Automatic (Offline) Configuration of Algorithms

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Part I

Automatic Algorithm Configuration (Overview)

Solving complex optimization problems

The algorithmic solution of hard optimization problems is one of the CS/OR success stories!

- Exact (systematic search) algorithms
  - branch&bound, branch&cut, constraint programming, ...
  - guarantees of optimality but often time/memory consuming
  - powerful general-purpose software available
- Approximation algorithms
  - heuristics, local search, metaheuristics, hyperheuristics ...
  - rarely provable guarantees but often fast and accurate
  - typically special-purpose software

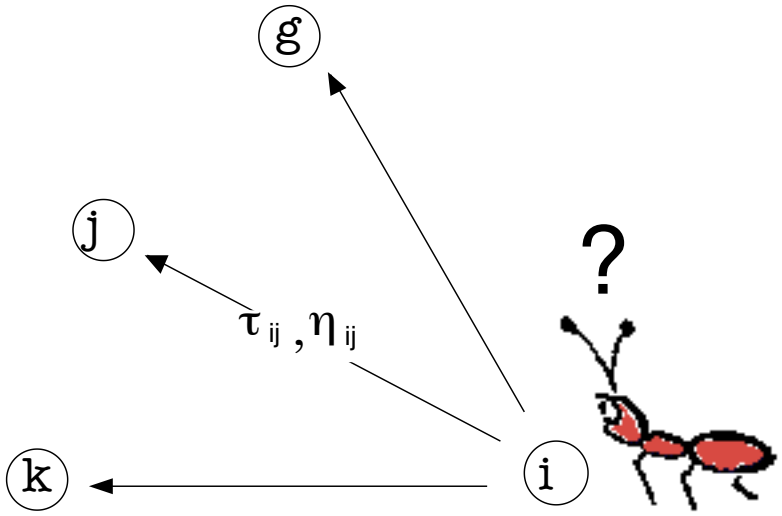
Very active research on hybrids of exact/approximate algorithms!

Design choices and parameters everywhere

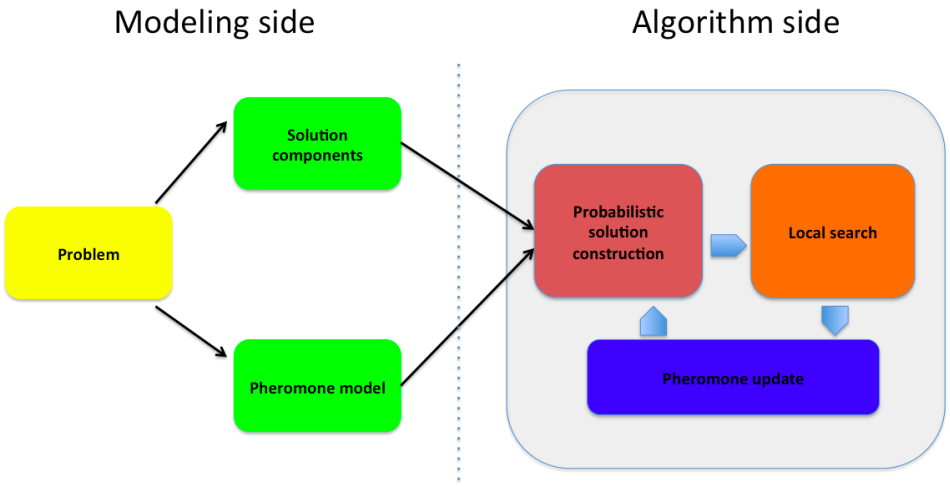
Modern high-performance optimizers involve a large number of design choices and parameter settings

- Exact solvers
  - Design choices: alternative models, pre-processing, variable selection, value selection, branching rules ...
    + numerical parameters
  - SCIP solver: more than 200 parameters that influence search
- (Meta)-heuristic solvers
  - Design choices: solution representation, operators, neighborhoods, pre-processing, strategies, ... + numerical parameters
  - Multi-objective ACO algorithms with 22 parameters (see part 2)

ACO, Probabilistic solution construction



Applying Ant Colony Optimization



ACO design choices and numerical parameters

- solution construction
  - choice of constructive procedure
  - choice of pheromone model
  - choice of heuristic information
  - numerical parameters
    - α, β influence the weight of pheromone and heuristic information, respectively
    - q_0 determines greediness of construction procedure
    - m, the number of ants
- pheromone update
  - which ants deposit pheromone and how much?
  - numerical parameters
    - ρ: evaporation rate
    - τ_0: initial pheromone level
- local search
  - . . . many more . . .

Parameter types

- *categorical* parameters **design**
  - choice of constructive procedure, choice of recombination operator, choice of branching strategy,. . .
- *ordinal* parameters **design**
  - neighborhoods, lower bounds, . . .
- *numerical* parameters **tuning, calibration**
  - integer or real-valued parameters
  - weighting factors, population sizes, temperature, hidden constants, . . .
- Parameters may be *conditional* to specific values of other parameters

Configuring algorithms involves setting categorical, ordinal and numerical parameters

Manual design and tuning

Human expert + trial-and-error/statistics

Towards more systematic 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

Can we make this approach more principled and automatic?

Towards automatic (offline) algorithm configuration

Automatic algorithm configuration

- apply powerful search techniques to design algorithms
- use computation power to explore algorithm design spaces
- free human creativity for higher level tasks

Offline configuration and online parameter control

Offline tuning / Algorithm configuration

- Learn best parameters *before* solving an instance
- Configuration done on training instances
- Performance measured over test ($\neq$ training) instances

Online tuning / Parameter control / Reactive search

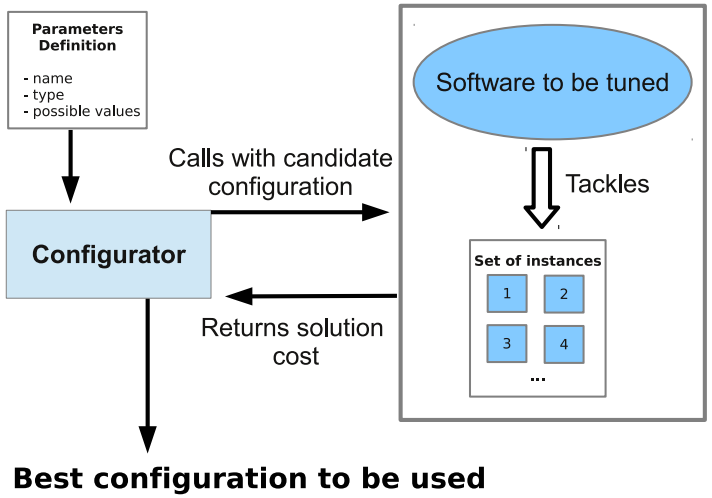
- Learn parameters *while* solving an instance
- No training phase
- Limited to very few crucial parameters
- Often static parameter tuning done online [Pellegrini et al., 2014]

