Automatic Algorithm Configuration based on Local Search

Frank Hutter¹ Holger Hoos¹ Thomas Stützle²

¹Department of Computer Science University of British Columbia Canada

²IRIDIA Université Libre de Bruxelles Belgium

Real-world example for algorithm configuration: Tree search for SAT-encoded software verification

▶ New DPLL-type SAT solver (SPEAR)

- Variable/value heuristics, clause learning, restarts, ...

Real-world example for algorithm configuration:

Tree search for SAT-encoded software verification

▶ New DPLL-type SAT solver (SPEAR)

- Variable/value heuristics, clause learning, restarts, ...
- 26 user-specifiable parameters:
 - 7 categorical, 3 boolean, 12 continuous, 4 integer parameters

Real-world example for algorithm configuration:

Tree search for SAT-encoded software verification

▶ New DPLL-type SAT solver (SPEAR)

- Variable/value heuristics, clause learning, restarts, ...
- 26 user-specifiable parameters:
 - 7 categorical, 3 boolean, 12 continuous, 4 integer parameters
- Minimize expected run-time

Real-world example for algorithm configuration:

Tree search for SAT-encoded software verification

- ▶ New DPLL-type SAT solver (SPEAR)
 - Variable/value heuristics, clause learning, restarts, ...
 - 26 user-specifiable parameters:
 - 7 categorical, 3 boolean, 12 continuous, 4 integer parameters
- Minimize expected run-time
- Problems:
 - Huge variation in runtime (with default setting):
 - < 1 second for some instances
 - $> 1 \mbox{ day for others}$
 - Good performance on a few instances does not generalise well
 - Many possible configurations (8.34×10^{17} after discretization)

Standard algorithm configuration approach

Choose a "representative" benchmark set for tuning

Standard algorithm configuration approach

- Choose a "representative" benchmark set for tuning
- Perform iterative manual tuning:

start with some parameter configuration repeat modify a single parameter if results on tuning set improve then keep new configuration

until no more improvement possible (or "good enough")

Slow and tedious, requires significant human time

- Slow and tedious, requires significant human time
- Not guaranteed to find global optimum
 - Hill climbing \rightsquigarrow local minimum only

- Slow and tedious, requires significant human time
- Not guaranteed to find global optimum
 - Hill climbing \rightsquigarrow local minimum only
- "Representative" benchmark set may not be representative
 - Constraints on tuning time
 vypically only few instances
 - \rightsquigarrow typically fairly easy instances

- Slow and tedious, requires significant human time
- Not guaranteed to find global optimum
 - Hill climbing \rightsquigarrow local minimum only
- "Representative" benchmark set may not be representative
 - - \rightsquigarrow typically fairly easy instances

Solution:

- Automate process
- Use more powerful search method

Search approaches

[Minton 1993, 1996], [Hutter 2004], [Cavazos & O'Boyle 2005], [Adenso-Diaz & Laguna 2006], [Audet & Orban 2006]

Search approaches

[Minton 1993, 1996], [Hutter 2004], [Cavazos & O'Boyle 2005], [Adenso-Diaz & Laguna 2006], [Audet & Orban 2006]

Racing algorithms/Bandit solvers

[Birattari et al. 2002], [Smith et al. 2004 - 2007]

Search approaches

[Minton 1993, 1996], [Hutter 2004], [Cavazos & O'Boyle 2005], [Adenso-Diaz & Laguna 2006], [Audet & Orban 2006]

Racing algorithms/Bandit solvers

[Birattari et al. 2002], [Smith et al. 2004 - 2007]

Stochastic Optimisation [Kiefer & Wolfowitz 1952], [Spall 1987]

Search approaches

[Minton 1993, 1996], [Hutter 2004], [Cavazos & O'Boyle 2005], [Adenso-Diaz & Laguna 2006], [Audet & Orban 2006]

Racing algorithms/Bandit solvers

[Birattari et al. 2002], [Smith et al. 2004 - 2007]

- Stochastic Optimisation [Kiefer & Wolfowitz 1952], [Spall 1987]
- Learning approaches
 - Regression trees [Bartz-Beielstein et al. 2004]
 - Response surface models, DACE

[Bartz-Beielstein et al. 2004-2006]

Search approaches

[Minton 1993, 1996], [Hutter 2004], [Cavazos & O'Boyle 2005], [Adenso-Diaz & Laguna 2006], [Audet & Orban 2006]

Racing algorithms/Bandit solvers

[Birattari et al. 2002], [Smith et al. 2004 - 2007]

- Stochastic Optimisation [Kiefer & Wolfowitz 1952], [Spall 1987]
- Learning approaches
 - Regression trees [Bartz-Beielstein et al. 2004]
 - Response surface models, DACE [Bartz-Beielstein et al. 2004–2006]

