

Automated Offline Design of Algorithms

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Part I

Automatic Algorithm Configuration (Overview)

Instructors

Manuel López-Ibáñez is a lecturer (Assistant Professor) at the Alliance Manchester Business School, University of Manchester, UK. He received the M.S. degree in computer science from the University of Granada, Granada, Spain, in 2004, and the Ph.D. degree from Edinburgh Napier University, U.K., in 2009. Between 2011 and 2015, he was a Postdoctoral Researcher of the Belgian F.R.S.-FNRS at the IRIDIA laboratory in the Université Libre de Bruxelles (ULB), Brussels, Belgium.



Thomas Stützle is a senior research associate of the Belgian F.R.S.-FNRS working at the IRIDIA laboratory of Université libre de Bruxelles (ULB), Belgium. He received the Diplom (German equivalent of M.S. degree) in business engineering from the Universität Karlsruhe (TH), Karlsruhe, Germany in 1994, and his PhD and his habilitation in computer science both from the Computer Science Department of Technische Universität Darmstadt, Germany, in 1998 and 2004, respectively. He is the co-author of two books about "Stochastic Local Search: Foundations and Applications" and "Ant Colony Optimization". His 2002 GECCO paper "A Racing Algorithm For Configuring Metaheuristics" (joint work with M. Birattari, L. Paquete, and K. Varrentapp) received the 2012 SIGEVO impact award.



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Automated Offline Design of Algorithms

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

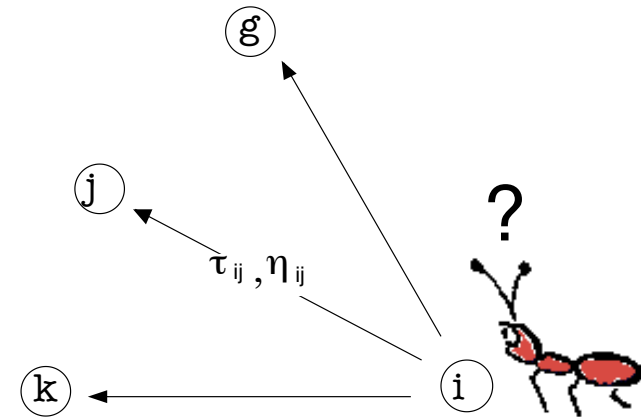
Very active research on hybrids of exact/approximate algorithms!

Design choices and parameters everywhere

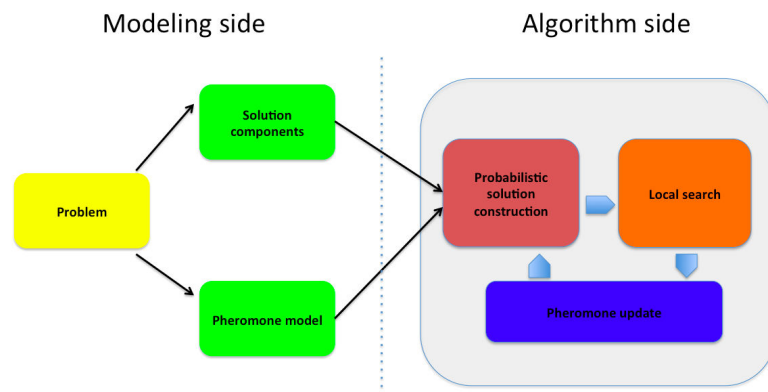
Modern high-performance optimizers involve a large number of design choices and parameter settings

- 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

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

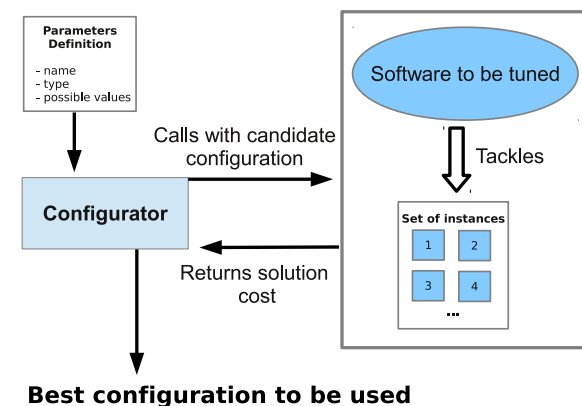
Can we make this approach more principled and automatic?

Towards automatic 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



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]

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

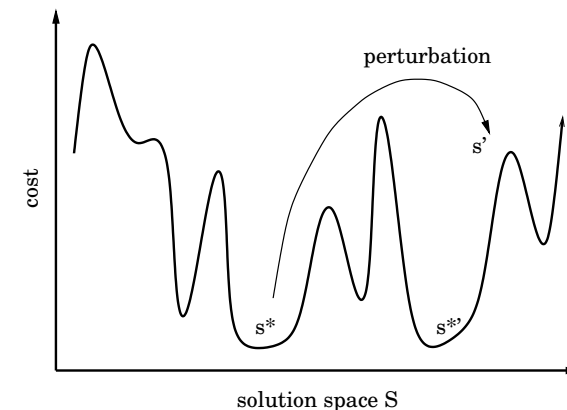
Other continuous optimizers [Yuan et al., 2012, 2013]

- 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

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

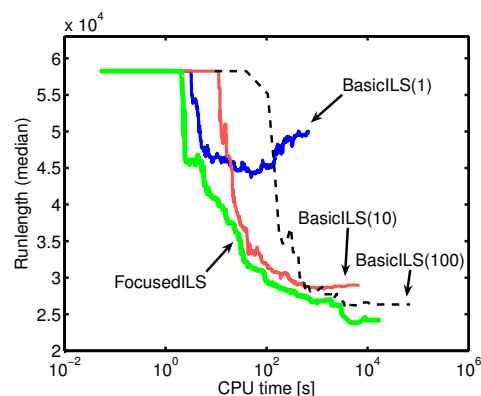
Evaluation of incumbent

- **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

The danger of over-tuning



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
 - ⇒ 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 Ipsolve (47 parameters) for various instance distributions of MIP encoded optimization problems
 - speed-ups ranged between a factor of 1 (none) to 153