Mario's Pizza Delivery Problem [Birattari, 2004; Birattari et al., 2002]

Mario collects phone orders for 30 minutes. He 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 amount of time for scheduling, say one minute
- Limited amount of time to implement an optimization algorithm, say one week

Offline configuration



AC is a stochastic optimization problem

Decision variables
- discrete (categorical, ordinal, integer) and continuous

Stochasticity
- of the target algorithm
- of the problem instances

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

AC requires specialized methods

Methods for Automatic Algorithm Configuration

experimental design, ANOVA
CALIBRA [Adenso-Díaz & Laguna, 2006]
others [Coy et al., 2001; Ridge & Kudenko, 2007; Ruiz & Maroto, 2005]

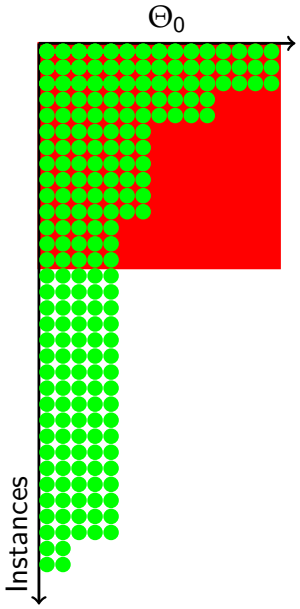
numerical optimization
MADS [Audet & Orban, 2006], CMA-ES, BOBYQA [Yuan et al., 2012]

heuristic optimization
meta-GA [Grefenstette, 1986], ParamILS [Hutter et al., 2007b, 2009], gender-based GA [Ansótegui et al., 2009], linear GP [Oltean, 2005], REVAC(++) [Nannen & Eiben, 2006; Smit & Eiben, 2009, 2010] ...

model-based
SPO [Bartz-Beielstein et al., 2005, 2010], SMAC [Hutter et al., 2011]

sequential statistical testing
F-race, iterated F-race [Balaprakash et al., 2007; Birattari et al., 2002]
irace [López-Ibáñez et al., 2011]

The racing approach [Birattari et al., 2002]



- start with a set of initial candidates
- consider a *stream* of instances
- sequentially evaluate candidates
- discard inferior candidates
  as sufficient evidence is gathered against them
- . . . repeat until a winner is selected
  or until computation time expires

The racing approach [Birattari et al., 2002]

How to discard?

Statistical testing!

- *F-Race:* Friedman two-way analysis of variance by ranks + Friedman post-hoc test [Conover, 1999]
- Alternative: paired t-test with/without p-value correction (against the best)

Some (early) applications of F-race

Vehicle routing and scheduling problem [Becker et al., 2005]
- first industrial application
- improved commercialized algorithm

International time-tabling competition [Chiarandini et al., 2006]
- winning algorithm configured by F-race
- interactive injection of new configurations

F-race in stochastic optimization [Birattari et al., 2006]
- evaluate "neighbors" using F-race
  (solution cost is a random variable)
- very good performance if variance of solution cost is high

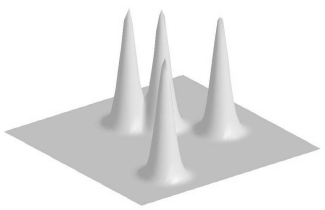
Sampling configuration

F-race is a method for the *selection of the best*
among a given set of algorithm configurations $\Theta_0 \subset \Theta$

How to sample algorithm configurations?

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

Iterative race: an illustration



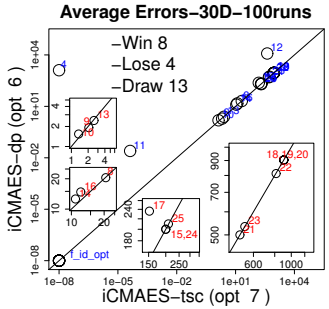
1: sample configurations from initial distribution
2: **while** not terminate() **do**
3: apply race
4: modify the distribution
5: sample configurations with selection probability

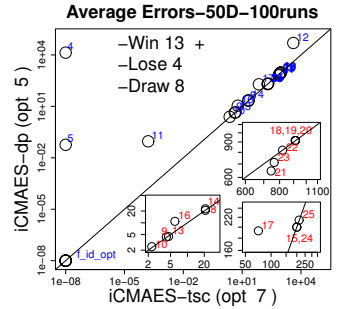
☞ more details, see part 2 of the tutorial

Example application: configuring IPOP-CMAES

[Liao et al., 2013]

- IPOP-CMAES is state-of-the-art continuous optimizer
- configuration done on benchmark problems (instances) distinct from test set (CEC'05 benchmark function set) using seven numerical parameters





Smit & Eiben [2010] configured another variant of IPOP-CMAES for three different objectives

Tuning in-the-loop: (re)design of continuous optimizers

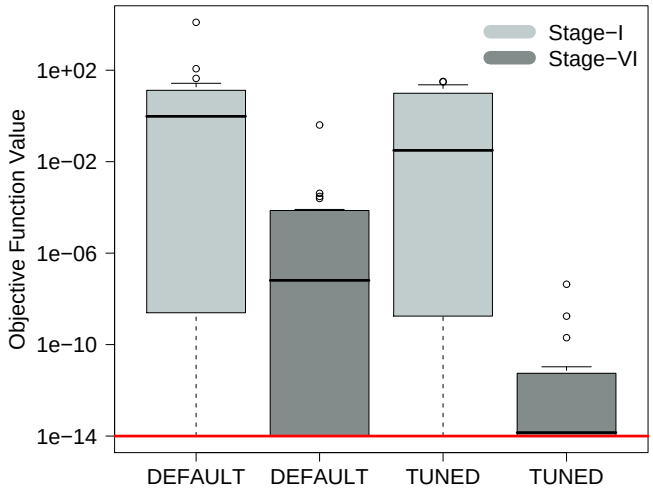
[Montes de Oca et al., 2011]

- re-design of an incremental PSO algorithm for large-scale continuous optimization
- steps: (1) local search, (2) call and control strategy of LS, (3) PSO rules, (4) bound constraint handling, (5) stagnation handling, (6) restarts
- iterated F-race used at each step to configure up to 10 parameters
- configuration done on 19 functions of dimension 10
- scaling examined until dimension 1000

configuration results may help the designer gain insight useful for further development