Lots of work on per-instance tuning / reactive search ~> orthogonal to the approach followed here

Hutter, Hoos, Stützle: Automatic Algorithm Configuration based on Local Search

1. Introduction

- 2. Iterated local search over parameter configurations
- 3. The BasicILS and FocusedILS algorithms
- 4. Sample applications and performance results
- 5. Conclusions and future work

Choose initial parameter configuration θ Perform *subsidiary local search* on θ

Choose initial parameter configuration θ Perform *subsidiary local search* on θ While tuning time left:

 $\begin{vmatrix} \theta' := \theta \\ \text{perform perturbation on } \theta \\ \text{perform subsidiary local search on } \theta \end{vmatrix}$

```
Choose initial parameter configuration \theta
Perform subsidiary local search on \theta
While tuning time left:
```

```
\begin{array}{l} \theta' := \theta \\ \text{perform } \textit{perturbation} \text{ on } \theta \\ \text{perform } \textit{subsidiary local search } \text{on } \theta \\ \text{based on } \textit{acceptance criterion,} \\ \text{keep } \theta \text{ or revert to } \theta := \theta' \end{array}
```

```
Choose initial parameter configuration \theta
Perform subsidiary local search on \theta
While tuning time left:
```

```
\begin{array}{l} \theta' := \theta \\ \text{perform } perfurbation \text{ on } \theta \\ \text{perform } subsidiary \ local \ search \ \text{on } \theta \end{array}
 based on acceptance criterion,
keep \theta or revert to \theta := \theta'
with probability p_{restart} randomly pick new \theta
```

~ Performs biased random walk over local optima

▶ Initialisation: pick *best* of default & *R* random configurations

- Initialisation: pick best of default & R random configurations
- Subsidiary local search: iterative first improvement, change one parameter in each step

- Initialisation: pick best of default & R random configurations
- Subsidiary local search: iterative first improvement, change one parameter in each step
- Perturbation: change s randomly chosen parameters

- Initialisation: pick best of default & R random configurations
- Subsidiary local search: iterative first improvement, change one parameter in each step
- Perturbation: change s randomly chosen parameters
- Acceptance criterion: always select better local optimum

Evaluation of a parameter configuration θ **(based on** *N* **runs)**

Sample N instances from given set (with repetitions)

Evaluation of a parameter configuration θ **(based on** *N* **runs)**

- Sample N instances from given set (with repetitions)
- ▶ For each of the *N* instances:
 - Execute algorithm with configuration θ
 - Record scalar cost of the run (user-defined: *e.g.* run-time, solution quality, ...)

Evaluation of a parameter configuration θ **(based on** *N* **runs)**

- Sample N instances from given set (with repetitions)
- ▶ For each of the *N* instances:
 - Execute algorithm with configuration θ
 - Record scalar cost of the run (user-defined: *e.g.* run-time, solution quality, ...)
- Compute scalar statistic ĉ_N(θ) of the N costs (user-defined: e.g. empirical mean, median, ...)

The BasicILS(N) algorithm

• Use a fixed number of N runs to evaluate each configuration θ

The BasicILS(N) algorithm

• Use a fixed number of N runs to evaluate each configuration θ

Question: How to choose number of runs N?

- ► Too many
 - \rightsquigarrow evaluating a configuration is very expensive
 - \rightsquigarrow optimisation process is very slow

The BasicILS(N) algorithm

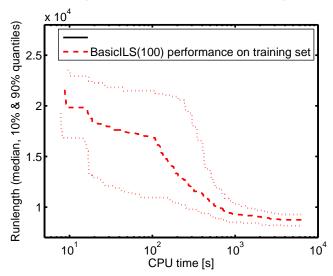
• Use a fixed number of N runs to evaluate each configuration θ

Question: How to choose number of runs N?

- Too many
 - \rightsquigarrow evaluating a configuration is very expensive
 - \rightsquigarrow optimisation process is very slow
- Too few
 - \rightsquigarrow very noisy approximations $\hat{c}_N(\theta)$
 - \rightsquigarrow poor generalisation to independent test runs

Generalisation to independent test set, large N (N=100)

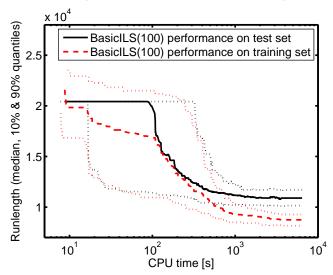
(SAPS on quasigroups with holes)



Hutter, Hoos, Stützle: Automatic Algorithm Configuration based on Local Search

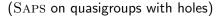
Generalisation to independent test set, large N (N=100)

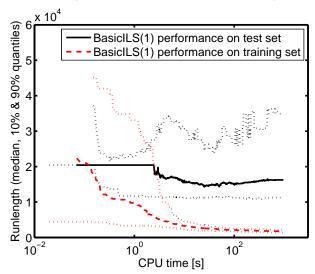
(SAPS on quasigroups with holes)



