Automated Offline Design of Algorithms

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Instructors

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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. Varrentrapp) received the 2012 SIGEVO impact award.

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

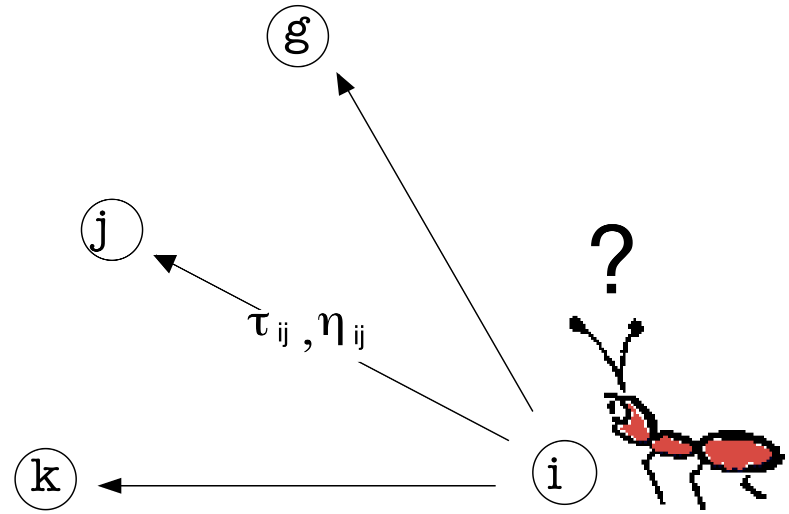
Very active research on hybrids of exact/approximate algorithms!

Design choices and parameters everywhere

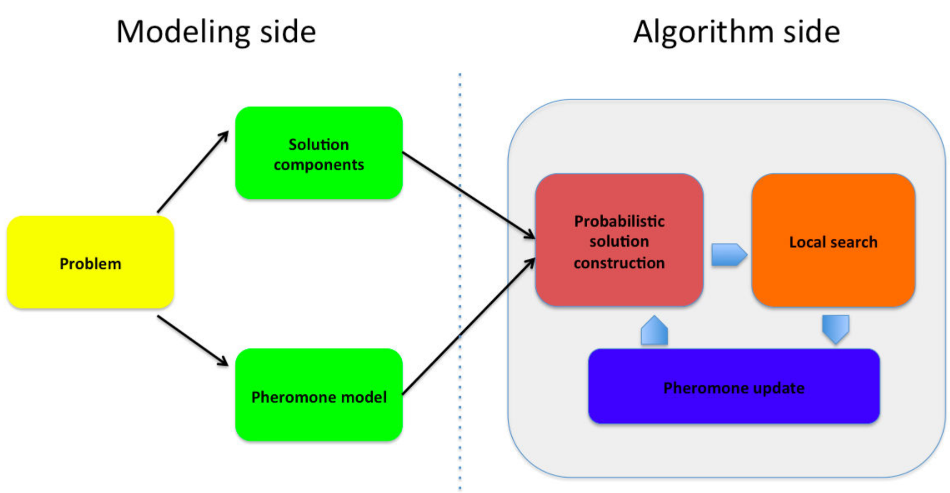
> Modern high-performance optimizers involve a large number of design choices and parameter settings

- 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

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

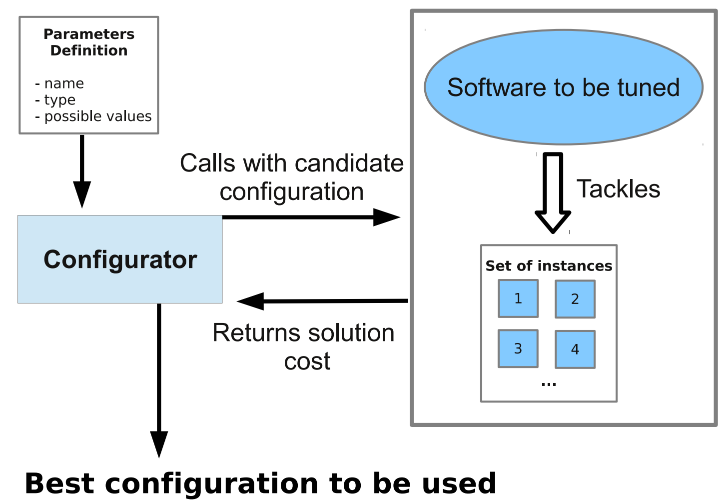
Can we make this approach more principled and automatic?