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: generate set of possible candidate configurations Θ
- 6: use model $\mathcal{M}$ to filter promising configurations $\Theta_p \subseteq \Theta$
- 7: evaluate configurations in Θ_p
- 8: $\Theta_0 := \Theta_0 \cup \Theta_p$
- 9: update $\theta^* \in \Theta_0$
- 10: **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 various analysis and visualization tools

Sequential model-based algorithm configuration (SMAC)

[Hutter et al., 2011]

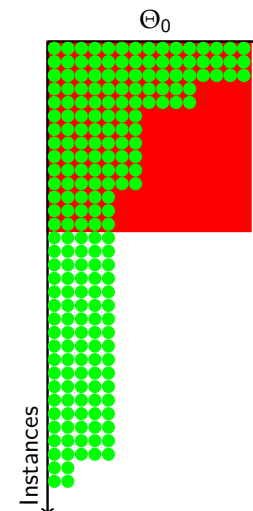
SMAC extends surrogate model-based configuration to complex algorithm configuration tasks and across multiple instances

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

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

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)

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
⇒ *Iterated F-Race (I/F-Race)* [Balaprakash et al., 2007]

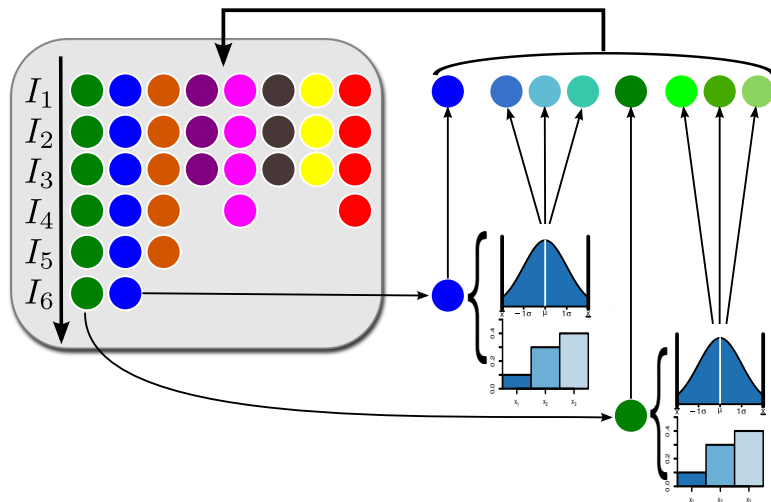
Iterated Racing (irace)

- 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]
 - Elitist variant proposed by López-Ibáñez, Dubois-Lacoste, Pérez Cáceres, Stützle, and Birattari [2016]
- 2 A software package implementing the latest variants.

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



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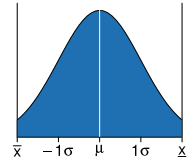
Iterated Racing: Sampling distributions

Numerical parameter $X_d \in [\underline{x}_d, \bar{x}_d]$
 $\Rightarrow$ *Truncated normal distribution*

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

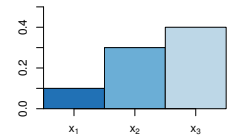
μ_d^z = value of parameter d in elite configuration z

σ_d^i = decreases with the number of iterations



Categorical parameter $X_d \in \{x_1, x_2, \dots, x_{n_d}\}$
 $\Rightarrow$ *Discrete probability distribution*

$$\Pr^z\{X_d = x_j\} = \begin{matrix} x_1 & x_2 & \dots & x_{n_d} \\ 0.1 & 0.3 & \dots & 0.4 \end{matrix}$$



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

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Elitist Iterated Racing

[López-Ibáñez et al., 2016]

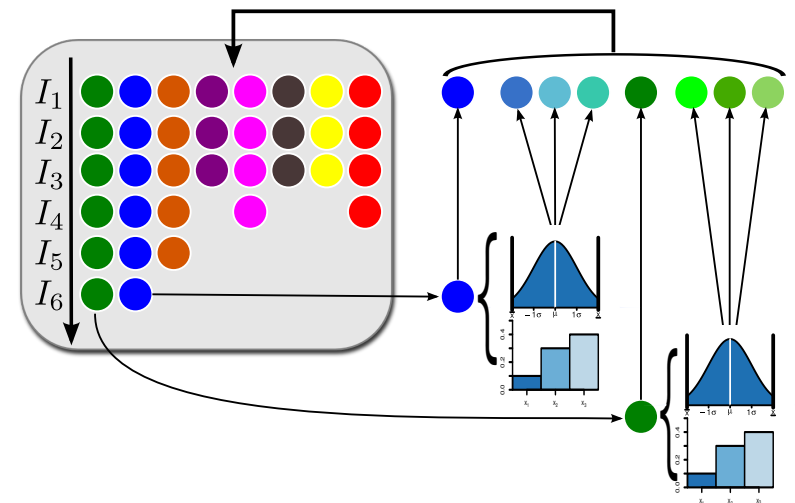
- ✗ Iterated F-race may “lose” the best-so-far configuration
 $\Rightarrow$ Each new iteration (race) forgets the results of the previous one
 - ✓ Protect the best configurations (*elites*) from being discarded unless all their results are considered
- 1 after race i , elites were evaluated in I_e instances
 - 2 race $i + 1$ will start with $I_{\text{new}} \cup I_e$ 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 $I_{\text{new}} \cup I_e$
(similar to ParamILS’s domination concept, but more strict)
 - 5 non-elites are discarded as usual

