

# Automating the Configuration of Algorithms for Solving Hard Computational Problems

Ph.D. Thesis Defence

Frank Hutter

Supervisory committee:

Prof. Holger Hoos (supervisor)

Prof. Kevin Leyton-Brown (co-supervisor)

Prof. Kevin Murphy (co-supervisor)

Prof. Alan Mackworth

University Examiners:

Prof. Michael Friedlander (CS)

Prof. Lutz Lampe (ECE)

External Examiner: Prof. ?

Chair: Prof. John Nelson (Forestry)

# 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)

# 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)
- ▶ Set to maximize empirical performance

## Real-world example for parameterized algorithms: commercial optimization tool CPLEX

---

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

## Real-world example for parameterized algorithms: commercial optimization tool CPLEX

---

- ▶ State of the art for mixed integer programming (MIP)
- ▶ Large user base
  - Over 1 300 corporations and over 1 000 universities

## Real-world example for parameterized algorithms: commercial optimization tool CPLEX

---

- ▶ State of the art for mixed integer programming (MIP)
- ▶ Large user base
  - Over 1 300 corporations and over 1 000 universities
- ▶ 63 parameters that affect search trajectory

## Real-world example for parameterized algorithms: commercial optimization tool CPLEX

---

- ▶ State of the art for mixed integer programming (MIP)
- ▶ Large user base
  - Over 1 300 corporations and over 1 000 universities
- ▶ 63 parameters that affect search trajectory
  - “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]

## Real-world example for parameterized algorithms: commercial optimization tool CPLEX

---

- ▶ State of the art for mixed integer programming (MIP)
- ▶ Large user base
  - Over 1 300 corporations and over 1 000 universities
- ▶ 63 parameters that affect search trajectory
  - “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”



## Real-world example for parameterized algorithms: commercial optimization tool CPLEX

---

- ▶ State of the art for mixed integer programming (MIP)
- ▶ Large user base
  - Over 1 300 corporations and over 1 000 universities
- ▶ 63 parameters that affect search trajectory
  - “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

## Real-world example for parameterized algorithms: commercial optimization tool CPLEX

---

- ▶ State of the art for mixed integer programming (MIP)
- ▶ Large user base
  - Over 1 300 corporations and over 1 000 universities
- ▶ 63 parameters that affect search trajectory
  - “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**

## Real-world example for parameterized algorithms: commercial optimization tool CPLEX

---

- ▶ State of the art for mixed integer programming (MIP)
- ▶ Large user base
  - Over 1 300 corporations and over 1 000 universities
- ▶ 63 parameters that affect search trajectory
  - “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

# 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

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

# Main Contribution of this thesis

---

Comprehensive study of the algorithm configuration problem

- ▶ Empirical analysis of configuration scenarios

# Main Contribution of this thesis

---

Comprehensive study of the algorithm configuration problem

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



# Main Contribution of this thesis

---

## Comprehensive study of the algorithm configuration problem

- ▶ Empirical analysis of configuration scenarios
- ▶ Two fundamentally different solution approaches
  
- ▶ Demonstrated practical relevance of algorithm configuration

# Main Contribution of this thesis

---

## Comprehensive study of the algorithm configuration problem

- ▶ Empirical analysis of configuration scenarios
- ▶ Two fundamentally different solution approaches
  - 1<sup>st</sup> and 2<sup>nd</sup> approach  
to configure algorithms with many categorical parameters
- ▶ Demonstrated practical relevance of algorithm configuration

# Main Contribution of this thesis

---

## Comprehensive study of the algorithm configuration problem

- ▶ Empirical analysis of configuration scenarios
- ▶ Two fundamentally different solution approaches
  - 1<sup>st</sup> and 2<sup>nd</sup> approach  
to configure algorithms with many categorical parameters
- ▶ Demonstrated practical relevance of algorithm configuration
  - CPLEX: up to 23-fold speedup