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]

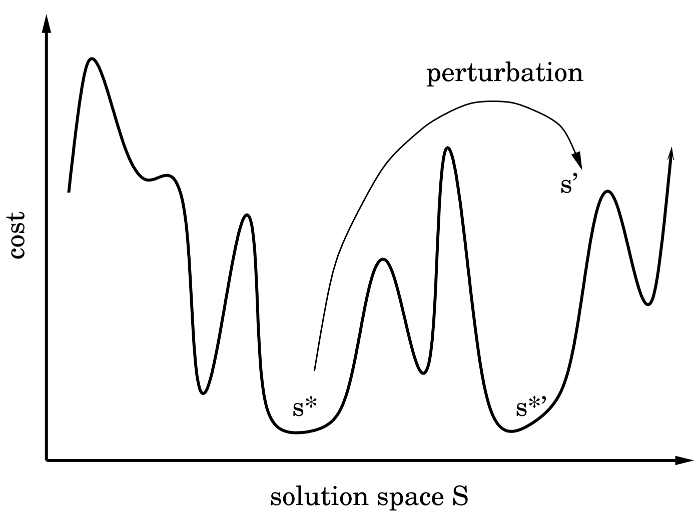
heuristic optimization
meta-GA [Grefenstette, 1986], ParamILS [Hutter et al., 2007b, 2009], gender-based GA [Ansótegui et al., 2009], linear GP [Oltean, 2005], REVAC(++) [Nannen & Eiben, 2006; Smit & Eiben, 2009, 2010] . . .

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]

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

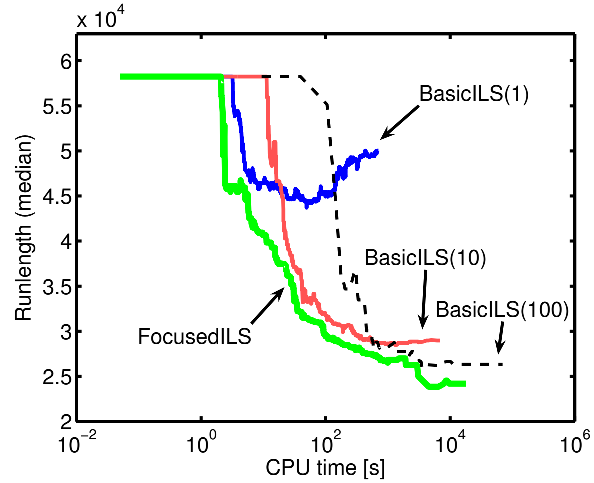
Evaluation of incumbent

- *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
    $\Rightarrow$ 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

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

generate and evaluate initial set of configurations Θ_0
choose best-so-far configuration $\theta^* \in \Theta_0$
while tuning budget available **do**
  learn surrogate model $\mathcal{M}\colon \Theta \mapsto R$
  generate set of possible candidate configurations Θ
  use model $\mathcal{M}$ to filter promising configurations $\Theta_p \subseteq \Theta$
  evaluate configurations in Θ_p
  $\Theta_0 := \Theta_0 \cup \Theta_p$
  update $\theta^* \in \Theta_0$
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]

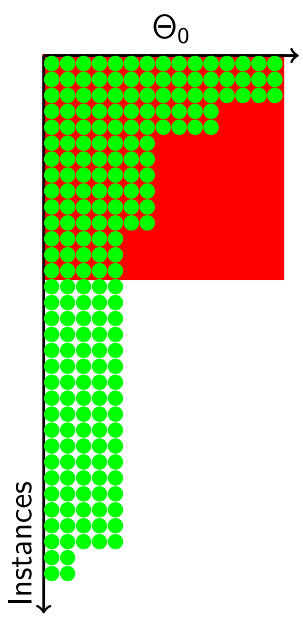
SMAC extends surrogate model-based configuration to complex algorithm configuration tasks and across multiple instances

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

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)

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]

What is Iterated Racing and irace?

Iterated Racing (irace)

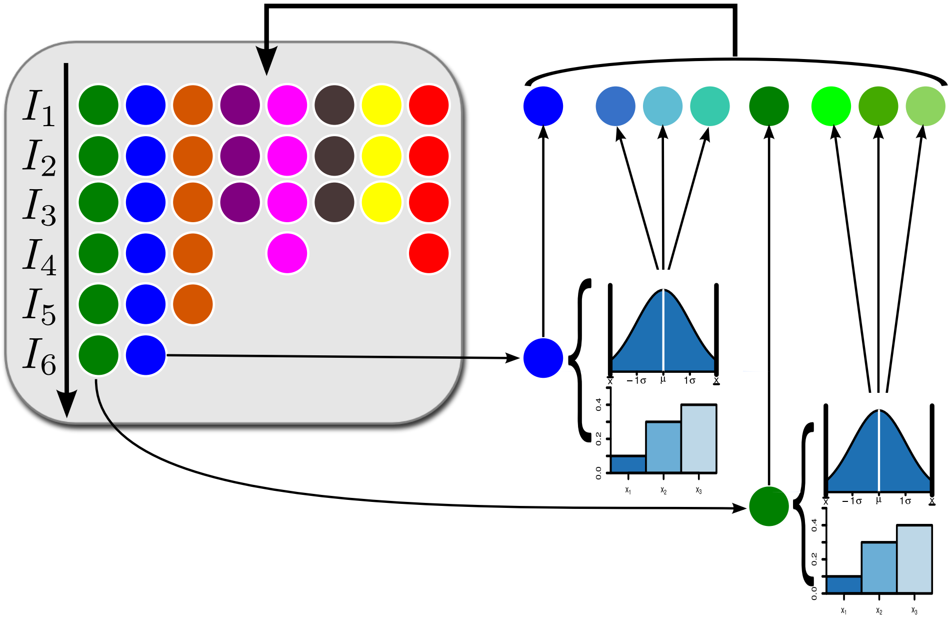
1. A variant of I/F-Race with several extensions
   - I/F-Race proposed by Balaprakash, Birattari, and Stützle [2007]
   - Refined by Birattari, Yuan, Balaprakash, and Stützle [2010]
   - Further refined and extended by López-Ibáñez, Dubois-Lacoste, Stützle, and Birattari [2011]
   - Elitist variant proposed by López-Ibáñez, Dubois-Lacoste, Pérez Cáceres, Stützle, and Birattari [2016]
2. A software package implementing the latest variants.