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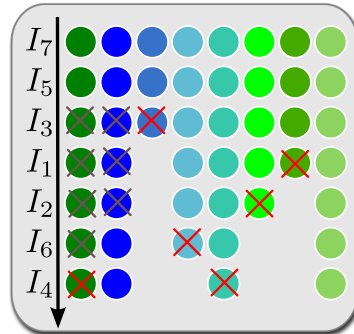
Elitist Iterated Racing

[López-Ibáñez et al., 2016]



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

- Implementation of Iterated Racing in R

Goal 1: Flexible

Goal 2: Easy to use

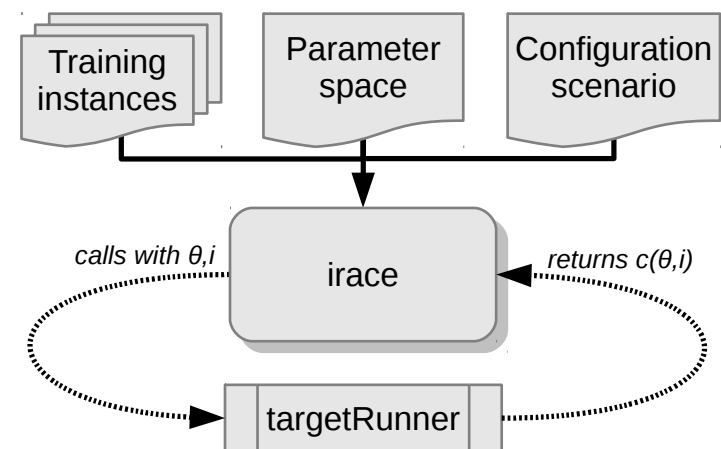
- R package available at CRAN

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

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

- ✓ No knowledge of R needed

- Elitist irace by default
- New interfaces with more intuitive names
- A detailed user-guide / tutorial:
<https://cran.r-project.org/web/packages/irace/vignettes/irace-package.pdf>
- Available from CRAN (GNU/Linux, Windows, OSX)
<https://cran.r-project.org/package=irace>
- Google group
<https://groups.google.com/forum/#!forum/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**)

```
$ 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: target-runner

- 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
 - ✓ “seed” irace with the default configuration
- 2 Parallel evaluation: MPI, multiple cores, batch job clusters (SGE, PBS, Torque, Slurm)
- 3 Forbidden configurations:

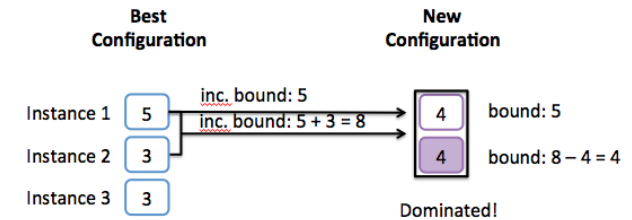
popsize < 5 & LS == "SA"
- 4 Recovery file: allows resuming an interrupted irace run
- 5 Test instances
 - ✓ Specify not only the training instances but also test instances for comparing results
- 6 Repair configurations before being evaluated (2.2)

Forthcoming version 3.0

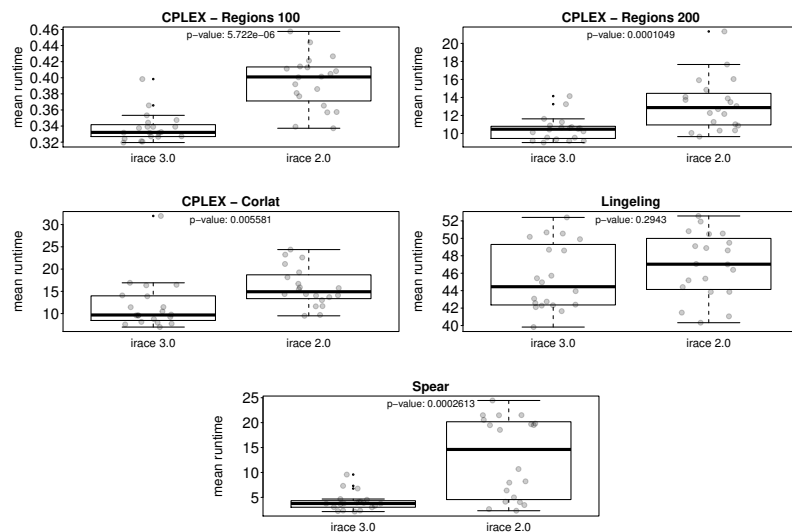
[Pérez Cáceres, López-Ibáñez, Hoos, and Stützle, 2017]

- Extension of irace to better handle run-time minimization
- Dominance: configuration θ_1 *dominates* θ_2 if

$$N_1 > N_2 \quad \text{and} \quad C(\theta_1, 1 \dots N_2) \leq C(\theta_2, 1 \dots N_2)$$
- Trajectory preserving capping



irace 3.0 vs. irace 2.0



An overview of applications of irace

- Parameter tuning
 - Exact MIP solvers (CPLEX, SCIP with > 200 parameters)
 - single-objective optimization metaheuristics
 - 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 [Miranda et al., 2014] (mlr R package, Bischl et al.)
- Automatic design of control software for robots [Francesca et al., 2015]

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 target runs)
- Target 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 target runs)
- Very large tuning budgets (millions of target runs)
- Target runs require days