# Main Contribution of this thesis

---

## Comprehensive study of the algorithm configuration problem

- ▶ Empirical analysis of configuration scenarios
- ▶ Two fundamentally different solution approaches
  - 1<sup>st</sup> and 2<sup>nd</sup> approach  
to configure algorithms with many categorical parameters
- ▶ Demonstrated practical relevance of algorithm configuration
  - CPLEX: up to 23-fold speedup
  - SAT solver: 500-fold speedup for software verification

# Outline

---

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

# Outline

---

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

# 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

- "Blackbox function"  $f : \mathbb{R}^n \rightarrow \mathbb{R}$
- 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

---

Deterministic algorithm with continuous parameters

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

$$\text{Find } \min_{\theta \in \mathbb{R}^n} f(\theta)$$

*Randomized* algorithm with continuous parameters

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

# Algorithm Configuration: General Case

---

## Difference to “standard” blackbox optimization

- ▶ Categorical parameters
- ▶ Distribution of costs
  - across multiple repeated runs for randomized algorithms
  - across problem instances
- ▶ Can *terminate* unsuccessful runs *early*

# Outline

---

1. Problem Definition & Intuition

2. Model-Free Search for Algorithm Configuration

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

3. Model-Based Search for Algorithm Configuration

4. Conclusions

# Outline

---

1. Problem Definition & Intuition
2. Model-Free Search for Algorithm Configuration  
ParamILS: Iterated Local Search in Configuration Space  
“Real-World” Applications of ParamILS
3. Model-Based Search for Algorithm Configuration
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”)*

## 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”)*

↔ Manually-executed **local search**

# The ParamLS Framework

---

## Iterated Local Search in parameter configuration space:

Choose initial parameter configuration  $\theta$

Perform *subsidiary local search* on  $\theta$

# The ParamLS Framework

---

## Iterated Local Search in parameter configuration space:

Choose initial parameter configuration  $\theta$

Perform *subsidiary local search* on  $\theta$

While tuning time left:

|  $\theta' := \theta$   
| Perform *perturbation* on  $\theta$   
| Perform *subsidiary local search* on  $\theta$

# The ParamLS Framework

---

## Iterated Local Search in parameter configuration space:

Choose initial parameter configuration  $\theta$

Perform *subsidiary local search* on  $\theta$

While tuning time left:

|  $\theta' := \theta$

| Perform *perturbation* on  $\theta$

| Perform *subsidiary local search* on  $\theta$

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

# The ParamLS Framework

---

## Iterated Local Search in parameter configuration space:

Choose initial parameter configuration  $\theta$

Perform *subsidiary local search* on  $\theta$

While tuning time left:

$\theta' := \theta$

Perform *perturbation* on  $\theta$

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**

# Instantiations of ParamLS Framework

---

How to evaluate each configuration?

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



# 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  $\theta$
- ▶ FocusedILS: adaptive choice of  $N(\theta)$ 
  - small  $N(\theta)$  for poor configurations  $\theta$
  - large  $N(\theta)$  only for good  $\theta$

# 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  $\theta$
- ▶ FocusedILS: adaptive choice of  $N(\theta)$ 
  - 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

# 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

Empirical comparison

- ▶ Focused ILS typically did better, never worse
- ▶ More importantly, much more general

## Adaptive Choice of Cutoff Time

---

- ▶ Evaluation of poor configurations takes especially long

## 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

# 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
- ▶ Results
  - Provably never hurts
  - Sometimes substantial speedups (factor 10)

# Outline

---

1. Problem Definition & Intuition

2. Model-Free Search for Algorithm Configuration

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

3. Model-Based Search for Algorithm Configuration

4. Conclusions



## Configuration of ILOG CPLEX

---

- ▶ Recall: 63 parameters,  $1.78 \times 10^{38}$  possible configurations
- ▶ Ran FocusedILS for 2 days on 10 machines