Tuning in-the-loop: (re)design of continuous optimizers

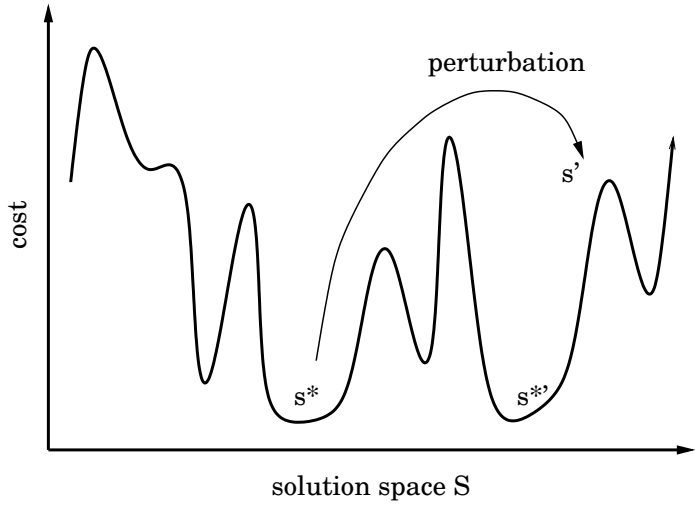
[Montes de Oca et al., 2011]



comparison on 100D, median values across 19 functions

ParamILS Framework [Hutter et al., 2007b, 2009]

ParamILS is an iterated local search method that works in the parameter space



Main design choices for ParamILS

Parameter encoding: only categorical parameters, numerical parameters need to be discretized

Initialization: select best configuration among default and several random configurations

Local search:
- 1-exchange neighborhood, where exactly one parameter changes a value at a time
- neighborhood is searched in random order

Perturbation: change several randomly chosen parameters

Acceptance criterion: always select the better configuration

Main design choices for ParamILS

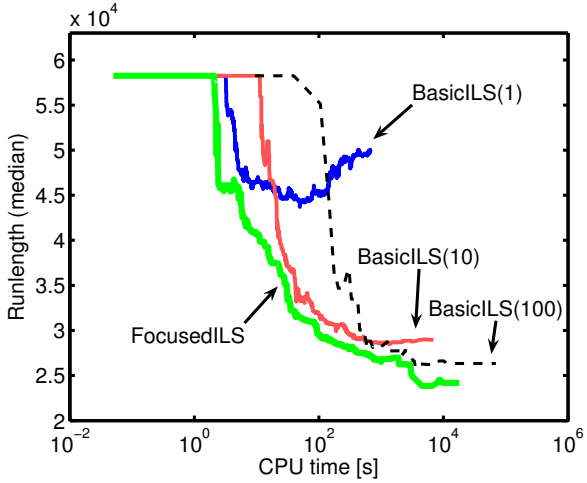
Evaluation of incumbent

- *BasicILS*: each configuration is evaluated on the same number of N instances
- *FocusedILS*: the number of instances on which the best configuration is evaluated increases at run time (intensification)

Adaptive Capping

- mechanism for early pruning the evaluation of poor candidate configurations
- particularly effective when configuring algorithms for minimization of computation time

ParamILS: BasicILS vs. FocusedILS



example: comparison of BasicILS and FocusedILS for configuring the SAPS solver for SAT-encoded quasi-group with holes, taken from [Hutter et al., 2007b]

Applications of ParamILS

- SAT-based verification [Hutter et al., 2007a]
  - SPEAR solver with 26 parameters
    $\Rightarrow$ speed-ups of up to 500 over default configuration
- Configuration of commercial MIP solvers [Hutter et al., 2010]
  - CPLEX (63 parameters), Gurobi (25 parameters) and lpsolve (47 parameters) for various instance distributions of MIP encoded optimization problems
  - speed-ups ranged between a factor of 1 (none) to 153

Mixed integer programming (MIP) solvers

[Hutter, Hoos, Leyton-Brown, and Stützle, 2009; Hutter, Hoos, and Leyton-Brown, 2010]

- MIP solvers widely used for tackling optimization problems
- powerful commercial (e.g. CPLEX) and non-commercial (e.g. SCIP) solvers
- large number of parameters (tens to hundreds)

Benchmark set	Default	Configured	Speedup
`Regions200`	72	10.5 (11.4 ± 0.9)	*6.8*
`Conic.SCH`	5.37	2.14 (2.4 ± 0.29)	*2.51*
`CLS`	712	23.4 (327 ± 860)	*30.43*
`MIK`	64.8	1.19 (301 ± 948)	*54.54*
`QP`	969	525 (827 ± 306)	*1.85*

FocusedILS, 10 runs, 2 CPU days, 63 parameters

Gender-based genetic algorithm [Ansótegui et al., 2009]

Parameter encoding

- variable structure that is inspired by *And*/*Or* trees
- *And* nodes separate variables that can be optimized independently
- instrumental for defining the crossover operator

Main details

- crossover between configurations from different sub-populations
- parallel evaluation of candidates supports early termination of poor performing candidates (inspired by racing / capping)
- designed for minimization of computation time

Promising initial results

Relevance Estimation and Value Calibration (REVAC)

[Nannen & Eiben, 2006; Smit & Eiben, 2009, 2010]

REVAC is an EDA for tuning *numerical* parameters

Main details

- variables are treated as independent
- multi-parent crossover of best parents to produce one child per iteration
- relevance of parameters is estimated by Shannon entropy

Extensions

- REVAC++ uses racing and sharpening [Smit & Eiben, 2009]
- training on more than one instance [Smit & Eiben, 2010]

Numerical optimization techniques

MADS / OPAL

- Mesh-adaptive direct search applied to parameter tuning of other direct-search methods [Audet & Orban, 2006]
- later extension to OPAL (*OP*timization of *AL*gorithms) framework [Audet et al., 2010]
- Limited experiments

Other continuous optimizers [Yuan et al., 2012, 2013]

- study of CMAES, BOBYQA, MADS, and irace for tuning continuous and quasi-continuous parameters
- BOBYQA best for few parameters; CMAES best for many
- post-selection mechanism appears promising

Model-based Approaches (SPOT, SMAC)

Idea: Use surrogate models to predict performance

Algorithmic scheme

1: generate and evaluate initial set of configurations Θ_0
2: choose best-so-far configuration $\theta^* \in \Theta_0$
3: **while** tuning budget available **do**
4: learn surrogate model $\mathcal{M}: \Theta \mapsto R$
5: use model $\mathcal{M}$ to generate promising configurations Θ_p
6: evaluate configurations in Θ_p
7: $\Theta_0 := \Theta_0 \cup \Theta_p$
8: update $\theta^* \in \Theta_0$
9: **output:** θ^*

Sequential parameter optimization (SPO) toolbox

[Bartz-Beielstein et al., 2005, 2010]

Main design decisions

- Gaussian stochastic processes for $\mathcal{M}$ (in most variants)
- Expected improv. criterion (EIC) $\Rightarrow$ promising configurations
- Intensification mechanism $\Rightarrow$ increase num. of evals. of θ^*

Practicalities

- SPO is implemented in the comprehensive SPOT R package
- Most applications to numerical parameters on one instance
- SPOT includes analysis and visualization tools

Sequential model-based algorithm configuration (SMAC)

[Hutter et al., 2011]

SMAC extends surrogate model-based configuration to complex algorithm configuration tasks and across multiple instances

Main design decisions

- Random forests for $\mathcal{M}$ $\Rightarrow$ categorical & numerical parameters
- Aggregate predictions from $\mathcal{M}_i$ for each instance i
- Local search on the surrogate model surface (EIC) $\Rightarrow$ promising configurations
- Instance features $\Rightarrow$ improve performance predictions
- Intensification mechanism (inspired by FocusedILS)
- Further extensions $\Rightarrow$ capping

Which method would you use?