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

Conclusions

“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)]

”

Part II

Automated Algorithm Design

Example #1

Example #1: Tuning 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	Label/switch	Type	Domain	Condition
	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 target-runner
```

```
#!/bin/bash
CONFIG.ID=$1
INSTANCE.ID=$2
SEED=$3
INSTANCE=$4
CONFIG.PARAMS=$*
FIXED.PARAMS=" --time 1 --tries 1 --quiet "
STDOUT="c$CONFIG.ID-$INSTANCE.ID.stdout"
acotsp $FIXED.PARAMS -i $INSTANCE --seed $SEED \
    $CONFIG.PARAMS > $STDOUT
COST=$(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 scenario.txt

trainInstancesDir = "./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

Configuring known algorithms

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)

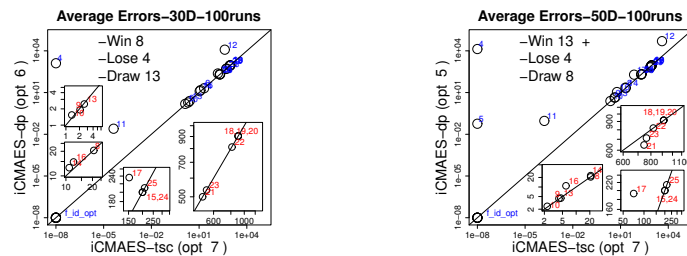
Benchmark set	Default	Configured	Speedup
Regions200	72	10.5 (11.4 ± 0.9)	6.8
Conic.SCH	5.37	2.14 (2.4 ± 0.29)	2.51
CLS	712	23.4 (327 ± 860)	30.43
MIK	64.8	1.19 (301 ± 948)	54.54
QP	969	525 (827 ± 306)	1.85

FocusedILS, 10 runs, 2 CPU days, 63 parameters

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

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Example #3

Automatically Improving the Anytime Behavior of Optimization Algorithms with irace

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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

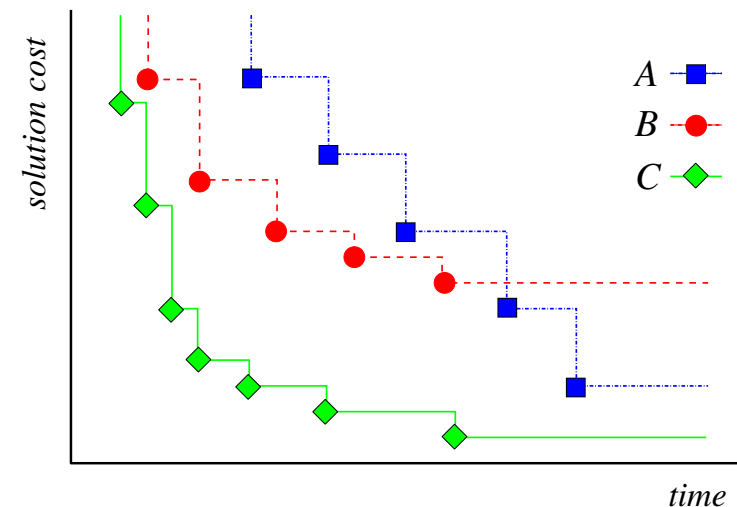
[Zilberstein, 1996]

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

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Automated Offline Design of Algorithms

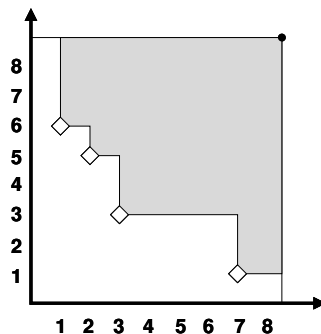
Automatically Improving the Anytime Behavior



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Automated Offline Design of Algorithms

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.

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

*Offline configuration techniques can be helpful
to configure online parameter control strategies*

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? $\Rightarrow$ 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*

Scenario #1: Brute-Force Approach

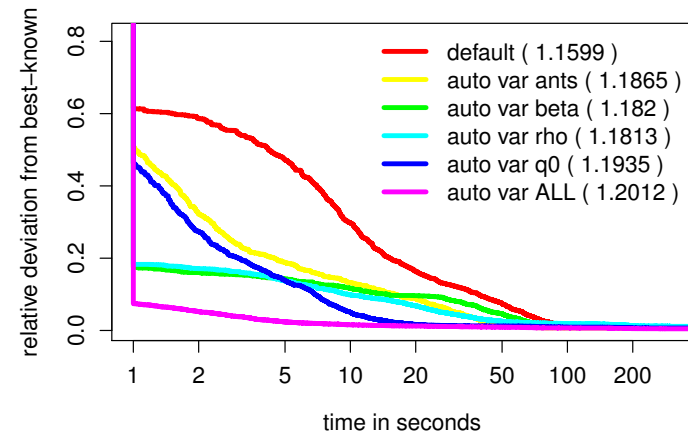
- 1 Devise *many* online strategies for parameter variation
- 2 Run lots of experiments
- 3 Visually compare SQT plots

After about year and a master thesis:

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

