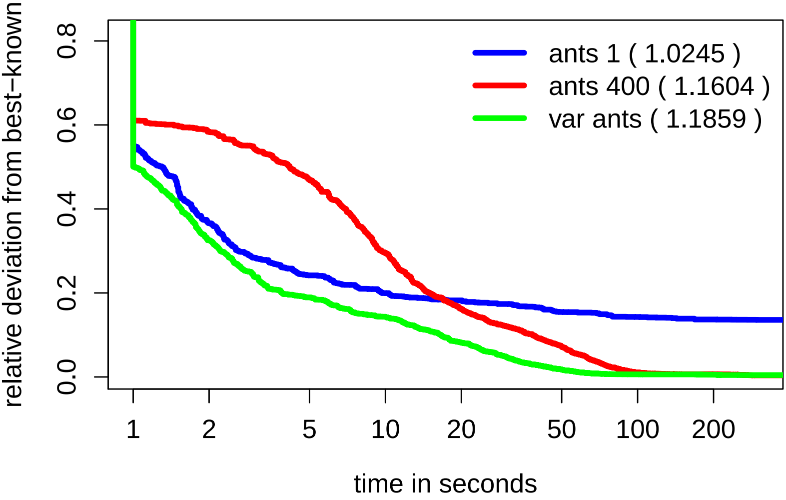
Bi-Objective Optimisation



Hypervolume measure



Hypervolume measure



Our Proposed Approach

`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

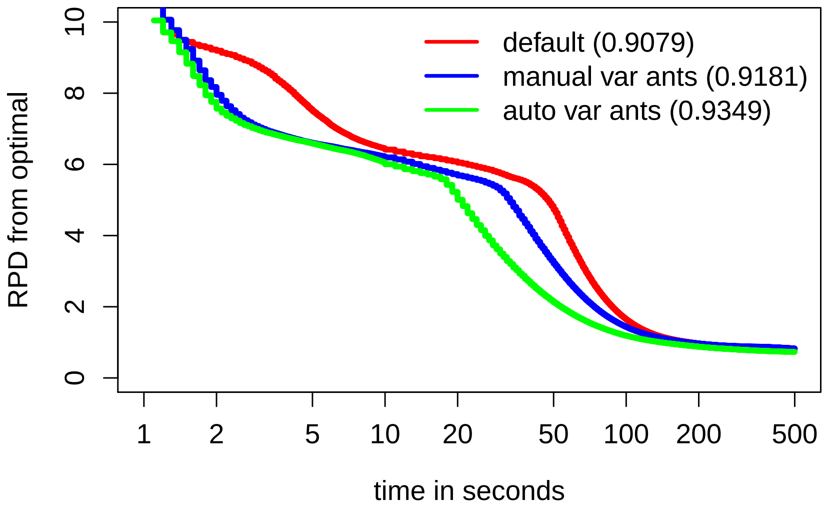
Experiments

- Time-varying *ants* (m): 6 parameters

Param.	Domain	Condition
m_{var}	{ *delta*, *switch*, *none* }	
m	[1, 100]	if var = *none*
Δm	$\{0.01, 0.05, 0.1, 0.25, 0.5, 1, 2, 5\}$	if var = *delta*
m_{switch}	[1, 500]	if var = *switch*
m_{start} m_{end}	1 [1, 500]	if var $\in$ {*delta*, *switch*}

- Other parameters are set to default
- Tuning budget: 1000 runs

Experiments

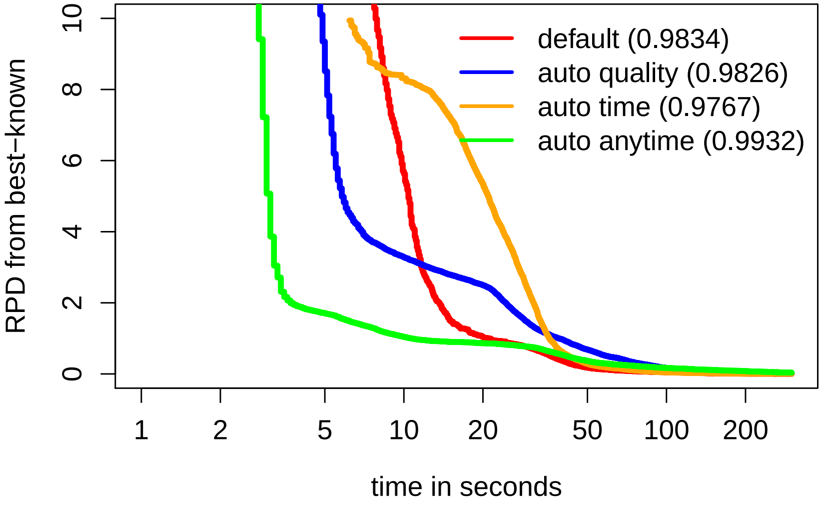


Automatically Improving the Anytime Behaviour of SCIP

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
- Tuning budget: 5 000 runs

Automatically Improving the Anytime Behaviour of SCIP



Automatically Improving Anytime Behavior

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- How to introduce a bias towards final quality?
  - ☞ Compute hypervolume on transformed y-axis
  - ☞ Weighted hypervolume [Zitzler et al., 2007]

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- How to introduce a bias towards final quality?
  - ☞ Compute hypervolume on transformed y-axis
  - ☞ Weighted hypervolume [Zitzler et al., 2007]
- How to define a cut-off time as short as possible?
  - ☞ Estimate point of diminishing returns [Woodruff et al., 2011]
  - ☞ Survival analysis techniques [Gagliolo & Legrand, 2010]

The End

irace

Easy, flexible, state-of-the-art automatic configuration tool

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`irace`

Easy, flexible, state-of-the-art automatic configuration tool

Automatic Design of Algorithms

Automatically find a good instantiation of an optimization algorithm from a large space of potential designs for a specific problem.

The End

irace

Easy, flexible, state-of-the-art automatic configuration tool

Automatic Design of Algorithms

Automatically find a good instantiation of an optimization algorithm from a large space of potential designs for a specific problem.

irace + hypervolume = automatic design of

- multi-objective optimization algorithms
- anytime optimization algorithms

Automatic Design of Algorithms with iRace for Multi-objective Optimization and Anytime Optimization

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IRIDIA Institut de Recherches Interdisciplinaires et de Développements en Intelligence Artificielle

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