## Configuration of ILOG CPLEX

---

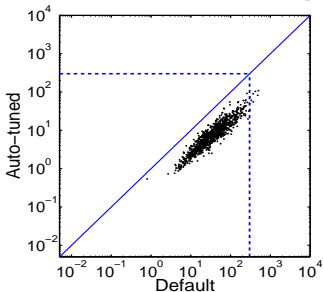
- ▶ Recall: 63 parameters,  $1.78 \times 10^{38}$  possible configurations
- ▶ Ran FocusedILS for 2 days on 10 machines
- ▶ Compared against default
  - “A great deal of algorithmic development effort has been devoted to establishing default ILOG CPLEX parameter settings that achieve good performance on a wide variety of MIP models.” [CPLEX 10.0 user manual, page 247]

# Configuration of ILOG CPLEX

---

- ▶ Recall: 63 parameters,  $1.78 \times 10^{38}$  possible configurations
- ▶ Ran FocusedILS for 2 days on 10 machines
- ▶ Compared against default

“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]

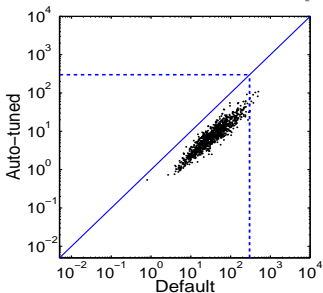


Combinatorial auctions: 7-fold speedup

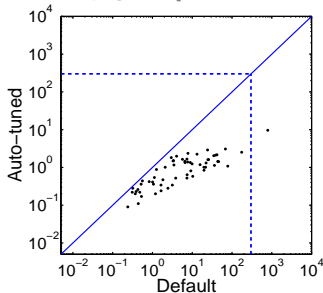
# Configuration of ILOG CPLEX

- ▶ Recall: 63 parameters,  $1.78 \times 10^{38}$  possible configurations
- ▶ Ran FocusedILS for 2 days on 10 machines
- ▶ Compared against default

“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]



Combinatorial auctions: 7-fold speedup



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

# Configuration of SAT Solver for Verification

---

SAT (propositional satisfiability problem)

- Prototypical  $\mathcal{NP}$ -hard problem
- Interesting theoretically and in practical applications

Formal verification

- Bounded model checking
- Software verification
- Recent progress based on SAT solvers

# Configuration of SAT Solver for Verification

---

SAT (propositional satisfiability problem)

- Prototypical  $\mathcal{NP}$ -hard problem
- Interesting theoretically and in practical applications

Formal verification

- Bounded model checking
- Software verification
- Recent progress based on SAT solvers

Spear, tree search solver for industrial SAT instances

- 26 parameters,  $8.34 \times 10^{17}$  configurations

# Configuration of SAT Solver for Verification

---

- ▶ Ran FocusedILS for 2 days on 10 machines



# Configuration of SAT Solver for Verification

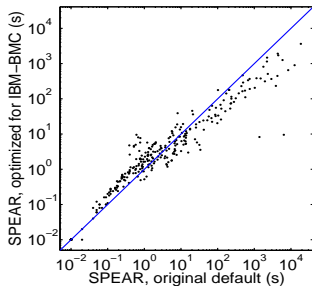
---

- ▶ Ran FocusedILS for 2 days on 10 machines
- ▶ Compared to manually-engineered default
  - 1 week of performance tuning
  - competitive with the state of the art

# Configuration of SAT Solver for Verification

---

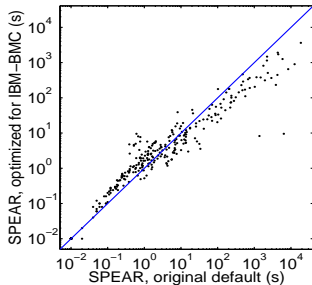
- ▶ Ran FocusedILS for 2 days on 10 machines
- ▶ Compared to manually-engineered default
  - 1 week of performance tuning
  - competitive with the state of the art



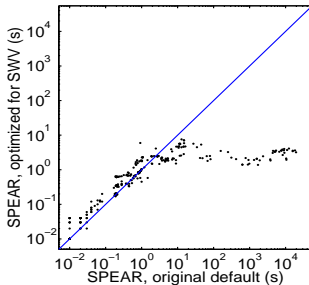
IBM Bounded Model Checking:  
4.5-fold speedup