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*

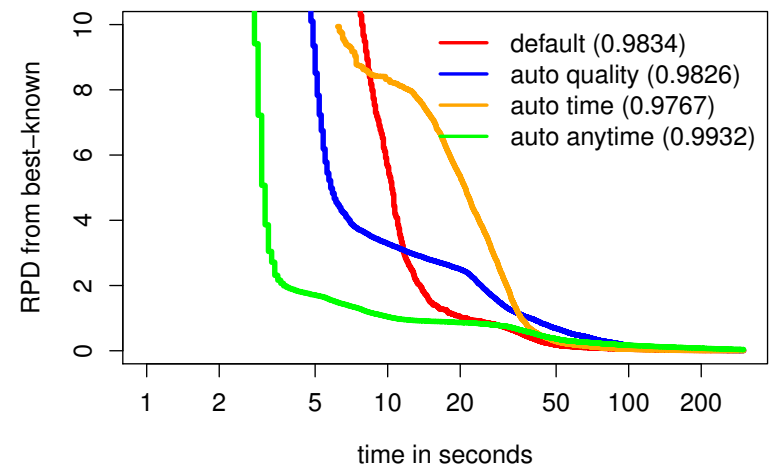


Scenario #2: SCIP

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]
1000 training + 1000 testing instances
- Single run timeout: 300 seconds
- irace budget (*maxExperiments*): 5000 runs

Scenario #2: SCIP



Example #4

Integration in algorithm (re-)engineering process

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

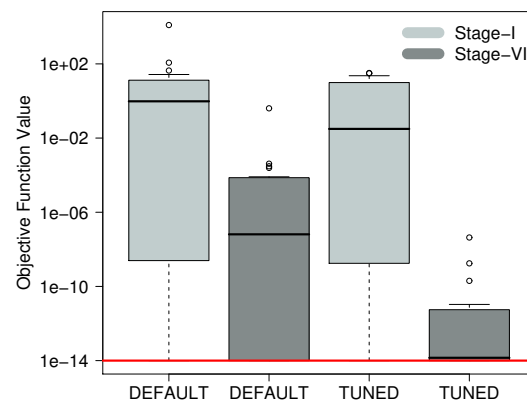
[Montes de Oca et al., 2011]

- 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

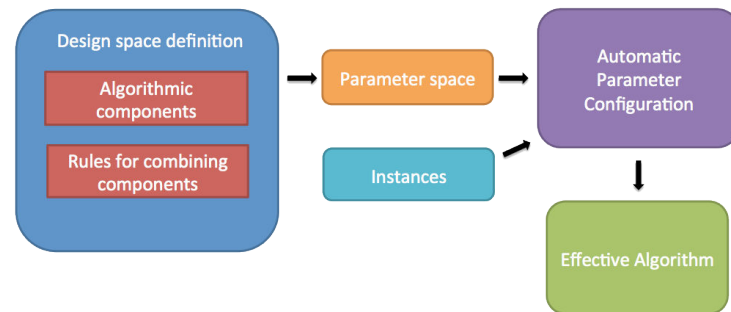
Tuning in-the-loop: (re)design of continuous optimizers

[Montes de Oca et al., 2011]



Automated design from (flexible) algorithm frameworks

General approach



Main approaches

Top-down approaches

- develop flexible framework following a fixed algorithm template with alternatives
- apply high-performing configurators
- Examples: Satenstein, MOACO, AutoMOEA, MIP Solvers

Bottom-up approaches

- flexible framework implementing algorithm components
- define rules for composing algorithms from components e.g. through grammars
- frequently usage of genetic programming, grammatical evolution etc.

Example #5

A more complex example: MOACO framework

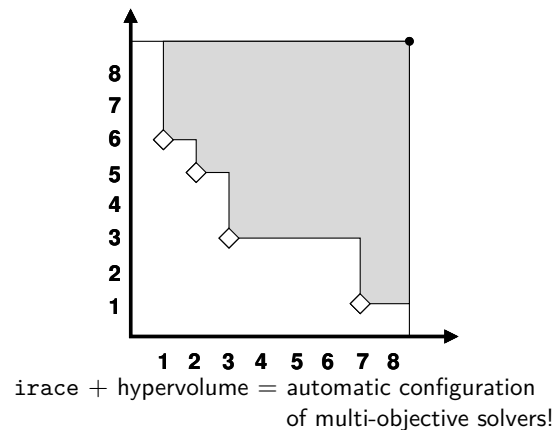
A more complex example: MOACO framework

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

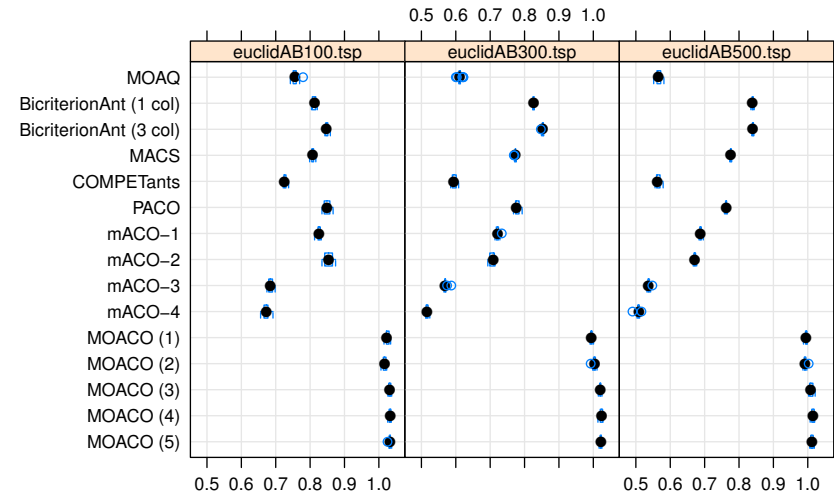
- A flexible framework of multi-objective ACO algorithms
- Parameters controlling multi-objective algorithmic design
- Parameters controlling underlying ACO settings
- Instantiates 9 MOACO algorithms from the literature
- Hundreds of potential **papers** algorithm designs

A more complex example: MOACO framework

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



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 #6

Top-down design approach: AutoMOEA

AutoMOEA

- ✓ Replicate as many well-known MOEAs as possible from the same *template*
- ✓ The template has a number of configurable algorithmic *components*
- ✓ Each component can be configured by choosing one *option* from various alternatives
- ✓ Aim to maximise the number of different configurations that are valid MOEAs



Leonardo C. T. Bezerra, Manuel López-Ibáñez, and Thomas Stützle.

Automatic Component-Wise Design of Multi-Objective Evolutionary Algorithms.
IEEE Transactions on Evolutionary Computation, 2016.

AutoMOEA: A MOEA template