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

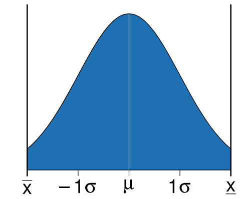
Numerical parameter $X_d \in [\underline{x}_d, \overline{x}_d]$

$\Rightarrow$ *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

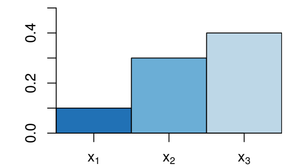
σ_d^i = decreases with the number of iterations



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

$\Rightarrow$ *Discrete probability distribution*

$$\Pr^z\{X_d = x_j\} = \begin{array}{cccc} x_1 & x_2 & \ldots & x_{n_d} \\ \hline 0.1 & 0.3 & \ldots & 0.4 \end{array}$$



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

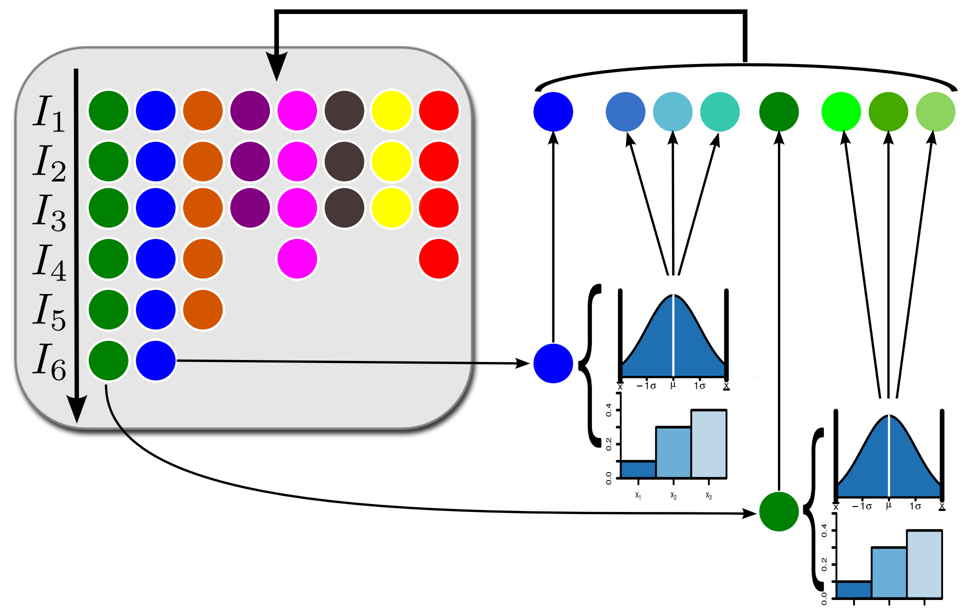
Iterated Racing: Elitist Iterated Racing [López-Ibáñez et al., 2016]

✘ irace may "*lose*" the best-so-far configuration
$\Rightarrow$ Each new iteration (race) forgets the results of the previous one

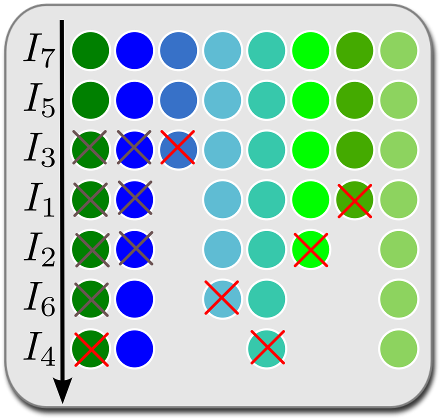
✔ Protect the best configurations (*elites*) from being discarded unless all their results are considered

1. after race i, elites were evaluated in I_e instances
2. race $i+1$ will start with $I_{new} \cup I_e$ 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 [López-Ibáñez et al., 2016]



Iterated Racing: Elitist Iterated Racing [López-Ibáñez et al., 2016]



The irace Package

Manuel López-Ibáñez, Jérémie Dubois-Lacoste, Leslie Pérez Cáceres, Thomas Stützle, and Mauro Birattari.
The irace package: Iterated Racing for Automatic Algorithm Configuration.
Operations Research Perspectives, 3:43–58, 2016. doi:10.1016/j.orp.2016.09.002
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`)