# Configuration of SAT Solver for Verification

- ▶ Ran FocusedILS for 2 days on 10 machines
- ▶ Compared to manually-engineered default
  - 1 week of performance tuning
  - competitive with the state of the art



IBM Bounded Model Checking:  
4.5-fold speedup



Software verification: 500-fold speedup  
↪ won 2007 SMT competition

## Other Fielded Applications of ParamLS

---

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

## Other Fielded Applications of ParamLS

---

- ▶ SAPS, local search for SAT
  - ↪ 8-fold and 130-fold speedup
- ▶ SAT4J, tree search for SAT
  - ↪ 11-fold speedup

## Other Fielded Applications of ParamILS

---

- ▶ SAPS, local search for SAT
  - ↪ 8-fold and 130-fold speedup
- ▶ SAT4J, tree search for SAT
  - ↪ 11-fold speedup
- ▶ GLS<sup>+</sup> for Most Probable Explanation (MPE) problem
  - ↪ > 360-fold speedup

## Other Fielded Applications of ParamILS

---

- ▶ SAPS, local search for SAT
  - ↪ 8-fold and 130-fold speedup
- ▶ SAT4J, tree search for SAT
  - ↪ 11-fold speedup
- ▶ GLS<sup>+</sup> for Most Probable Explanation (MPE) problem
  - ↪ > 360-fold speedup
- ▶ Applications by others
  - Protein folding [Thatchuk, Shmygelska & Hoos '07]
  - Time-tabling [Fawcett, Hoos & Chiarandini '09]
  - Local Search for SAT [Khudabukhsh, Xu, Hoos, & Leyton-Brown '09]

## Other Fielded Applications of ParamILS

---

- ▶ SAPS, local search for SAT
  - ↪ 8-fold and 130-fold speedup
- ▶ SAT4J, tree search for SAT
  - ↪ 11-fold speedup
- ▶ GLS<sup>+</sup> for Most Probable Explanation (MPE) problem
  - ↪ > 360-fold speedup
- ▶ Applications by others
  - Protein folding [Thatchuk, Shmygelska & Hoos '07]
  - Time-tabling [Fawcett, Hoos & Chiarandini '09]
  - Local Search for SAT [Khudabukhsh, Xu, Hoos, & Leyton-Brown '09]
  - ↪ demonstrates versatility & maturity



# Outline

---

1. Problem Definition & Intuition
2. Model-Free Search for Algorithm Configuration
3. Model-Based Search for Algorithm Configuration
  - State of the Art
  - Improvements for Stochastic Blackbox Optimization
  - Beyond Stochastic Blackbox Optimization
4. Conclusions

# Model-Based Optimization: Motivation

---

Fundamentally different approach for algorithm configuration

- ▶ So far: discussed local search approach
- ▶ Now: alternative choice, based on predictive models

# Model-Based Optimization: Motivation

---

Fundamentally different approach for algorithm configuration

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

# Model-Based Optimization: Motivation

---

Fundamentally different approach for algorithm configuration

- ▶ So far: discussed local search approach
- ▶ Now: alternative choice, based on predictive models
  - Model-based optimization was less well developed
  - ↪ emphasis on methodological improvements
- ▶ In the end: state-of-the-art configuration tool

# Outline

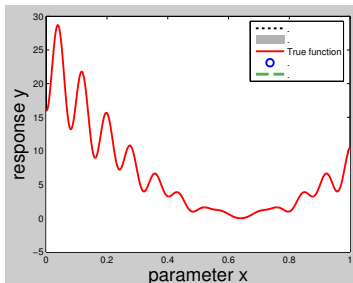
---

1. Problem Definition & Intuition
2. Model-Free Search for Algorithm Configuration
3. Model-Based Search for Algorithm Configuration
  - State of the Art
  - Improvements for Stochastic Blackbox Optimization
  - Beyond Stochastic Blackbox Optimization
4. Conclusions