```

1: pop ← Initialization ()
2: if type(pop_ext) != none then
3:   pop_ext ← pop
4: repeat
5:   pool ← BuildMatingPool (pop)
6:   pop_new ← Variation (pool)
7:   pop_new ← Evaluation (pop_new)
8:   pop ← Replacement (pop, pop_new)
9:   if type(pop_ext) == bounded then
10:    pop_ext ← Archiving (pop_ext, pop_new)
11:   else if type(pop_ext) == unbounded then
12:    pop_ext ← pop_ext ∪ pop
13: until termination criteria met
14: if type(pop_ext) == none then
15:   return pop
16: else
17:   return pop_ext

```

AutoMOEA: Main components

Component	Parameters
BuildMatingPool	$\langle \text{Preference}_{Mat}, \text{Selection} \rangle$
Replacement	$\langle \text{Preference}_{Rep}, \text{Removal} \rangle$
Archiving	$\langle \text{Preference}_{Ext}, \text{Removal}_{Ext} \rangle$
Preference	$\langle \text{Fitness}, \text{Diversity} \rangle$

Algorithm	Fitness	Diversity
NSGA-II	dominance depth	crowding distance
SPEA2	dom. strength	kNN
IBEA	binary indicator	
HypE		I_H^h
SMS-EMOA	dom. depth-rank	I_H^l

AutoMOEA: Redesign of main components [Zitzler et al., 2010]

Component	Parameters
BuildMatingPool	$\langle \text{Preference}_{Mat}, \text{Selection} \rangle$
Replacement	$\langle \text{Preference}_{Rep}, \text{Removal} \rangle$
Archiving	$\langle \text{Preference}_{Ext}, \text{Removal}_{Ext} \rangle$
Preference	$\langle \text{Fitness}, \text{Diversity} \rangle$ $\langle \text{Set-partitioning}, \text{Quality}, \text{Diversity} \rangle$

	BuildMatingPool			Replacement		
	SetPart	Quality	Diversity	SetPart	Quality	Diversity
MOGA	dom. rank	—	niche-sharing	—	—	—
NSGA-II	dom. depth	—	crowding dist.	dom. depth	—	crowding dist.
SPEA2	dom. strength	—	kNN	dom. strength	—	kNN
IBEA	—	binary indicator	—	—	binary ind.	—
HypE	—	I_H^h	—	dom. depth	I_H^h	—
SMS-EMOA	—	—	—	dom. depth-rank	I_H^l	—

AutoMOEA: Automatic Design

Automatic configuration ([irace](#))
 + Flexible algorithmic framework (AutoMOEA)
 = Automatic design of state-of-the-art MOEAs

BuildMatingPool				Replacement		
SetPart	Quality	Diversity	SetPart	Quality	Diversity	
MOGA	rank	—	niche-sharing	—	—	—
NSGA-II	depth	—	crowding dist.	depth	—	crowding dist.
SPEA2	strength	—	kNN	strength	—	kNN
IBEA	—	binary indicator	—	—	binary ind.	—
HypE	—	I_H^h	—	depth	I_H^h	—
SMS-EMOA	—	—	depth-rank	I_H^h	—	—
DTLZ 2-obj	—	—	crowding	depth-rank	I_ϵ	sharing
DTLZ 3-obj	depth-rank	I_ϵ	kNN	rank	I_H^1	sharing
DTLZ 5-obj	rank	I_H^1	crowding	depth	I_H^1	—
WFG 2-obj	rank	—	crowding	depth-rank	I_H^1	—
WFG 3-obj	count	I_H^1	crowding	strength	I_H^1	sharing
WFG 5-obj	count	I_H^h	crowding	—	I_H^1	—

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Experimental results

DTLZ			WFG		
2-obj $\Delta R = 126$	3-obj $\Delta R = 127$	5-obj $\Delta R = 107$	2-obj $\Delta R = 169$	3-obj $\Delta R = 130$	5-obj $\Delta R = 97$
Autop₂ (1339)	Autop₃ (1500)	Autop₅ (1002)	Autow₂ (1692)	Autow₃ (1375)	Autow₅ (1170)
SPEA2 _{D2} (1562)	IBEA _{D3} (1719)	SMS _{D5} (1550)	SPEA2 _{W2} (2097)	SMS _{W3} (1796)	SMS _{W5} (1567)
IBEA _{D2} (1940)	SMS _{D3} (1918)	IBEA _{D5} (1867)	NSGA-II _{W2} (2542)	IBEA _{W3} (1843)	IBEA _{W5} (1746)
NSGA-II _{D2} (2143)	HypE _{D3} (2019)	SPEA2 _{D5} (2345)	SMS _{W2} (2621)	SPEA2 _{W3} (2600)	SPEA2 _{W5} (2747)
HypE _{D2} (2338)	SPEA2 _{D3} (2164)	NSGA-II _{D5} (2346)	IBEA _{W2} (2777)	NSGA-II _{W3} (3315)	NSGA-II _{W5} (3029)
SMS _{D2} (2406)	NSGA-II _{D3} (2528)	HypE _{D5} (2674)	HypE _{W2} (2851)	HypE _{W3} (3431)	MOGA _{W5} (4268)
MOGA _{D2} (2970)	MOGA _{D3} (2851)	MOGA _{D5} (2915)	MOGA _{W2} (4320)	MOGA _{W3} (4540)	HypE _{W5} (4373)

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AutoMOEA: Automatic Design

Automatic configuration ([irace](#))
 + Flexible algorithmic framework (AutoMOEA)
 = Automatic design of state-of-the-art MOEAs

- Fair to compare with untuned traditional MOEAs?
- Why is our setup representative?
 ⇒ Different AutoMOEAs for termination criterion in FEs or seconds
- How do you define “state-of-the-art”?
- What is a “novel” MOEA?

Exactly!

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Automatic Design: The End of the Game

“The Journal of Heuristics does not endorse the up-the-wall game. [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?

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Example #7

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

Automatic design of hybrid SLS algorithms

[Marmion, Mascia, López-Ibáñez, Stützle, 2013]

Approach

- decompose single-point SLS methods into components
- derive generalized metaheuristic structure
- component-wise implementation of metaheuristic part

Implementation

- present possible algorithm compositions by a grammar
- instantiate grammar using a parametric representation
 - allows use of standard automatic configuration tools
 - shows good performance when compared to, e.g., grammatical evolution [Mascia, López-Ibáñez, Dubois-Lacoste, and Stützle, 2014]

General Local Search Structure: ILS

