# Automatic Algorithm Configuration based on Local Search

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## Motivation for automatic algorithm configuration

- Want to design 'best' algorithm to solve a problem
  - Many design choices need to be made
  - Some choices deferred to later: free parameters of algorithm
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  - Many parameters, discrete & continuous
  - Dependencies between parameters
  - Many test instances needed to generalize
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  - Many test instances needed to generalize
  - Many runs per instance needed for randomised algorithms
- Algorithm configuration / tuning still often done manually, using ad-hoc methods
  - $\rightsquigarrow\,$  tedious and time-consuming, sub-optimal results
  - $\rightsquigarrow$  big incentive for automation

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- Minimize expected run-time
- Problems:
  - default settings  $\rightsquigarrow \approx$  300 seconds / run
  - good performance on a few instances may not generalise

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")

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- manual search = iterative improvement (hill climbing) ~ finds local optimum only

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## 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]

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

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- Racing algorithms/Bandit solvers [Birattari et al. 2002], [Smith et al. 2004, 2006]
- 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 / reactive tuning ~→ orthogonal to the approach followed here

# Outline

### 1. Introduction

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

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### → performs biased random walk over local minima

subsidiary local search: iterative first improvement, change on parameter in each step

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- ▶ initialisation: pick *best* of default + *R* random configurations

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- Compute scalar statistic  $\hat{c}_N(\theta)$  of  $\widehat{CD}$  (mean, median, ...)
- ▶ Note: For large *N*,  $\hat{c}_N(\theta)$  approaches true cost  $c(\theta)$

#### Solution quality over time achieved by ParamILS



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- 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 runs (1)



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#### Generalisation to independent test runs (2)



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- Idea: Use high  $N(\theta)$  only for good  $\theta$ 
  - start with  $N(\theta) = 0$  for all  $\theta$
  - increment  $N(\theta)$  whenever  $\theta$  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  $\theta^*$ 

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Key ideas in proof:

1. For  $N(\theta), N(\theta') \to \infty$ , comparisons between  $\theta, \theta'$  become precise.

#### Theorem:

As number of FocusedILS iterations  $\rightarrow \infty$ , it converges to true optimal configuration  $\theta^*$ 

Key ideas in proof:

- 1. For  $N(\theta), N(\theta') \to \infty$ , comparisons between  $\theta, \theta'$  become precise.
- 2. Underlying ILS eventually reaches any configuration  $\theta$ .



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#### **Experiment: Comparison to CALIBRA**

| Scenario | Default           | CALIBRA(100)    | BasicILS(100)   | FocusedILS                           |
|----------|-------------------|-----------------|-----------------|--------------------------------------|
| GLS-GRID | $\epsilon = 1.81$ | $1.234\pm0.492$ | $0.951\pm0.004$ | $\textbf{0.949} \pm \textbf{0.0001}$ |

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| SAPS-SW  | 5.60 s              | $0.053\pm0.010$ | $0.046\pm0.01$  | $\textbf{0.043} \pm \textbf{0.005}$  |

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| SAPS-SW  | 5.60 s              | $\textbf{0.053} \pm \textbf{0.010}$ | $\textbf{0.046} \pm \textbf{0.01}$ | $\textbf{0.043} \pm \textbf{0.005}$  |
| SAT4J-SW | 7.02 s              | (too many param.)                   | $1.19\pm0.58$                      | $\textbf{0.65} \pm \textbf{0.2}$     |

### **Speedup obtained by automated tuning** (SAPS default *vs* tuned on test set SW-GCP)



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# Two 'real-world" applications

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  - 26 parameters
  - Software verification: 500-fold speedup
  - Hardware verification: 4.5-fold speedup
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- 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 (under review)

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- Publically available at: http://www.cs.ubc.ca/labs/beta/Projects/ParamILS

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