# Model-Based Deterministic Blackbox Optimization (BBO)

---

EGO algorithm [Jones, Schonlau & Welch '98]

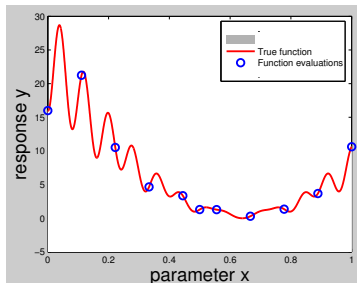


# Model-Based Deterministic Blackbox Optimization (BBO)

---

EGO algorithm [Jones, Schonlau & Welch '98]

1. Get response values at initial design points

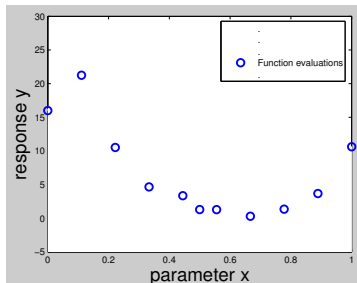


# Model-Based Deterministic Blackbox Optimization (BBO)

---

EGO algorithm [Jones, Schonlau & Welch '98]

1. Get response values at initial design points

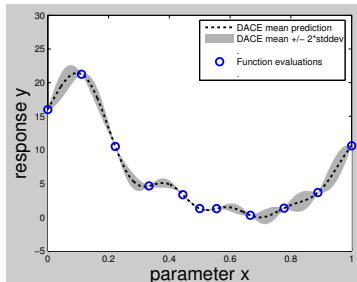




# Model-Based Deterministic Blackbox Optimization (BBO)

EGO algorithm [Jones, Schonlau & Welch '98]

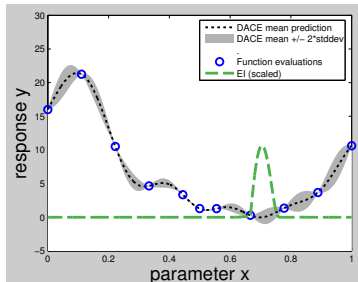
1. Get response values at initial design points
2. Fit a model to the data



# Model-Based Deterministic Blackbox Optimization (BBO)

EGO algorithm [Jones, Schonlau & Welch '98]

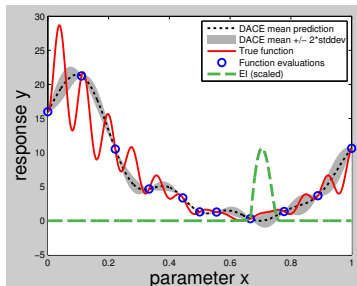
1. Get response values at initial design points
2. Fit a model to the data
3. Use model to pick most promising next design point



# Model-Based Deterministic Blackbox Optimization (BBO)

EGO algorithm [Jones, Schonlau & Welch '98]

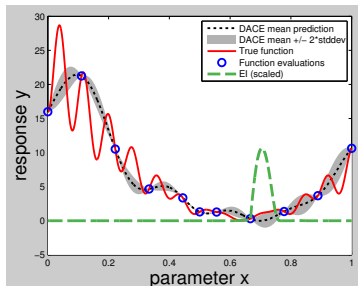
1. Get response values at initial design points
2. Fit a model to the data
3. Use model to pick most promising next design point
4. Repeat 2. and 3. until time is up



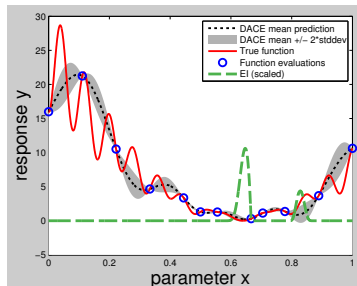
# Model-Based Deterministic Blackbox Optimization (BBO)

EGO algorithm [Jones, Schonlau & Welch '98]