```
s0 := initSolution
s* := ls(s0)
repeat
  s' := perturb(s*, history)
  s*' := ls(s')
  s* := accept(s*, s*', history)
until termination criterion met
```

- many SLS methods instantiable from this structure
- abilities
 - hybridization through recursion
 - problem specific implementation at low-level
 - separation of generic and problem-specific components

Example instantiations of some metaheuristics

	<i>perturb</i>	<i>ls</i>	<i>accept</i>
SA	random move	∅	Metropolis
PII	random move	∅	Metropolis, fixed T
TS	∅	TS	∅
ILS	any	any	any
IG	destruct/construct	any	any
GRASP	rand. greedy sol.	any	∅

Grammar

```

<algorithm> ::= <initialization> <ils>
<initialization> ::= random | <pbs_initialization>
<ils> ::= ILS(<perturb>, <ls>, <accept>, <stop>)

<perturb> ::= none | <initialization> | <pbs_perturb>
<ls> ::= <ils> | <descent> | <sa> | <rii> | <pii> | <vns> | <ig> | <pbs_ls>
<accept> ::= alwaysAccept | improvingAccept <comparator>
           | prob(<value_prob_accept>) | probRandom | <metropolis>
           | threshold(<value_threshold_accept>) | <pbs_accept>

<descent> ::= bestDescent(<comparator>, <stop>)
           | firstImprDescent(<comparator>, <stop>)
<sa> ::= ILS(<pbs_move>, no_ls, <metropolis>, <stop>)
<rii> ::= ILS(<pbs_move>, no_ls, probRandom, <stop>)
<pii> ::= ILS(<pbs_move>, no_ls, prob(<value_prob_accept>), <stop>)
<vns> ::= ILS(<pbs_variable_move>, firstImprDescent(improvingStrictly),
           improvingAccept(improvingStrictly), <stop>)
<ig> ::= ILS(<deconst-construct_perturb>, <ls>, <accept>, <stop>)

<comparator> ::= improvingStrictly | improving
<value_prob_accept> ::= [0, 1]
<value_threshold_accept> ::= [0, 1]
<metropolis> ::= metropolisAccept(<init_temperature>, <final_temperature>,
                                <decreasing_temperature_ratio>, <span>)

<init_temperature> ::= {1, 2, ..., 10000}
<final_temperature> ::= {1, 2, ..., 100}
<decreasing_temperature_ratio> ::= [0, 1]
<span> ::= {1, 2, ..., 10000}

```

Grammar

```

<algorithm> ::= <initialization> <ils>
<initialization> ::= random | <pbs_initialization>
<ils> ::= ILS(<perturb>, <ls>, <accept>, <stop>)
<perturb> ::= none | <initialization> | <pbs_perturb>
<ls> ::= <ils> | <descent> | <sa> | <rii> | <pii> | <vns> | <ig> | <pbs_ls>
<accept> ::= alwaysAccept | improvingAccept <comparator>
           | prob(<value_prob_accept>) | probRandom | <metropolis>
           | threshold(<value_threshold_accept>) | <pbs_accept>

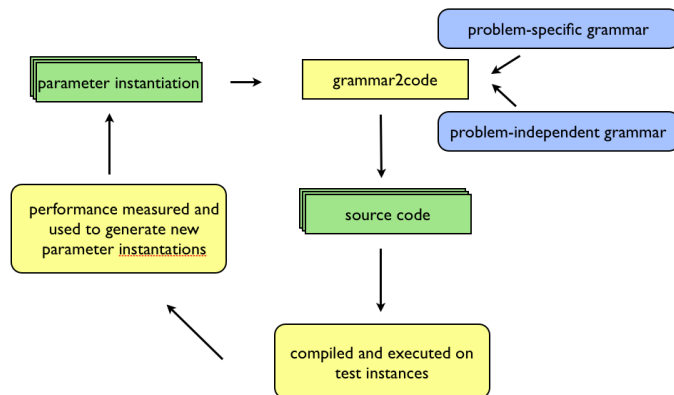
<descent> ::= bestDescent(<comparator>, <stop>)
           | firstImprDescent(<comparator>, <stop>)
<sa> ::= ILS(<pbs_move>, no_ls, <metropolis>, <stop>)
<rii> ::= ILS(<pbs_move>, no_ls, probRandom, <stop>)
<pii> ::= ILS(<pbs_move>, no_ls, prob(<value_prob_accept>), <stop>)
<vns> ::= ILS(<pbs_variable_move>, firstImprDescent(improvingStrictly),
           improvingAccept(improvingStrictly), <stop>)
<ig> ::= ILS(<deconst-construct_perturb>, <ls>, <accept>, <stop>)