- Only numerical parameters:
  - Homogeneous instances ⇒ numerical optimizers, e.g.,
    BOBYQA (few parameters), **CMA-ES** (many)
  - Expensive homogeneous instances ⇒ **SPO**
  - Heterogeneous instances ⇒
    numerical optimizers + (racing or post-selection)
- Categorical and numerical parameters
  - Tuning goal is time ⇒ **SMAC**
  - Tuning goal is quality ⇒ **IRACE**

Disclaimer: *This is a personal opinion based on our own experience*

AClib: A Benchmark Library for Algorithm Configuration

F. Hutter, M. López-Ibáñez, C. Fawcett, M. Lindauer, H. H. Hoos, K. Leyton-Brown and T. Stützle. **AClib: a Benchmark Library for Algorithm Configuration**, Learning and Intelligent Optimization Conference (LION 8), 2014.

http://www.aclib.net/

- Standard benchmark for experimenting with configurators
- 326 heterogeneous scenarios
- SAT, MIP, ASP, time-tabling, TSP, multi-objective, machine learning
- Extensible ⇒ new scenarios welcome !

Why automatic algorithm configuration?

- improvement over manual, ad-hoc methods for tuning
- reduction of development time and human intervention
- increased number of potential designs
- empirical studies, comparisons of algorithms
- support for end-users of algorithms

... and it has become feasible due
to increase in computational power!

Scaling to expensive instances

What if my problem instances are too difficult/large?

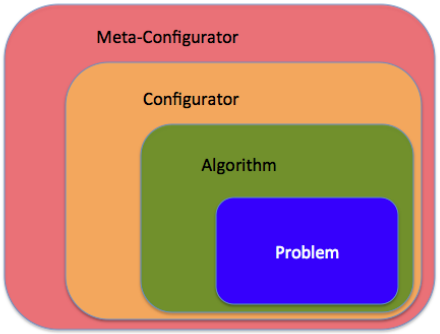
- Cloud computing / Large computing clusters
- J. Styles and H. H. Hoos. **Ordered racing protocols for automatically configuring algorithms for scaling performance.** GECCO, 2013

  Tune on easy instances,
  then ordered F-race on increasingly difficult ones
- F. Mascia, M. Birattari, and T. Stützle. **Tuning algorithms for tackling large instances: An experimental protocol.** Learning and Intelligent Optimization, LION 7, 2013.

  Tune on easy instances,
  then scale parameter values to difficult ones

Configuring configurators

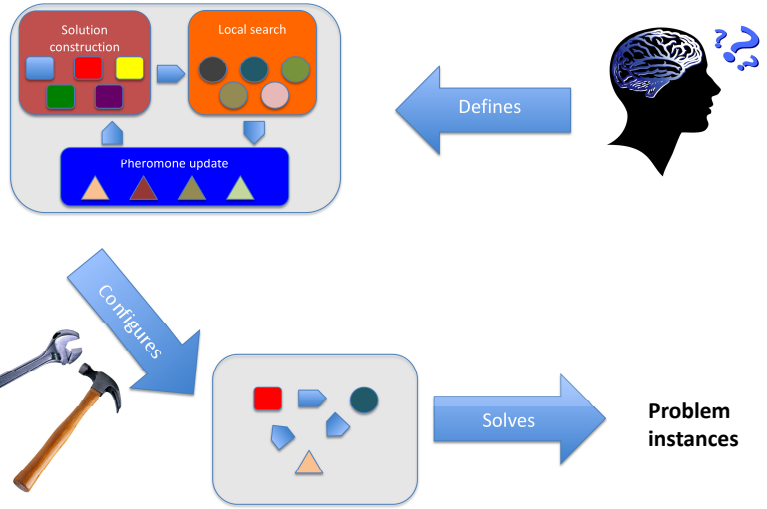
What about configuring automatically the configurator?
. . . and configuring the configurator of the configurator?



✔ it can be done [Hutter et al., 2009] but . . .

✘ it is costly and iterating further leads to diminishing returns

Towards a paradigm shift in algorithm design



Part II

Iterated Racing (irace)

What is Iterated Racing and irace?

Iterated Racing (irace)

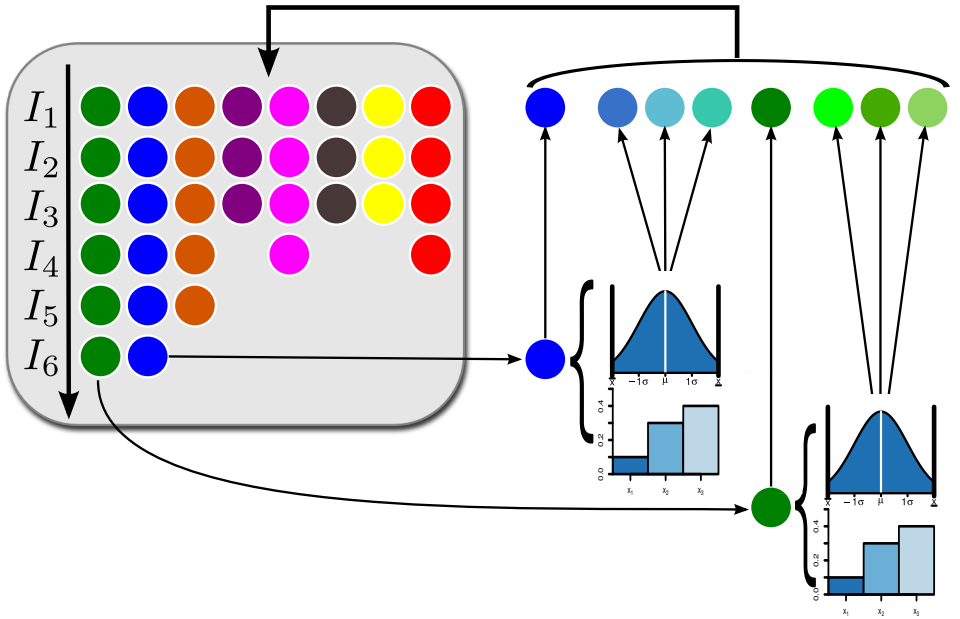
1. A variant of I/F-Race with several extensions
   - I/F-Race proposed by Balaprakash, Birattari, and Stützle [2007]
   - Refined by Birattari, Yuan, Balaprakash, and Stützle [2010]
   - Further refined and extended by López-Ibáñez, Dubois-Lacoste, Stützle, and Birattari [2011]
2. A software package implementing the variant proposed by López-Ibáñez, Dubois-Lacoste, Stützle, and Birattari [2011]

