Automating the Configuration of Algorithms for Solving Hard Computational Problems

Ph.D. Thesis Defence

Frank Hutter

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Parameters in Algorithms

Most algorithms have parameters

▶ Decisions that are left open during algorithm design
  – numerical parameters (e.g., real-valued thresholds)
  – categorical parameters (e.g., which heuristic to use)
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- Decisions that are left open during algorithm design
  - numerical parameters (e.g., real-valued thresholds)
  - categorical parameters (e.g., which heuristic to use)
- Set to maximize empirical performance
Real-world example for parameterized algorithms: commercial optimization tool CPLEX

- State of the art for mixed integer programming (MIP)

“Integer programming problems are more sensitive to specific parameter settings, so you may need to experiment with them.” [CPLEX 10.0 user manual, page 130]

- “Experiment with them” – Perform manual optimization in 63-dimensional space – Complex, unintuitive interactions between parameters – Humans are not good at that

→ developed the first automated tools for this type of problem
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- State of the art for mixed integer programming (MIP)
- Large user base
  - Over 1300 corporations and over 1000 universities

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Automated Algorithm Configuration

Automate the setting of algorithm parameters

- Eliminate most tedious part of algorithm design and end use
- Save development time
- Improve performance
Automated Algorithm Configuration

Automate the setting of algorithm parameters

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First to consider the general problem, in particular **many categorical parameters**
  - E.g. 50/63 CPLEX parameters are categorical
  - Algorithm configuration
Main Contribution of this thesis

Comprehensive study of the algorithm configuration problem
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Comprehensive study of the algorithm configuration problem

- Empirical analysis of configuration scenarios

- Demonstrated practical relevance of algorithm configuration
  - CPLEX: up to 23-fold speedup
  - SAT solver: 500-fold speedup for software verification
Main Contribution of this thesis

Comprehensive study of the algorithm configuration problem

- Empirical analysis of configuration scenarios
- Two fundamentally different solution approaches

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Outline

1. Problem Definition & Intuition
2. Model-Free Search for Algorithm Configuration
3. Model-Based Search for Algorithm Configuration
4. Conclusions
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Algorithm Configuration as Function Optimization

Deterministic algorithm with continuous parameters

- “Blackbox function” $f : \mathbb{R}^n \rightarrow \mathbb{R}$
- Can query function at arbitrary points $\theta \in \mathbb{R}^n$

Find $\min_{\theta \in \mathbb{R}^n} f(\theta)$
Algorithm Configuration as Function Optimization

Deterministic algorithm with continuous parameters

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- Can query function at arbitrary points $\theta \in \mathbb{R}^n$
  \[
  \text{Find } \min_{\theta \in \mathbb{R}^n} f(\theta)
  \]

Randomized algorithm with continuous parameters

- For each $\theta$: distribution $D_\theta$
- Optimize statistical parameter $\tau$ (e.g., expected value)
Algorithm Configuration as Function Optimization

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Randomized algorithm with continuous parameters

- For each $\theta$: distribution $D_\theta$
- Optimize statistical parameter $\tau$ (e.g., expected value)
- Can sample from distribution $D_\theta$ at arbitrary points $\theta \in \Theta$

$$\text{Find } \min_{\theta \in \mathbb{R}^n} \tau(D_\theta)$$
Algorithm Configuration: General Case

Difference to “standard” blackbox optimization

- Categorical parameters
Algorithm Configuration: General Case

Difference to “standard” blackbox optimization

- Categorical parameters
- Distribution of costs
  - across multiple repeated runs for randomized algorithms
  - across problem instances
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- Categorical parameters
- Distribution of costs
  - across multiple repeated runs for randomized algorithms
  - across problem instances
- Can terminate unsuccessful runs early
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   ParamILS: Iterated Local Search in Configuration Space
   “Real-World” Applications of ParamILS

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4. Conclusions
Simple manual approach for configuration

Start with some parameter configuration
Simple manual approach for configuration

Start with some parameter configuration

Modify a single parameter
Simple manual approach for configuration

Start with some parameter configuration

Modify a single parameter

if results on benchmark set improve then
   keep new configuration
Simple manual approach for configuration