1. Get response values at initial design points
2. Fit a model to the data
3. Use model to pick most promising next design point
4. Repeat 2. and 3. until time is up



First step



Second step

# 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)

[Huang, Allen, Notz & Zeng, '06]

# 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)

[Huang, Allen, Notz & Zeng, '06]

Application domain for stochastic BBO

- ▶ *Randomized* algorithms with continuous parameters
- ▶ Optimization for single instances

# 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)

[Huang, Allen, Notz & Zeng, '06]

## Application domain for stochastic BBO

- ▶ *Randomized* algorithms with continuous parameters
- ▶ Optimization for single instances

## Empirical Evaluation

- ▶ SPO more robust

# Outline

---

1. Problem Definition & Intuition
2. Model-Free Search for Algorithm Configuration
3. Model-Based Search for Algorithm Configuration
  - State of the Art
  - Improvements for Stochastic Blackbox Optimization
  - Beyond Stochastic Blackbox Optimization
4. Conclusions



# 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

---

## I: Studied SPO components

- ▶ Improved component: “intensification mechanism”
  - Increase  $N(\theta)$  similarly as in FocusedILS
  - Improved robustness

## II: Better Models

- ▶ Compared various probabilistic models
  - Model SPO uses
  - Approximate Gaussian process (GP)
  - Random forest (RF)

# Improvements for stochastic BBO

---

## I: Studied SPO components

- ▶ Improved component: “intensification mechanism”
  - Increase  $N(\theta)$  similarly as in FocusedILS
  - Improved robustness

## II: Better Models

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

# Improvements for stochastic BBO

---

## I: Studied SPO components

- ▶ Improved component: “intensification mechanism”
  - Increase  $N(\theta)$  similarly as in FocusedILS
  - Improved robustness

## II: Better Models

- ▶ Compared various probabilistic models
  - Model SPO uses
  - Approximate Gaussian process (GP)
  - Random forest (RF)
- ▶ New models much better
  - Resulting configuration procedure: ActiveConfigurator
  - **Improved state of the art** for model-based stochastic BBO
  - *Randomized* algorithm with continuous parameters
  - Optimization for single instances

# Outline

---

1. Problem Definition & Intuition
2. Model-Free Search for Algorithm Configuration
3. Model-Based Search for Algorithm Configuration
  - State of the Art
  - Improvements for Stochastic Blackbox Optimization
  - Beyond Stochastic Blackbox Optimization**
4. Conclusions

## 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 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

## Application domain

- ▶ Algorithms with categorical parameters
- ▶ Single instances

# 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

## Application domain

- ▶ Algorithms with categorical parameters
- ▶ Single instances

## Empirical evaluation

- ▶ **ActiveConfigurator outperformed FocusedILS**



## Extension II: Multiple Instances

---

### Models incorporating multiple instances

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

## Extension II: Multiple Instances

---

### Models incorporating multiple instances

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

### General algorithm configuration

- ▶ Algorithms with categorical parameters
- ▶ Multiple instances

## Extension II: Multiple Instances

---

### Models incorporating multiple instances

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

### General algorithm configuration

- ▶ Algorithms with categorical parameters
- ▶ Multiple instances

### Empirical evaluation

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

# Outline

---

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

# Conclusions

---

## Algorithm configuration

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

# Conclusions

---

## Algorithm configuration

- ▶ Is a high-dimensional optimization problem
  - Can be solved by automated approaches
  - Sometimes much better than by human experts
- ▶ Can cut development time & improve results

# Conclusions

---

## Algorithm configuration

- ▶ Is a high-dimensional optimization problem
  - Can be solved by automated approaches
  - Sometimes much better than by human experts
- ▶ Can cut development time & improve results

## 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

# Conclusions

---

## Algorithm configuration

- ▶ Is a high-dimensional optimization problem
  - Can be solved by automated approaches
  - Sometimes much better than by human experts
- ▶ Can cut development time & improve results