Iterated Racing

Iterated Racing $\supseteq$ I/F-Race

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

Iterated Racing



Iterated Racing: Sampling distributions

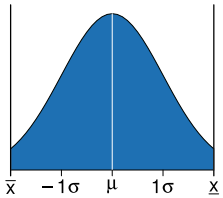
Numerical parameter $X_d \in [\underline{x}_d, \overline{x}_d]$

$\Rightarrow$ *Truncated normal distribution*

$$\mathcal{N}(\mu_d^z, \sigma_d^i) \in [\underline{x}_d, \overline{x}_d]$$

μ_d^z = value of parameter d in elite configuration z

σ_d^i = decreases with the number of iterations

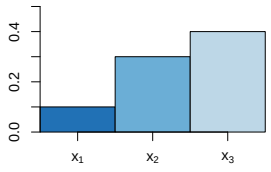


Categorical parameter $X_d \in \{x_1, x_2, \ldots, x_{n_d}\}$

$\Rightarrow$ *Discrete probability distribution*

$\Pr^z\{X_d = x_j\} =$

x_1	x_2	...	x_{n_d}
0.1	0.3	...	0.4



- Updated by increasing probability of parameter value in elite configuration
- Other probabilities are reduced

Iterated Racing: Soft-restart

✘ irace may converge too fast
⇒ the same configurations are sampled again and again

✔ Soft-restart !

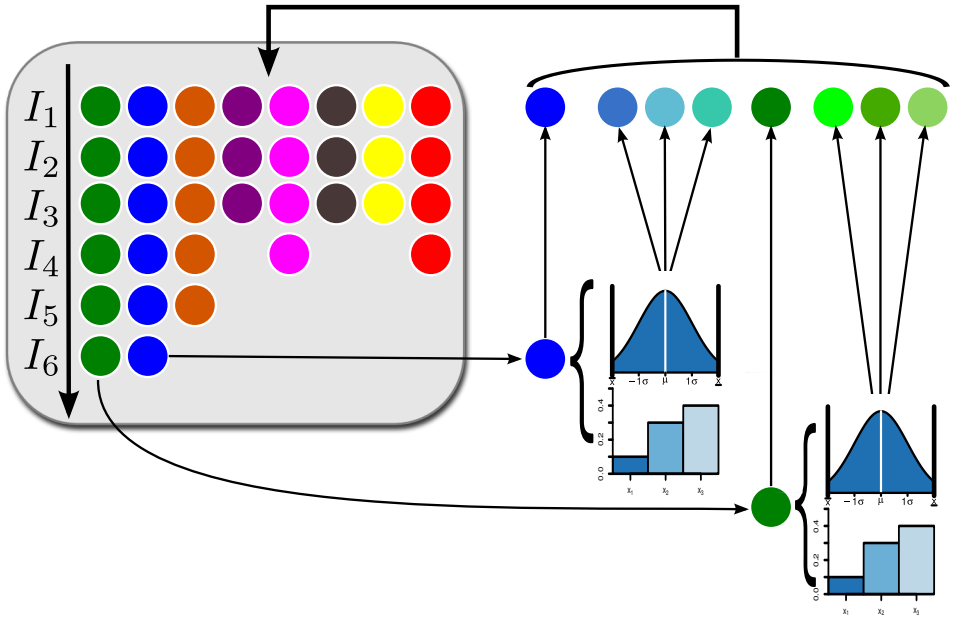
1. *Compute distance* between sampled candidate configurations
2. If distance is zero, *soft-restart* the sampling distribution of the parents
   Numerical parameters : σ_d^i is "brought back" to its value at two iterations earlier, approx. σ_d^{i-2}
   Categorical parameters : "smoothing" of probabilities, increase low values, decrease high values.
3. *Resample*

Iterated Racing: Elitist Iterated Racing [Pérez-Cáceres, et al.]

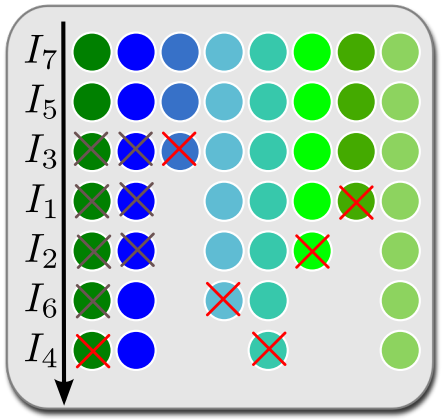
- ✘ irace may "*lose*" the best-so-far configuration
  ⇒ Each new iteration (race) forgets the results of the previous one
- ✔ Protect the best configurations (*elites*) from being discarded unless all their results are considered

1. after race i, elites were evaluated in I_e instances
2. race $i+1$ will start with $I_{new} \cup I_e$ instances
3. irace remembers the values of the elites on I_e
4. elites can only be discarded after alive configurations are evaluated on at least all $I_{new} \cup I_e$
   (similar to ParamILS's domination concept, but more strict)
5. non-elites are discarded as usual

Iterated Racing: Elitist Iterated Racing [Pérez-Cáceres, et al.]



Iterated Racing: Elitist Iterated Racing [Pérez-Cáceres, et al.]