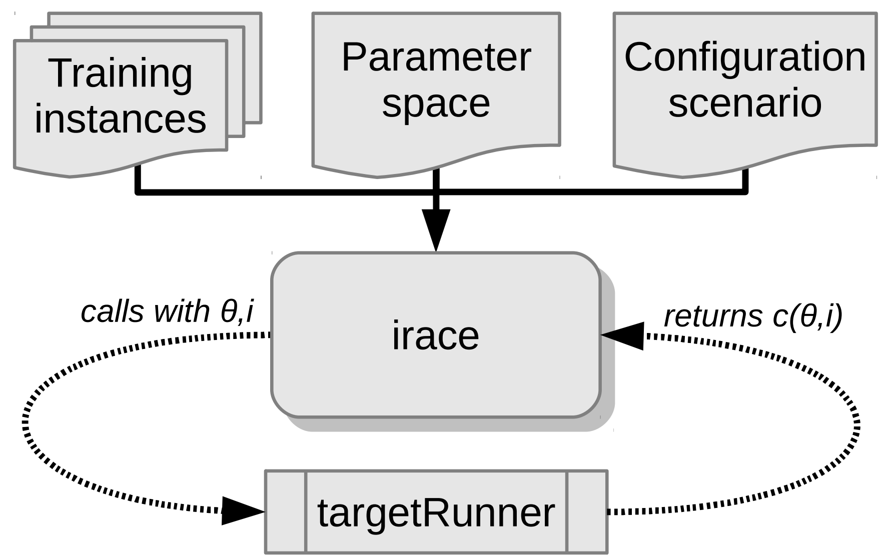
```
irace --max-experiments 1000 --param-file parameters.txt
```

✔ No knowledge of R needed

The irace Package: version 2.3

- 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

The irace Package



The irace Package: Instances

- TSP instances

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

- Continuous functions

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

- Parameters for an instance generator

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

- Script / R function that generates instances
  ☞ if you need this, tell us!