Hutter, Hoos, Stützle: Automatic Algorithm Configuration based on Local Search

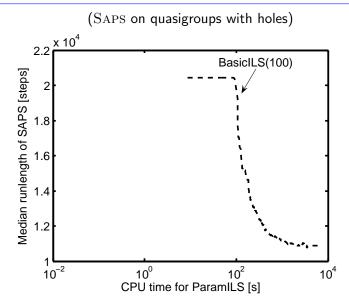
Generalisation to independent test set, small N (N=1)





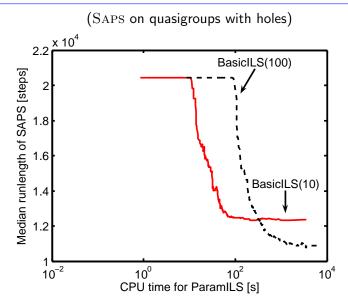
Hutter, Hoos, Stützle: Automatic Algorithm Configuration based on Local Search

Test performance of BasicILS with different N



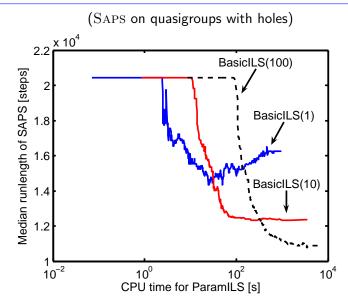
Hutter, Hoos, Stützle: Automatic Algorithm Configuration based on Local Search

Test performance of BasicILS with different N



Hutter, Hoos, Stützle: Automatic Algorithm Configuration based on Local Search

Test performance of BasicILS with different N



Hutter, Hoos, Stützle: Automatic Algorithm Configuration based on Local Search

▶ Use different numbers of runs, $N(\theta)$, for each configuration θ

- ▶ Use different numbers of runs, $N(\theta)$, for each configuration θ
- ▶ Idea: Use high $N(\theta)$ only for good θ
 - start with $N(\theta) = 0$ for all θ
 - increment $N(\theta)$ whenever θ is visited
 - additional runs upon finding new, better configuration heta

- Use different numbers of runs, $N(\theta)$, for each configuration θ
- Idea: Use high $N(\theta)$ only for good θ
 - start with N(heta) = 0 for all heta
 - increment $N(\theta)$ whenever θ is visited
 - additional runs upon finding new, better configuration $\boldsymbol{\theta}$

Theorem:

As number of FocusedILS iterations $\rightarrow \infty$,

it converges to true optimal configuration θ^{\ast}

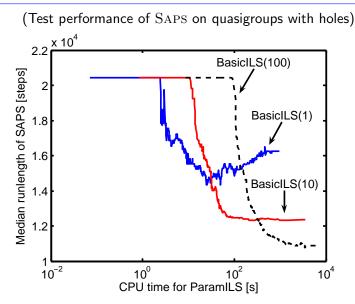
- Use different numbers of runs, $N(\theta)$, for each configuration θ
- Idea: Use high $N(\theta)$ only for good θ
 - start with N(heta) = 0 for all heta
 - increment $N(\theta)$ whenever θ is visited
 - additional runs upon finding new, better configuration $\boldsymbol{\theta}$

Theorem:

As number of FocusedILS iterations $\rightarrow\infty$,

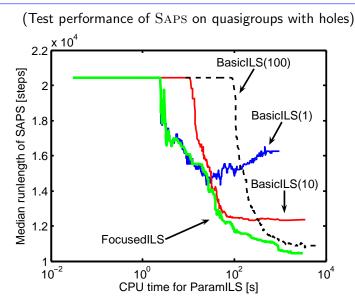
- it converges to true optimal configuration θ^*
 - ► Key ideas in proof
 - 1. For $N(heta) o \infty$, $\hat{c}_N(heta) o c(heta)$
 - 2. Underlying ILS eventually reaches any configuration θ .

Performance of FocusedILS vs BasicILS



Hutter, Hoos, Stützle: Automatic Algorithm Configuration based on Local Search

Performance of FocusedILS vs BasicILS



Hutter, Hoos, Stützle: Automatic Algorithm Configuration based on Local Search

- ► CALIBRA: limited to 5 continuous/integer parameters
- ParamILS better results with same tuning time

- ► CALIBRA: limited to 5 continuous/integer parameters
- ParamILS better results with same tuning time

Scenario	Metric	Default	FocusedILS	BasicILS(100)	CALIBRA(100)
Saps on GC	Runtime	5.60 s	0.043 ± 0.005	$\textbf{0.046} \pm \textbf{0.01}$	$\textbf{0.053} \pm \textbf{0.010}$