Elitist iterated racing will be in irace 2.0

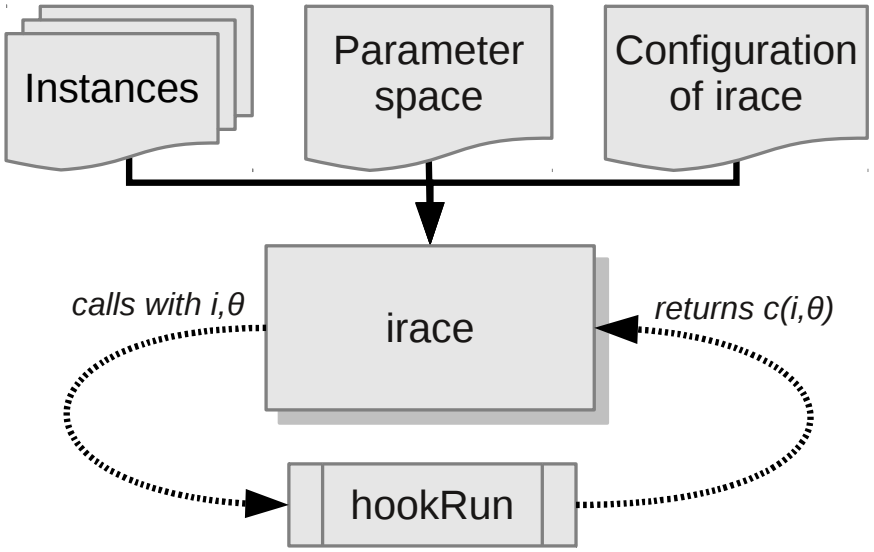
The irace Package

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

- Implementation of Iterated Racing in R
  Goal 1: Flexible
  Goal 2: Easy to use
- R package available at CRAN
- 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: 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`)

```
$ cat parameters.txt
```

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

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

The irace Package: Options

- *maxExperiments*: maximum number of runs of the target algorithm (tuning budget)
- *digits*: number of decimal places to be considered for the real parameters (default: 4)
- *testType*: either F-test or t-test
- *firstTest*: specifies how many instances are seen before the first test is performed (default: 5)
- *eachTest*: specifies how many instances are seen between tests (default: 1)

The irace Package: hook-run

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

```
./hook-run instance candidate-number candidate-parameters ...
```

- An R function

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

The irace Package: Other features

1. Initial configurations
   - seed irace with the default configuration
2. Parallel evaluation: MPI, multiple cores, Grid Engine / qsub
3. Forbidden configurations
   - `popsize < 5 & LS == "SA"`
4. Recovery file: allows resuming a previous irace run
5. Test instances *(new in 1.07)*
   - Specify not only the training instances but also test instances for comparing results

Example #1

ACOTSP

Example: ACOTSP

Thomas Stützle. **ACOTSP: A software package of various ant colony optimization algorithms applied to the symmetric traveling salesman problem**, 2002.

Command-line program:

```
$ ./acotsp -i instance -t 20 --mmas --ants 10 --rho 0.95 ...
```

Goal: find best parameter settings of ACOTSP for solving random Euclidean TSP instances with $n \in [500, 5000]$ within 20 CPU-seconds

Example: ACOTSP

```
$ cat parameters-acotsp.txt

# name       switch            type  values     conditions
algorithm    "--"              c (as,mmas,eas,ras,acs)
localsearch  "--localsearch "  c (0, 1, 2, 3)
alpha        "--alpha "        r (0.00, 5.00)
beta         "--beta "         r (0.00, 10.00)
rho          "--rho  "         r (0.01, 1.00)
ants         "--ants "         i (5, 100)
q0           "--q0 "           r (0.0, 1.0) | algorithm == "acs"
rasrank      "--rasranks "     i (1, 100)   | algorithm == "ras"
elitistants  "--elitistants "  i (1, 750)   | algorithm == "eas"
nnls         "--nnls "         i (5, 50)    | localsearch %in% c(1,2,3)
dlb          "--dlb "          c (0, 1)     | localsearch %in% c(1,2,3)
```


Example: ACOTSP

```
$ cat hook-run

#!/bin/bash
INSTANCE=$1
CANDIDATENUM=$2
CAND_PARAMS=$*
STDOUT="c${CANDIDATENUM}.stdout"
FIXED_PARAMS=" --time 1 --tries 1 --quiet "
acotsp $FIXED_PARAMS -i $INSTANCE $CAND_PARAMS 1> $STDOUT
COST=$(grep -oE 'Best [-+0-9.e]+' $STDOUT |cut -d' ' -f2)
echo "${COST}"
exit 0
```


Example: ACOTSP

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

instanceDir = "./Instances"
maxExperiments = 1000
digits = 2
```

✔ Good to go:

```
$ irace --parallel 2 --debug-level 1
```

- `--parallel` to execute in parallel
- `--debug-level` to see what irace is executing

Example: ACOTSP: and more

- Initial configurations:

```
$ cat default.txt

algorithm localsearch alpha beta rho  ants nnls dlb q0
as        0           1.0   1.0  0.95 10   NA   NA  NA
```

- Logical expressions that forbid configurations:

```
$ cat forbidden.txt

(alpha == 0.0) & (beta == 0.0)
```

Example #2

A more complex example:
MOACO framework

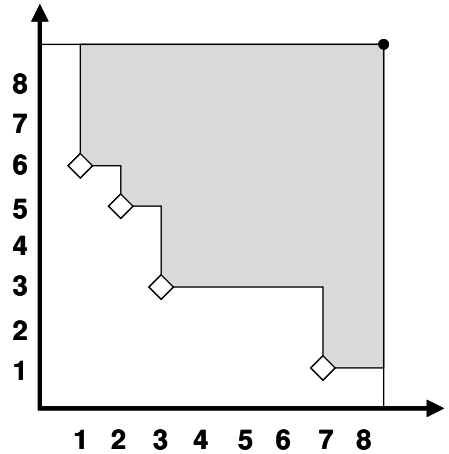
A more complex example: MOACO framework

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

- A flexible framework of multi-objective ACO algorithms
- Parameters controlling multi-objective algorithmic design
- Parameters controlling underlying ACO settings
- Instantiates 9 MOACO algorithms from the literature
- Hundreds of potential ~~papers~~ algorithm designs

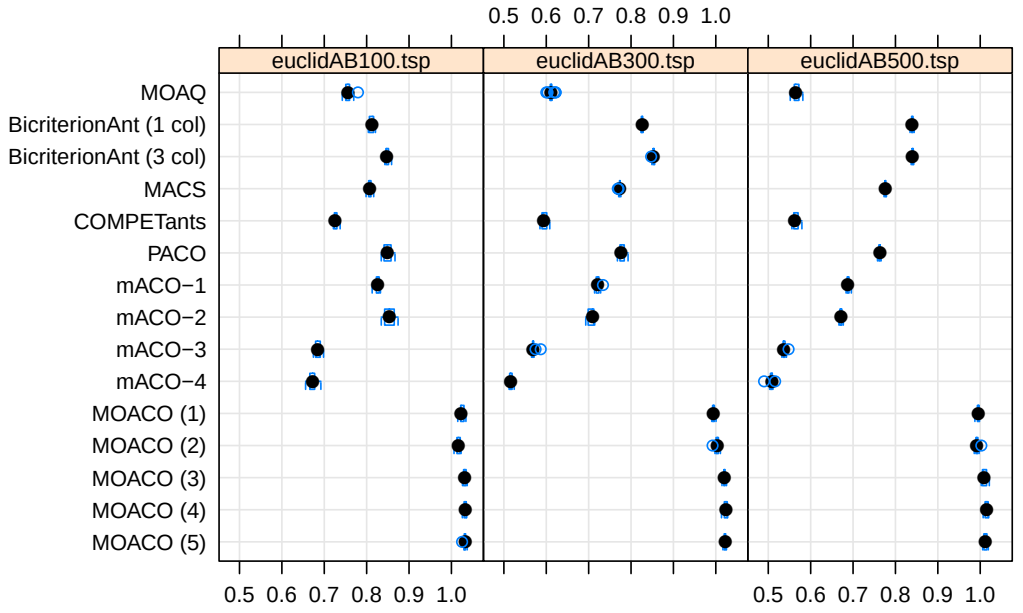
A more complex example: MOACO framework

✘ Multi-objective! Output is an approximation to the Pareto front!



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

Results: Multi-objective components



Summary

- ~~We propose a new MOACO algorithm that...~~
- We propose an approach to automatically design MOACO algorithms:
  1. Synthesize state-of-the-art knowledge into a flexible MOACO framework
  2. Explore the space of potential designs automatically using irace
- Other examples:
  - Single-objective top-down frameworks for MIP: CPLEX, SCIP
  - Single-objective top-down framework for SAT: SATenstein *[KhudaBukhsh, Xu, Hoos, and Leyton-Brown, 2009]*
  - Multi-objective automatic configuration with SPO *[Wessing, Beume, Rudolph, and Naujoks, 2010]*
  - Multi-objective framework for PFSP, TP+PLS *[Dubois-Lacoste, López-Ibáñez, and Stützle, 2011]*

Example #3

Automatically Improving the Anytime Behavior of Optimization Algorithms with irace

Automatically Improving the Anytime Behavior

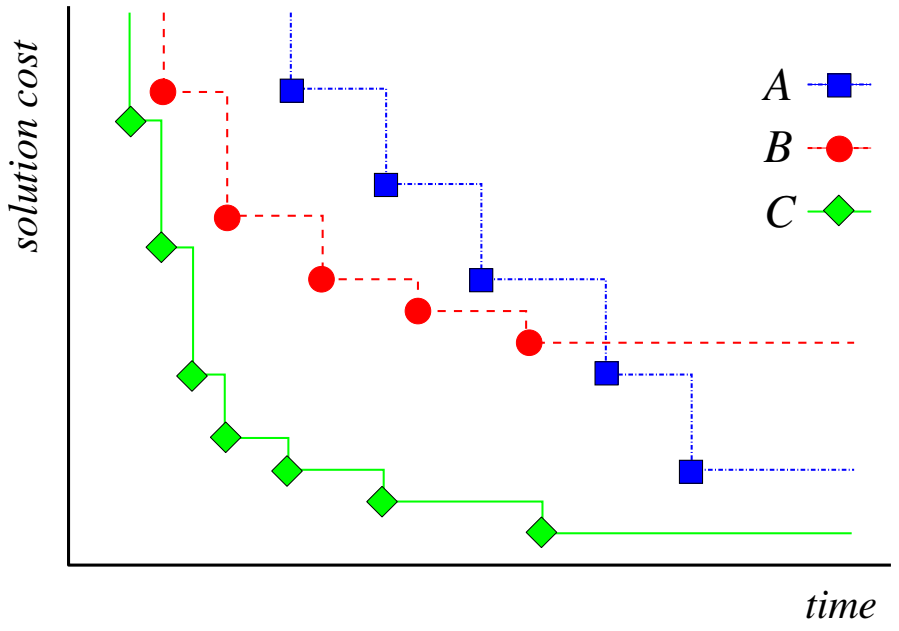
Anytime Algorithm [Dean & Boddy, 1988]

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

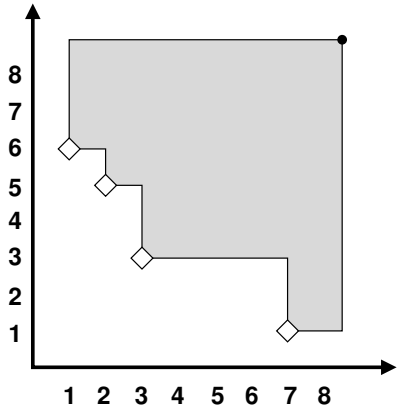
Good Anytime Behavior [Zilberstein, 1996]

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

Automatically Improving the Anytime Behavior



Automatically Improving the Anytime Behavior



Hypervolume measure $\approx$ Anytime behaviour

Manuel López-Ibáñez and Thomas Stützle.
Automatically improving the anytime behaviour of optimisation algorithms.
European Journal of Operational Research, 2014.

Automatically Improving the Anytime Behavior

Scenario #1

Online parameter adaptation to make an algorithm more robust to different termination criteria

- ✘ Which parameters to adapt? How? ⇒ More parameters!
- ✔ Use irace (offline) to select the best parameter adaptation strategies

Scenario #2

General purpose black-box solvers (CPLEX, SCIP, . . .)

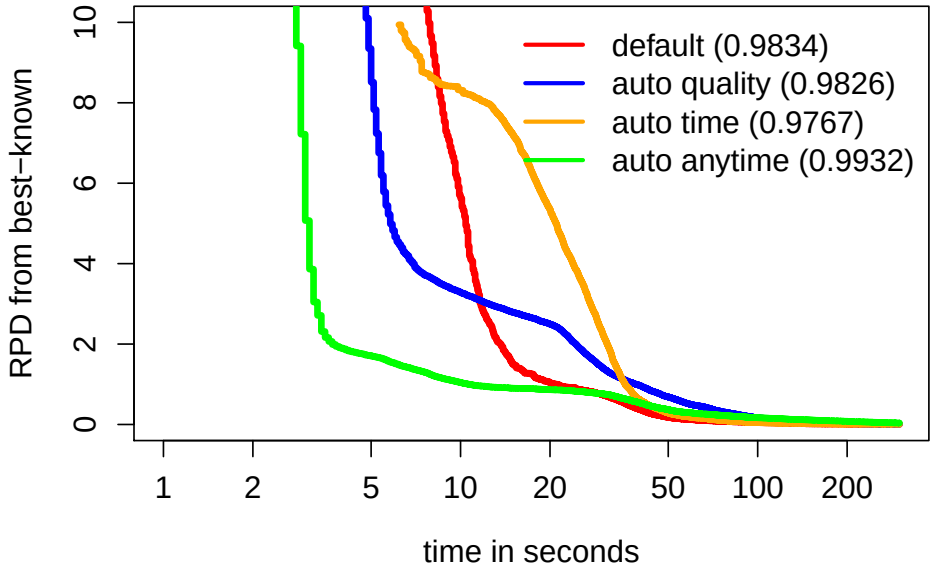
- Hundred of parameters
- Tuned by default for solving fast to *optimality*

Automatically Improving the Anytime Behavior

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

Automatically Improving the Anytime Behavior



Example #4

From Grammars to Parameters:
How to use irace to design algorithms from a grammar description?

Automatic Design of Algorithms: Top-down vs. Bottom-up

Top-down approaches

- Flexible frameworks:
  - *SATenstein* [KhudaBukhsh et al., 2009]
  - *MOACO framework* [López-Ibáñez and Stützle, 2012]
  - *MIP solvers: CPLEX, SCIP*
- Automatic configuration tools:
  - *ParamILS* [Hutter et al., 2009]
  - *irace* [Birattari et al., 2010; López-Ibáñez et al., 2011]

Bottom-up approaches

- Based on GP and trees [Vázquez-Rodríguez & Ochoa, 2010]
- Based on GP and Lisp-like S-expressions [Fukunaga, 2008]
- Based on GE and a grammar description [Burke et al., 2012]

Bottom-up approach using grammars + irace
[Mascia, López-Ibáñez, Dubois-Lacoste, and Stützle, 2014]

Iterated Greedy (IG) for One-Dimensional Bin Packing

Burke, E.K., Hyde, M.R., Kendall, G.: **Grammatical evolution of local search heuristics**. *IEEE Transactions on Evolutionary Computation* 16(7), 406–417 (2012)