The irace Package: Parameter space

- Categorical (c), ordinal (o), integer (i) and real (r)
- Subordinate parameters (| condition)

```
$ 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, Grid Engine / qsub
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

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: 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 #1

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)

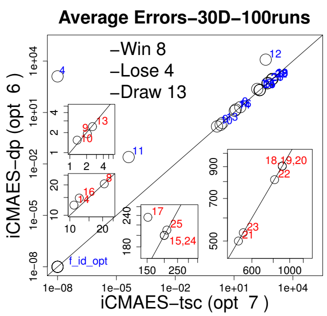
Benchmark set	Default	Configured	Speedup
`Regions200`	72	10.5 (11.4 ± 0.9)	*6.8*
`Conic.SCH`	5.37	2.14 (2.4 ± 0.29)	*2.51*
`CLS`	712	23.4 (327 ± 860)	*30.43*
`MIK`	64.8	1.19 (301 ± 948)	*54.54*
`QP`	969	525 (827 ± 306)	*1.85*

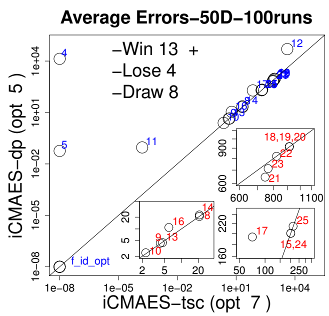
FocusedILS, 10 runs, 2 CPU days, 63 parameters

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

Example #2

Automatically Improving the Anytime Behavior of Optimization Algorithms with irace

Automatically Improving the Anytime Behavior

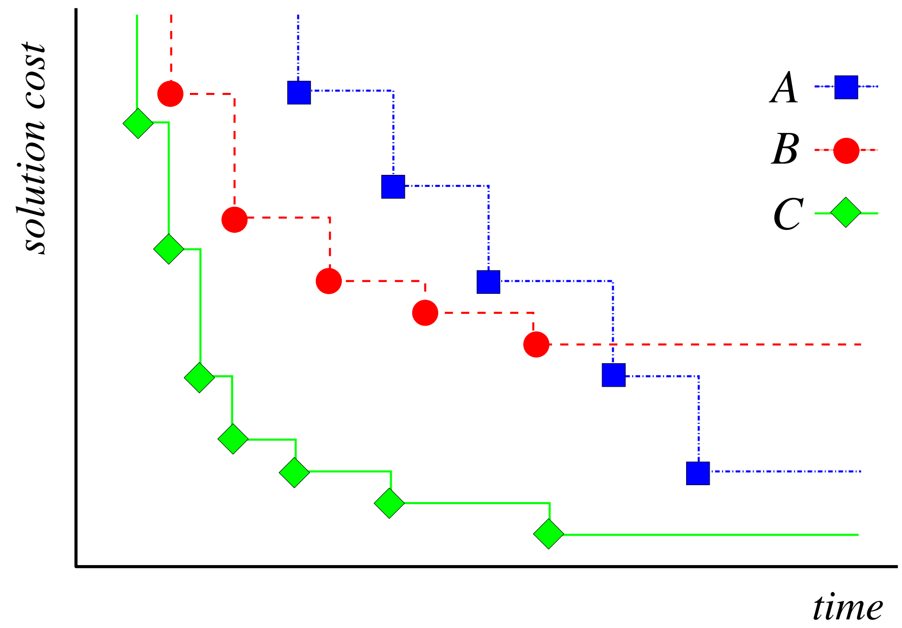
Anytime Algorithm [Dean & Boddy, 1988]

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

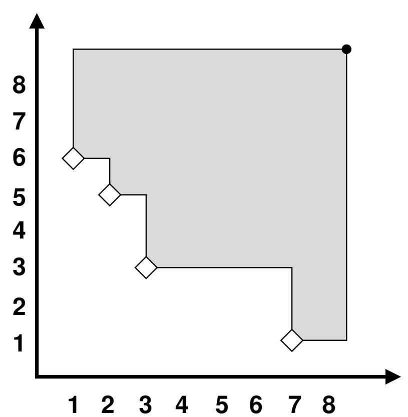
Good Anytime Behavior [Zilberstein, 1996]

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 ≈ 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? ⇒ 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*

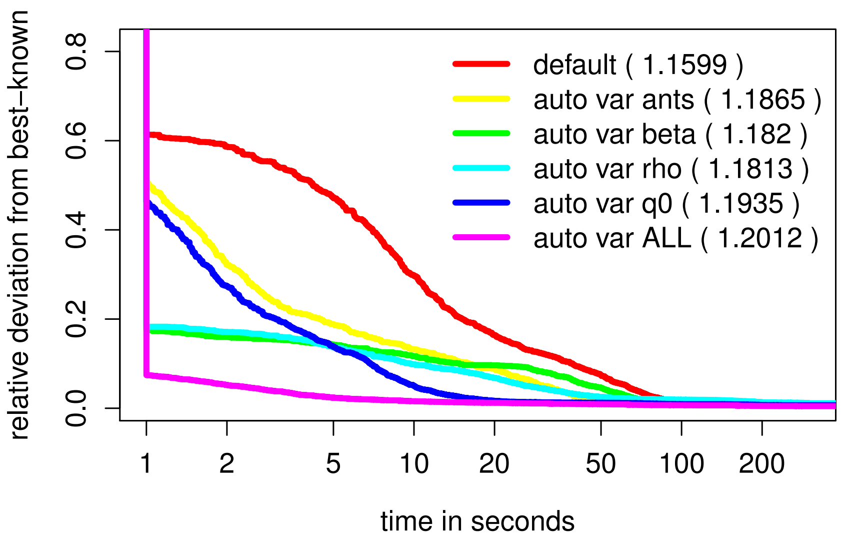
Scenario #1: Brute-Force Approach

1. Choose *many* parameter settings
2. Run lots of experiments
3. Visually compare SQT plots

After about one year:

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

Scenario #2: Experimental comparison

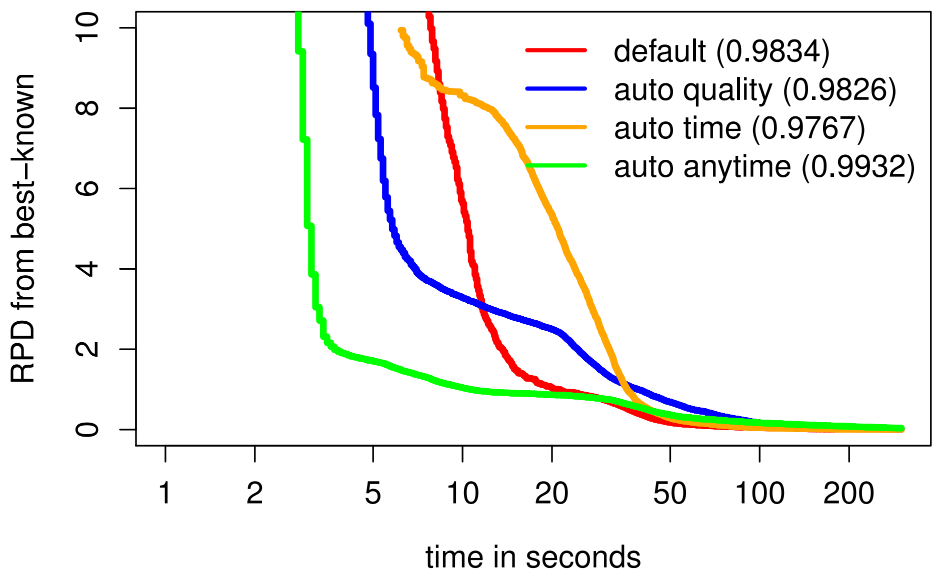


Scenario #2: SCIP

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]
  1 000 training + 1 000 testing instances
- Single run timeout: 300 seconds
- irace budget (*maxExperiments*): 5 000 runs