- CALIBRA: limited to 5 continuous/integer parameters
- ParamILS better results with same tuning time

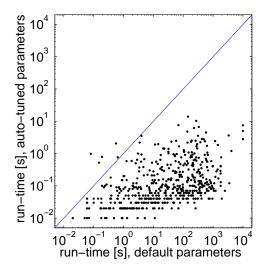
Scenario	Metric	Default	FocusedILS	BasicILS(100)	CALIBRA(100)
Saps on GC	Runtime	5.60 s	0.043 ± 0.005	0.046 ± 0.01	$\textbf{0.053} \pm \textbf{0.010}$
${\rm GLS}^+$ for MPE	Approx. error	$\epsilon = 1.81$	0.949 ± 0.0001	0.951 ± 0.004	1.234 ± 0.492

- CALIBRA: limited to 5 continuous/integer parameters
- ParamILS better results with same tuning time

Scenario	Metric	Default	FocusedILS	BasicILS(100)	CALIBRA(100)
Saps on GC	Runtime	5.60 s	0.043 ± 0.005	0.046 ± 0.01	0.053 ± 0.010
GLS^+ for MPE	Approx. error	$\epsilon = 1.81$	0.949 ± 0.0001	0.951 ± 0.004	1.234 ± 0.492
${\rm Sat4j}$ on GC	Runtime	7.02 s	0.65 ± 0.2	1.19 ± 0.58	(too many param.)

Speedup obtained by automated tuning

(SAPS default vs tuned on graph colouring, test set performance)



Hutter, Hoos, Stützle: Automatic Algorithm Configuration based on Local Search

Two "real-world" applications

- ▶ New DPLL-type SAT solver SPEAR
 - ► 26 parameters
 - Software verification: 500-fold speedup (won QB_FQ category in SMT'07 competition)
 - Hardware verification: 4.5-fold speedup
 - \rightsquigarrow New state of the art for those instances
 - → [Hutter, Babić, Hoos & Hu: FMCAD '07 (to appear)]

Two "real-world" applications

- ▶ New DPLL-type SAT solver SPEAR
 - ► 26 parameters
 - Software verification: 500-fold speedup (won QB_FQ category in SMT'07 competition)
 - Hardware verification: 4.5-fold speedup
 - \rightsquigarrow New state of the art for those instances
 - → [Hutter, Babić, Hoos & Hu: FMCAD '07 (to appear)]
- New replica exchange Monte Carlo algorithm for protein structure prediction
 - ► 3 parameters
 - 2-fold improvement
 - \rightsquigarrow New state of the art for 2D/3D protein structure prediction
 - →→ [Thachuk, Shmygelska & Hoos: BMC Bioinformatics '07 (to appear)]

- ParamILS: Simple and efficient framework for automatic parameter optimization
 - Arbitrary number and types of parameters
 - User-defined objective function

- ParamILS: Simple and efficient framework for automatic parameter optimization
 - Arbitrary number and types of parameters
 - User-defined objective function
- FocusedILS:
 - Converges provably towards optimal configuration
 - Excellent performance in practice (outperforms BasicILS, CALIBRA)

- ParamILS: Simple and efficient framework for automatic parameter optimization
 - Arbitrary number and types of parameters
 - User-defined objective function
- FocusedILS:
 - Converges provably towards optimal configuration
 - Excellent performance in practice (outperforms BasicILS, CALIBRA)
- Huge speedups:
 - $\blacktriangleright~\approx 100 \times$ for $\rm SAPS$ (local search) on graph colouring
 - $\blacktriangleright~\approx 500\times$ for $\rm SPEAR$ (tree search) on software verification

- ParamILS: Simple and efficient framework for automatic parameter optimization
 - Arbitrary number and types of parameters
 - User-defined objective function
- FocusedILS:
 - Converges provably towards optimal configuration
 - Excellent performance in practice (outperforms BasicILS, CALIBRA)
- Huge speedups:
 - $\blacktriangleright~\approx 100 \times$ for $\rm SAPS$ (local search) on graph colouring
 - $\blacktriangleright~\approx 500\times$ for $\rm SPEAR$ (tree search) on software verification
- Publically available at: http://www.cs.ubc.ca/labs/beta/Projects/ParamILS

Continuous parameters (currently discretised)

- Continuous parameters (currently discretised)
- Statistical tests (cf. racing algorithms)

- Continuous parameters (currently discretised)
- Statistical tests (cf. racing algorithms)
- Learning approaches, sequential design of experiments

- Continuous parameters (currently discretised)
- Statistical tests (cf. racing algorithms)
- Learning approaches, sequential design of experiments
- Per-instance tuning

- Continuous parameters (currently discretised)
- Statistical tests (cf. racing algorithms)
- Learning approaches, sequential design of experiments
- Per-instance tuning
- Automatic algorithm design