<comparator> ::= improvingStrictly | improving
<value_prob_accept> ::= [0, 1]
<value_threshold_accept> ::= [0, 1]
<metropolis> ::= metropolisAccept(<init_temperature>, <final_temperature>,
                                <decreasing_temperature_ratio>, <span>)

<init_temperature> ::= {1, 2, ..., 10000}
<final_temperature> ::= {1, 2, ..., 100}
<decreasing_temperature_ratio> ::= [0, 1]
<span> ::= {1, 2, ..., 10000}

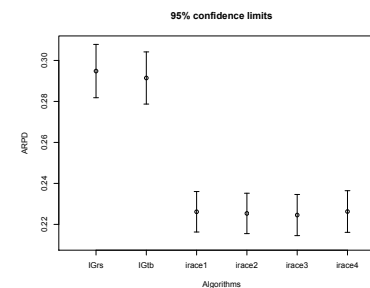
```

System overview [Mascia, López-Ibáñez, Dubois-Lacoste, and Stützle, 2014]



Flow-shop problem with makespan objective [Pagnozzi, Stützle, 2017]

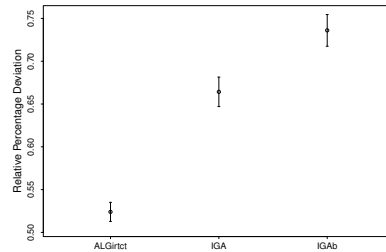
- Automatic configuration:
 - max. three levels of recursion
 - biased / unbiased grammar resulting in 262 and 502 parameters, respectively
 - budget: 200 000 trials of $n \cdot m \cdot 0.03$ seconds



Results are clearly superior to state-of-the-art

Flow-shop problem with total completion time objective [Pagnozzi, Stützle, 2017]

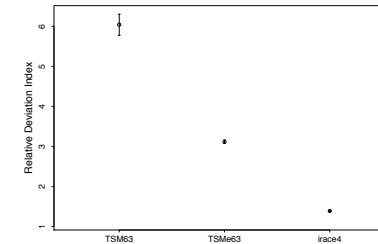
- Automatic configuration:
 - max. three levels of recursion
 - budget: 100 000 trials of $n \cdot m \cdot 0.03$ seconds



Results are clearly superior to state-of-the-art

Flow-shop problem with total tardiness objective [Pagnozzi, Stützle, 2017]

- Automatic configuration:
 - max. three levels of recursion
 - budget: 100 000 trials of $n \cdot m \cdot 0.03$ seconds



Results are clearly superior to state-of-the-art

Summary

Contributions

- approach to automate design and analysis of (hybrid) metaheuristics
- not a silver bullet, but needs right components, especially problem-specific ones
- better or equal performance to state-of-the-art for UBQP, TSP-TW, many (flow-shop) scheduling problems
- directly extendible for automated comparison of metaheuristics

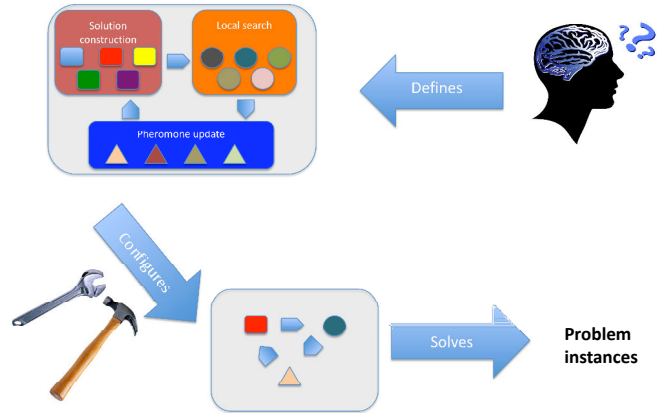
Current/future work

- extensions to other methods and templates
- dealing with complexity of hybrid algorithms
- increase generality, tackling wide problem classes

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

Towards a paradigm shift in algorithm design



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Configurable, flexible (SLS) frameworks XXL

- paradigm shift in SLS algorithm development
- configurable frameworks XXL
- solve = model + configure + search

Many challenges remain on (i) problem representations, (ii) algorithmic structure, (iii) algorithmic components and generation thereof, (iv) automatic configuration techniques, and (v) extensions to other techniques and challenging problems, ...

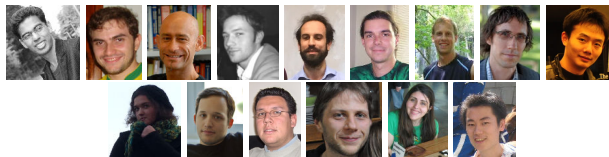
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- PAI project COMEX funded by the Interuniversity Attraction Poles Programme of the Belgian Science Policy Office
- and the EU FP7 ICT Project COLOMBO, Cooperative Self-Organizing System for Low Carbon Mobility at Low Penetration Rates (agreement no. 318622)

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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 $\Rightarrow$ new scenarios welcome !

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

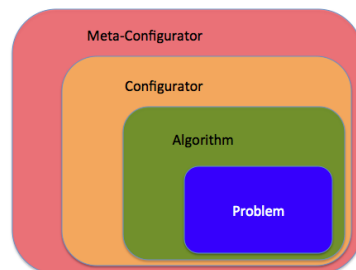
Tune on easy instances,
then ordered F-race on increasingly difficult ones

- 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