Scenario #2: SCIP



Example #3

Integration in algorithm (re-)engineering process

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

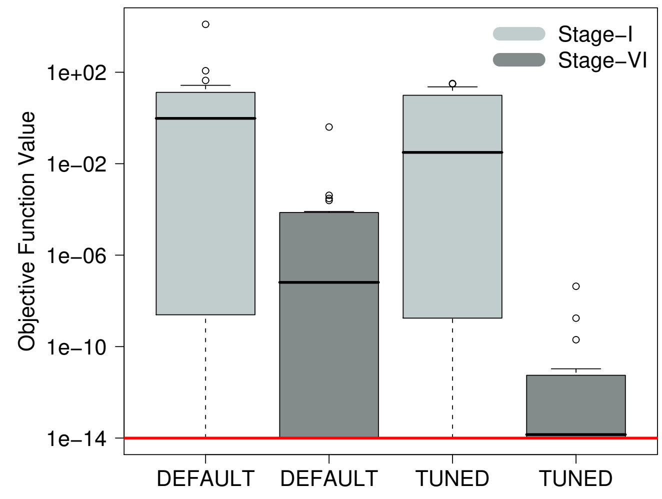
[Montes de Oca et al., 2011]

- 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

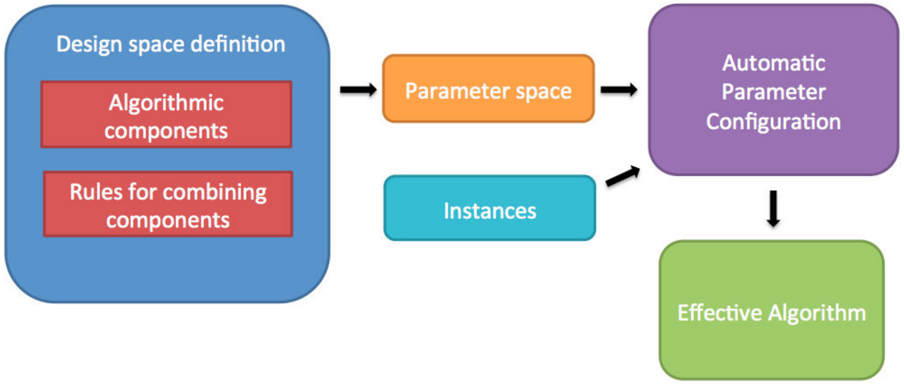
Tuning in-the-loop: (re)design of continuous optimizers

[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 #4

Top-down design approach: MOACO framework

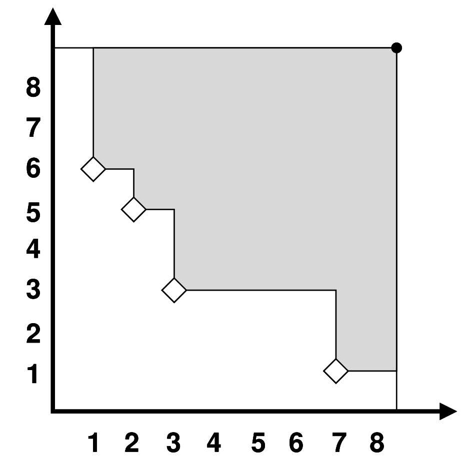
A more complex example: MOACO framework

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

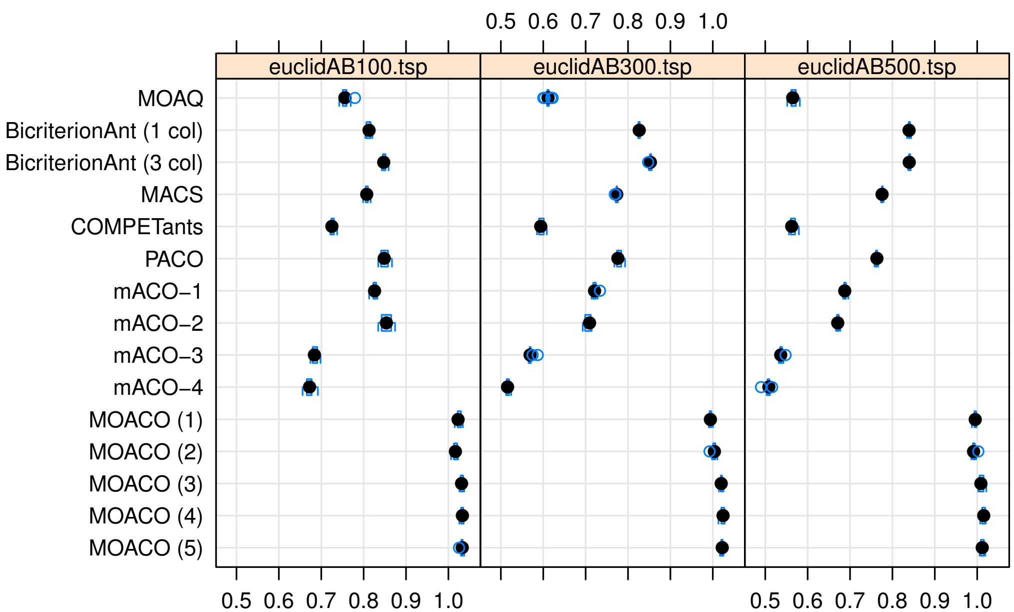
A more complex example: MOACO framework

✘ 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 #5

Top-down design approach: MOEA framework

An even more complex example: MOEA framework

- ✔ 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

AutoMOEA: A MOEA template

$\texttt{pop} := \texttt{Initialization}\ ()$
if *type*$(\texttt{pop}_{\texttt{ext}})$!= *none* **then**
  $\texttt{pop}_{\texttt{ext}} := \texttt{pop}$
repeat
  $\texttt{pool} := \texttt{BuildMatingPool}\ (\texttt{pop})$
  $\texttt{pop}_{\texttt{new}} := \texttt{Variation}\ (\texttt{pool})$
  $\texttt{pop}_{\texttt{new}} := \texttt{Evaluation}\ (\texttt{pop}_{\texttt{new}})$
  $\texttt{pop} := \texttt{Replacement}\ (\texttt{pop}, \texttt{pop}_{\texttt{new}})$
  if *type*$(\texttt{pop}_{\texttt{ext}})$ == *bounded* **then**
    $\texttt{pop}_{\texttt{ext}} := \texttt{Archiving}\ (\texttt{pop}_{\texttt{ext}}, \texttt{pop}_{\texttt{new}})$
  else if *type*$(\texttt{pop}_{\texttt{ext}})$ == *unbounded* **then**
    $\texttt{pop}_{\texttt{ext}} := \texttt{pop}_{\texttt{ext}} \cup \texttt{pop}$
until *termination criteria met*
if *type*$(\texttt{pop}_{\texttt{ext}})$ == *none* **then**
  return pop
else
  return $\texttt{pop}_{\texttt{ext}}$