```
<program> ::= <choosebins>
              remove_pieces_from_bins()
              <repack>

<choosebins> ::= <type> | <type> <choosebins>

<type> ::= highest_filled(<num>, <ignore>, <remove>)
         | lowest_filled(<num>, <ignore>, <remove>)
         | random_bins(<num>, <ignore>, <remove>)
         | gap_lessthan(<num>, <threshold>, <ignore>, <remove>)
         | num_of_pieces(<num>, <numpieces>, <ignore>, <remove>)

      <num> ::= 2 | 5 | 10 | 20 | 50
<threshold> ::= average | minimum | maximum
<numpieces> ::= 1 | 2 | 3 | 4 | 5 | 6
   <ignore> ::= 0.995 | 0.997 | 0.999 | 1.0 | 1.1
   <remove> ::= ALL | ONE
   <repack> ::= best_fit | worst_fit | first_fit
```


GE representation

codons = | 3 | 5 | 1 | 2 | 7 | 4 |

1. Start at <program>
2. Expand until rule with alternatives
3. Compute $(3 \bmod 2) + 1 = 2 \Rightarrow$ <type> <choosebins>
4. Compute $(5 \bmod 5) + 1 = 1 \Rightarrow$ highest_filled(<num>,)
5. ... until complete expansion or maximum number of wrappings

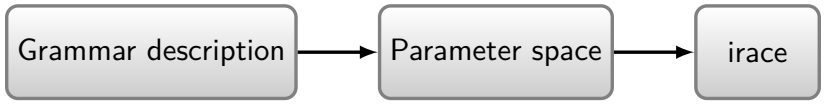
```
<program> ::= highest_filled(<num>, <ignore>)
              <choosebins>
              remove_pieces_from_bins()
              <repack>

      <num> ::= 2 | 5 | 10 | 20 | 50
```

Parametric representation

Parametric representation ⇒ Grammar expansion ?

```
--type highest-filled --num 5 --remove ALL ...
```



Grammar ⇒ Parameter space ?

Parametric representation

Grammar ⇒ Parameter space ?

- Rules without alternatives ⇒ no parameter

```
<highest_filled> ::= highest_filled(<num>, <ignore>)
```


Parametric representation

Grammar ⇒ Parameter space ?

- Rules with alternative choices ⇒ categorical parameters

```
<type> ::= highest_filled(<num>, <ignore>, <remove>)
         | lowest_filled(<num>, <ignore>, <remove>)
         | random_bins(<num>, <ignore>, <remove>)
```

becomes

```
--type (highest_filled, lowest_filled, random_bins)
```


Parametric representation

Grammar ⇒ Parameter space ?

- Rules with numeric terminals ⇒ numerical parameters

```
<num> ::= [0, 100]
```

becomes

```
--num   [0, 100]
```

Parametric representation

Grammar ⇒ Parameter space ?

- Rules that can be applied more than once
  ⇒ one extra parameter per application

```
<choosebins> ::= <type> | <type> <choosebins>
      <type> ::= highest(<num>) | lowest(<num>)
```

can be represented by

```
--type1   {highest, lowest}
--num1    (1, 5)
--type2   {highest, lowest, ""}
--num2    (1, 5)                    if type2 ≠ ""
--type3   {highest, lowest, ""}     if type2 ≠ ""
...       ...
```


Summary

✔ irace works better than GE for designing IG algorithms for bin-packing and PFSP-WT

Franco Mascia, Manuel López-Ibáñez, Jérémie Dubois-Lacoste, and Thomas Stützle.
Grammar-based Generation of Stochastic Local Search Heuristics Through Automatic Algorithm Configuration Tools. *Computers & Operations Research*, 2014.

✔ Not limited to IG!

Marie-Eléonore Marmion, Franco Mascia, Manuel López-Ibáñez, and Thomas Stützle.
Automatic Design of Hybrid Stochastic Local Search Algorithms.
In *Hybrid Metaheuristics*, vol. 7919 of LNCS, 2013.

An overview of applications of irace

Done already

- Parameter tuning
  - single-objective optimization metaheuristics
  - MIP solvers (SCIP) with > 200 parameters.
  - multi-objective optimization metaheuristics
  - anytime algorithms (improve time-quality trade-offs)
- Automatic algorithm design
  - From a flexible framework of algorithm components
  - From a grammar description
- Machine learning
  - Automatic model selection for high-dimensional survival analysis [Lang et al., 2014]
  - Hyperparameter tuning (mlr R package, Bischl et al.)

An overview of applications of irace

irace (and others) works great for

- Complex parameter spaces:
  numerical, categorical, ordinal, subordinate (conditional)
- Large parameter spaces (few hundred parameters)
- Heterogeneous instances
- Medium to large tuning budgets (thousands of runs)
- Individual runs require from seconds to hours
- Multi-core CPUs, MPI, Grid-Engine clusters

An overview of applications of irace

What we haven't deal with yet

- Extremely large parameter spaces (thousands of parameters)
- Extremely heterogeneous instances
- Small tuning budgets (500 or less runs)
- Very large tuning budgets (millions of runs)
- Individual runs require days
- Parameter tuning of decision algorithms / minimize time

We are looking for interesting benchmarks / applications!
Talk to us!

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Questions

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

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