Start with some parameter configuration
repeat
  Modify a single parameter
  if results on benchmark set improve then
    keep new configuration
until no more improvement possible (or “good enough”)
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⇝ Manually-executed local search
The ParamILS Framework

Iterated Local Search in parameter configuration space:

Choose initial parameter configuration \( \theta \)
Perform \textit{subsidiary local search} on \( \theta \)
The ParamILS Framework

Iterated Local Search in parameter configuration space:

1. Choose initial parameter configuration $\theta$
2. Perform *subsidiary local search* on $\theta$
3. While tuning time left:
   - $\theta' := \theta$
   - Perform *perturbation* on $\theta$
   - Perform *subsidiary local search* on $\theta$
The ParamILS Framework

Iterated Local Search in parameter configuration space:

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

1. $\theta' := \theta$
2. Perform perturbation on $\theta$
3. Perform subsidiary local search on $\theta$

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
The ParamILS Framework

Iterated Local Search in parameter configuration space:

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

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Based on *acceptance criterion*,
keep $\theta$ or revert to $\theta := \theta'$

With probability $p_{\text{restart}}$ randomly pick new $\theta$

$\rightsquigarrow$ Performs *biased random walk over local optima*
Instantiations of ParamILS Framework

How to evaluate each configuration?

- **BasicILS\((N)\):** perform fixed number of \(N\) runs to evaluate a configuration \(\theta\)
  - Blocking: use same \(N\) (instance, seed) pairs for each \(\theta\)

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- **BasicILS(\(N\))**: perform fixed number of \(N\) runs to evaluate a configuration \(\theta\)
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- **FocusedILS**: adaptive choice of \(N(\theta)\)
  - small \(N(\theta)\) for poor configurations \(\theta\)
  - large \(N(\theta)\) only for good \(\theta\)
How to evaluate each configuration?

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  - small $N(\theta)$ for poor configurations $\theta$
  - large $N(\theta)$ only for good $\theta$
  - typically outperforms BasicILS
Empirical Comparison to Previous Configuration Procedure

CALIBRA system [Adenso-Diaz & Laguna, '06]

- Based on fractional factorial designs
- Limited to continuous parameters
- Limited to 5 parameters
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Empirical comparison

- FocusedILS typically did better, never worse
- More importantly, much more general
Adaptive Choice of Cutoff Time

- Evaluation of poor configurations takes especially long

Results
- Provably never hurts
- Sometimes substantial speedups (factor 10)
Adaptive Choice of Cutoff Time

- Evaluation of poor configurations takes especially long
- Can terminate evaluations early
  - Incumbent solution provides bound
  - Can stop evaluation once bound is reached

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   ParamILS: Iterated Local Search in Configuration Space
   “Real-World” Applications of ParamILS

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Configuration of ILOG CPLEX

- Recall: 63 parameters, $1.78 \times 10^{38}$ possible configurations
- Ran FocusedILS for 2 days on 10 machines
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“A great deal of algorithmic development effort has been devoted to establishing default ILOG CPLEX parameter settings that achieve good performance on a wide variety of MIP models.” [CPLEX 10.0 user manual, page 247]
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Combinatorial auctions: 7-fold speedup
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Mixed integer knapsack: 23-fold speedup
Configuration of SAT Solver for Verification

SAT (propositional satisfiability problem)

- Prototypical $\mathcal{NP}$-hard problem
- Interesting theoretically and in practical applications
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Formal verification
- Bounded model checking
- Software verification
- Recent progress based on SAT solvers
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Spear, tree search solver for industrial SAT instances
- 26 parameters, \(8.34 \times 10^{17}\) configurations
Configuration of SAT Solver for Verification

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Compared to manually-engineered default

- 1 week of performance tuning
- competitive with the state of the art
Configuration of SAT Solver for Verification

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IBM Bounded Model Checking: 4.5-fold speedup
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Software verification: 500-fold speedup
\( \sim \) won 2007 SMT competition
Other Fielded Applications of ParamILS