AutoMOEA: Main components

Component	Parameters
BuildMatingPool	$\langle$ Preference$_{Mat}$, Selection $\rangle$
Replacement	$\langle$ Preference$_{Rep}$, Removal $\rangle$
Archiving	$\langle$ Preference$_{Ext}$, Removal$_{Ext}$ $\rangle$
Preference	$\langle$ Fitness, 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^1

AutoMOEA: Main components

"*On Set-Based Multiobjective Optimization*"[Zitzler, Thiele, and Bader, 2010]

Set-partitioning
- dominance count
- dominance rank
- dominance strength
- dominance depth
- dominance depth-rank

Pareto-compliant quality measures
- binary indicator (I_ϵ or I_H^-)
- exclusive hypervolume contribution (I_H^1)
- shared hypervolume contribution (I_H^h)

Diversity measures (not Pareto-compliant)
- niche sharing
- k-th nearest neighbor (kNN)
- crowding distance

AutoMOEA: Main components

Component	Parameters
`BuildMatingPool`	⟨ `Preference`$_{Mat}$, `Selection` ⟩
`Replacement`	⟨ `Preference`$_{Rep}$, `Removal` ⟩
`Archiving`	⟨ `Preference`$_{Ext}$, `Removal`$_{Ext}$ ⟩
`Preference`	~~⟨ `Fitness`, `Diversity` ⟩~~
	⟨ `Set-partitioning`, `Quality`, `Diversity` ⟩

	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^1	—

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^1	—
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	—

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!

Automatic Design: The End of the Game

> *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?

Example #6

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]

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

s_0 :=initSolution
s^* := ls(s_0)
repeat
  s' :=perturb(s^*,*history*)
  $s^{*\prime}$:=ls(s')
  s^* :=accept(s^*,$s^{*\prime}$,*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

	perturb	*ls*	*accept*
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	∅

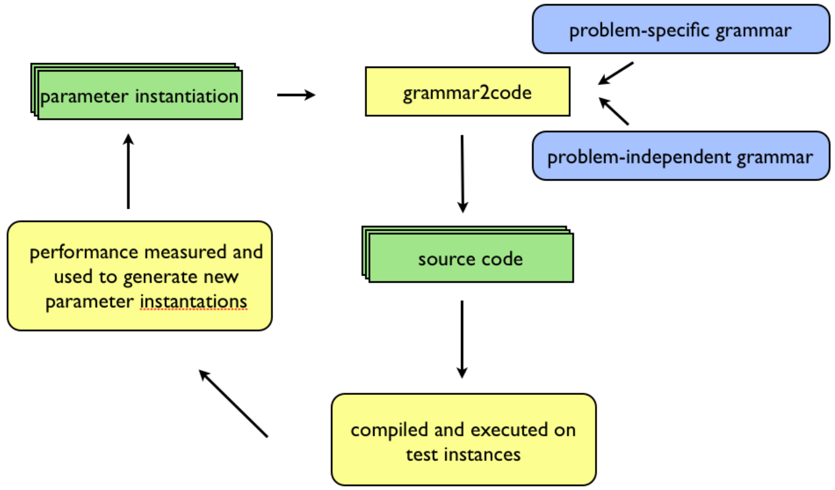
Grammar