## 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

## Blackbox approaches

- ▶ Very general
- ▶ Can be used to optimize *your* parameters



# Main Contribution of this thesis

---

Comprehensive study of the algorithm configuration problem

# Main Contribution of this thesis

---

Comprehensive study of the algorithm configuration problem

- ▶ Empirical analysis of configuration scenarios
- ▶ Two fundamentally different solution approaches
- ▶ Demonstrated practical relevance of algorithm configuration

# Main Contribution of this thesis

---

Comprehensive study of the algorithm configuration problem

- ▶ Empirical analysis of configuration scenarios
- ▶ Two fundamentally different solution approaches
- ▶ Demonstrated practical relevance of algorithm configuration

# Main Contribution of this thesis

---

Comprehensive study of the algorithm configuration problem

- ▶ Empirical analysis of configuration scenarios
- ▶ Two fundamentally different solution approaches
  - Model-free Iterated Local Search approach
- ▶ Demonstrated practical relevance of algorithm configuration

# Main Contribution of this thesis

---

Comprehensive study of the algorithm configuration problem

- ▶ Empirical analysis of configuration scenarios
- ▶ Two fundamentally different solution approaches
  - Model-free Iterated Local Search approach
  - Improved & Extended Sequential Model-Based Optimization
- ▶ Demonstrated practical relevance of algorithm configuration

# Main Contribution of this thesis

---

Comprehensive study of the algorithm configuration problem

- ▶ Empirical analysis of configuration scenarios
- ▶ Two fundamentally different solution approaches
  - Model-free Iterated Local Search approach
  - Improved & Extended Sequential Model-Based Optimization
- ▶ Demonstrated practical relevance of algorithm configuration

# Main Contribution of this thesis

---

## Comprehensive study of the algorithm configuration problem

- ▶ Empirical analysis of configuration scenarios
- ▶ Two fundamentally different solution approaches
  - Model-free Iterated Local Search approach
  - Improved & Extended Sequential Model-Based Optimization
- ▶ Demonstrated practical relevance of algorithm configuration
  - CPLEX: up to 23-fold speedup
  - SPEAR: 500-fold speedup for software verification

# Main Contribution of this thesis

---

## Comprehensive study of the algorithm configuration problem

- ▶ Empirical analysis of configuration scenarios  
[Ready for submission]
- ▶ Two fundamentally different solution approaches
  - Model-free Iterated Local Search approach [AAAI'07]
  - Improved & Extended Sequential Model-Based Optimization [GECCO'09; EMOA'09]
- ▶ Demonstrated practical relevance of algorithm configuration
  - CPLEX: up to 23-fold speedup [JAIR'09]
  - SPEAR: 500-fold speedup for software verification [FMCAD'07]



# Important Directions for the Next Few Years

---

- ▶ Improve configuration procedures from practical point of view
  - Mixed categorical/numerical optimization
  - Make easier to use off the shelf

# Important Directions for the Next Few Years

---

- ▶ Improve configuration procedures from practical point of view
  - Mixed categorical/numerical optimization
  - Make easier to use off the shelf
- ▶ More sophisticated model-based methods
  - Use model to select most informative instance
  - Use model to select best cutoff time
  - Per-instance setting of parameters

# Important Directions for the Next Few Years

---

- ▶ Improve configuration procedures from practical point of view
  - Mixed categorical/numerical optimization
  - Make easier to use off the shelf
- ▶ More sophisticated model-based methods
  - Use model to select most informative instance
  - Use model to select best cutoff time
  - Per-instance setting of parameters
- ▶ Explore other fields of applications

# Thanks to

---

- ▶ Supervisory committee
  - Holger Hoos (supervisor)
  - Kevin Leyton-Brown (co-supervisor)
  - Kevin Murphy (co-supervisor)
  - Alan Mackworth
- ▶ Further collaborators
  - Domagoj Babić
  - Thomas Bartz-Beielstein
  - Youssef Hamadi
  - Alan Hu
  - Thomas Stützle
  - Dave Tompkins
  - Lin Xu
- ▶ LCI and BETA lab faculty and students