- SAPS, local search for SAT
  - 8-fold and 130-fold speedup

- Applications by others
  - Protein folding [Thatchuk, Shmygelska & Hoos '07]
  - Time-tabling [Fawcett, Hoos & Chiarandini '09]
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- Demonstrates versatility & maturity
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  \[\Rightarrow\] demonstrates versatility & maturity
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3. Model-Based Search for Algorithm Configuration
   - State of the Art
   - Improvements for Stochastic Blackbox Optimization
   - Beyond Stochastic Blackbox Optimization

4. Conclusions
Fundamentally different approach for algorithm configuration

- So far: discussed local search approach
- Now: alternative choice, based on predictive models
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- Now: alternative choice, based on predictive models
  - Model-based optimization was less well developed
  - emphasis on methodological improvements
Model-Based Optimization: Motivation

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- Now: alternative choice, based on predictive models
  - Model-based optimization was less well developed
  ~ emphasis on methodological improvements
- In then end: state-of-the-art configuration tool
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EGO algorithm [Jones, Schonlau & Welch ’98]
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1. Get response values at initial design points
2. Fit a model to the data

![Graph showing the EGO algorithm process with DACE mean prediction and function evaluations.](image)
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3. Use model to pick most promising next design point

![Graphical representation of EGO algorithm](image)
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Stochastic Blackbox Optimization (BBO): State of the Art

Extensions of EGO algorithm for stochastic case

- Sequential Parameter Optimization (SPO)
  [Bartz-Beielstein, Preuss, Lasarczyk, '05-'09]
- Sequential Kriging Optimization (SKO)
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Application domain for stochastic BBO

- *Randomized* algorithms with continuous parameters
- Optimization for single instances
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Empirical Evaluation

- SPO more robust
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Improvements for stochastic BBO

I: Studied SPO components

▶ Improved component: “intensification mechanism”
  – Increase $N(\theta)$ similarly as in FocusedILS
  – Improved robustness
Improvements for stochastic BBO

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II: Better Models
   ▶ Compared various probabilistic models
     – Model SPO uses
       – Approximate Gaussian process (GP)
       – Random forest (RF)
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  – Model SPO uses
    – Approximate Gaussian process (GP)
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▶ New models much better
  – Resulting configuration procedure: ActiveConfigurator
  – **Improved state of the art** for model-based stochastic BBO
Improvements for stochastic BBO

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  - *Randomized* algorithm with continuous parameters
  - Optimization for single instances
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Extension I: Categorical Parameters

Models that can handle categorical inputs

▶ Random forests: out of the box
▶ Extended (approximate) Gaussian processes
  – new kernel based on weighted Hamming distance
Extension 1: Categorical Parameters

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Application domain

- Algorithms with categorical parameters
- Single instances
Extension 1: Categorical Parameters

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Application domain

▶ Algorithms with categorical parameters
▶ Single instances

Empirical evaluation

▶ ActiveConfigurator outperformed FocusedILS
Models incorporating multiple instances

- Can still learn probabilistic models of algorithm performance
- Model inputs:
  - algorithm parameters
  - instance features
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General algorithm configuration

- Algorithms with categorical parameters
- Multiple instances
Extension II: Multiple Instances

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  - algorithm parameters
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General algorithm configuration

- Algorithms with categorical parameters
- Multiple instances

Empirical evaluation

- ActiveConfigurator never worse than FocusedILS
- Overall: model-based approaches very promising
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Algorithm configuration

- Is a high-dimensional optimization problem
  - Can be solved by automated approaches
  - Sometimes much better than by human experts
Conclusions

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Scaling to very complex problems allows us to

- Build very flexible algorithm frameworks
- Apply automated tool to instantiate framework
  - Generate custom algorithms for different problem types
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Blackbox approaches

- Very general
- Can be used to optimize your parameters
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  - Model-free Iterated Local Search approach

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- Two fundamentally different solution approaches
  - Model-free Iterated Local Search approach
  - Improved & Extended Sequential Model-Based Optimization

- Demonstrated practical relevance of algorithm configuration
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Comprehensive study of the algorithm configuration problem

- Empirical analysis of configuration scenarios

- Two fundamentally different solution approaches
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[Ready for submission]

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- Explore other fields of applications
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