```
     <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

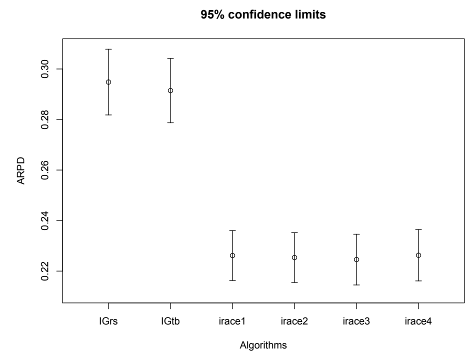
```
     <algorithm> ::= <initialization> <ils>
<initialization> ::= random | <pbs_initialization>
           <ils> ::= ILS(<perturb>, <ls>, <accept>, <stop>)
<perturb> ::= none | <initialization> | <pbs_perturb>
     <ls> ::= <ils> | <descent> | <sa> | <rii> | <pii> | <vns> | <ig> | <pbs_ls>
 <accept> ::= 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]

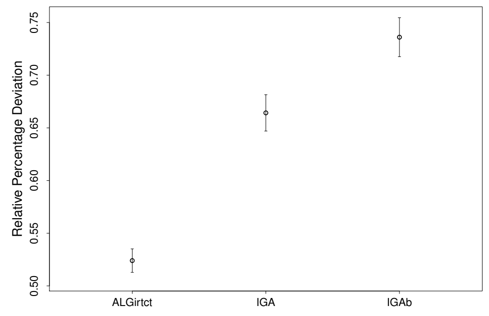
- Automatic configuration:
  - max. three levels of recursion
  - biased / unbiased grammar resulting in 262 and 502 parameters, respectively
  - budget: 200 000 trials of $n \cdot m \cdot 0.03$ seconds



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

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

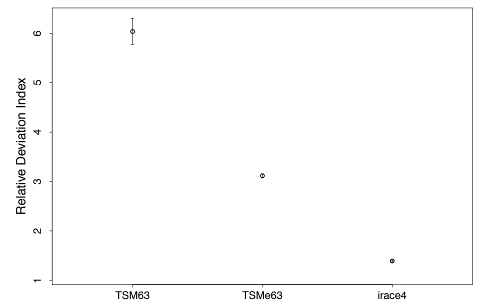
- Automatic configuration:
  - max. three levels of recursion
  - budget: 100 000 trials of $n \cdot m \cdot 0.03$ seconds



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

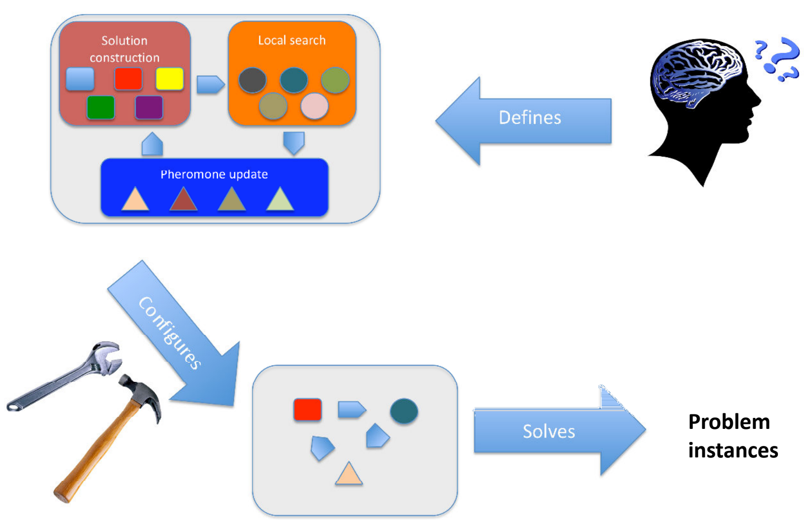
Current/future work

- 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



Conclusions

Automatic Configuration

- leverages computing power for software design
- is rewarding w.r.t. development time and algorithm performance

Future work

- more powerful configurators
- more and more complex applications
- paradigm shift in optimization software development

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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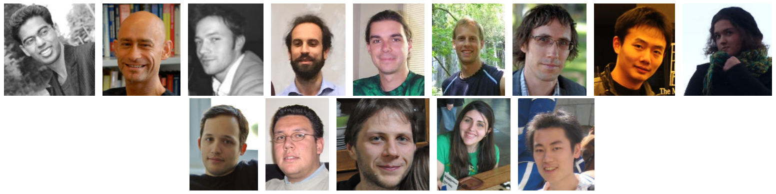

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AClib: A Benchmark Library for Algorithm Configuration

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

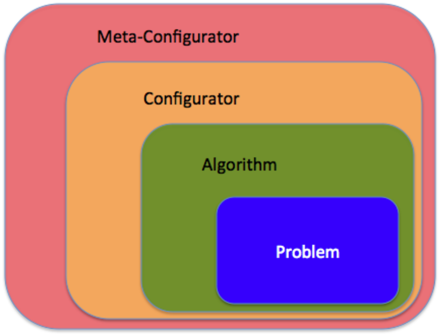
  Tune on easy instances,
  then ordered F-race on increasingly difficult ones

- 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