Automatic solver configuration using SMAC How to boost performance of your SAT solver?

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SAT Industrial Day 2016, Bordeaux





¹Thanks to Frank Hutter!

Ever looked into --help?

MiniSat (10 parameters)

```
CORE OPTIONS:
 -rnd-init, -no-rnd-init
                                        (default: off)
  -luby. -no-luby
                                        (default: on)
 -rnd-freq = <double> [ 0 .. 1] (default: 0)
 -rnd-seed = <double> ( 0 .. inf) (default: 9.16483e+07)
 -var-decay = <double> ( 0 .. 1) (default: 0.95)
 -cla-decay = <double> ( 0 .. 1) (default: 0.95)
-rinc = <double> ( 1 .. inf) (default: 2)
 -gc-frac = <double> ( 0 .. inf) (default: 0.2)
 -rfirst = <int32> [ 1 .. imax] (default: 100)
 -ccmin-mode = <int32> [ 0 .. 2] (default: 2)
 -phase-saving = \langle int32 \rangle [ 0 .. 2] (default: 2)
MAIN OPTIONS:
 -verb = <int32> [ 0 .. 2] (default: 1)
 -cpu-lim = <int32> [ 0 .. imax] (default: 2147483647)
 -mem-lim
               = <int32> [ 0 .. imax] (default: 2147483647)
HELP OPTIONS:
 --help Print help message.
 <u>--help-ver</u>b Print verbose help message.
```

Ever looked into --help?

Glucose (20 parameters)

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- K	= <double> (</double>) (default:	0.8)
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SIMP OPTION				
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-simp-gc-	frac = <double> (</double>) (default:	0.5)
-grow] (default:	
-sub-lim	= <int32> [</int32>	-1 inax] (default:	
-cl-lim	= <int32> [</int32>] (default:	
HELP OPTION:				
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Algorithm Configuration

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lingeling (> 300 parameters)

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Algorithm Configuration

Importance of Algorithm Configuration?

SAT Competition

- Submission of a solver
- Same parameter configuration on all instances
- → Robust performance across instances
- \rightsquigarrow Similar to downloading a solver and using its defaults
 - \$ lingeling inst.cnf

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Configurable SAT Solver Challenge (CSSC)

- Submission of a solver
- We tuned the parameter configuration for each instance set
- → Peak performance on each set
 - \$ lingeling inst.cnf cce3wait=2 deco=1 saturating=73 lkhdmisifelmrtc=0

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Importance of Algorithm Configuration? (from CSSC)

Lingeling on CircuitFuzz (#TOs: $30 \rightarrow 18$)



Importance of Algorithm Configuration? (from CSSC)





Importance of Algorithm Configuration? (from CSSC)

ProbSAT on 5SAT500 (#TOs: $250 \rightarrow 0$)



In a Nutshell: Algorithm Configuration

How to automatically determine a well-performing parameter configuration with SMAC?

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How to automatically determine a well-performing parameter configuration with SMAC?

Focus on basics

- State-of-the-art in algorithm configuration (Focus: SMAC)
- 2 Parameter importance
- Advanced Topics

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In a Nutshell: Algorithm Configuration

How to automatically determine a well-performing parameter configuration with SMAC?

Focus on basics

- State-of-the-art in algorithm configuration (Focus: SMAC)
- Parameter importance
- 3 Advanced Topics
 - Please ask questions
 - All literature references are hyperlinks

Slides at: www.ml4aad.org

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1 The Algorithm Configuration Problem

- Problem Statement
- Overview of Methods

2 Using AC Systems

- 3 Importance of Parameters
- 4 Advanced Topics

Manual Tuning

- Requires a lot of expert knowledge about the solver and the instances
- Tedious and time-intensive task for a human
- Error-prone to human bias

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Automatic Tuning

- More systematic search (less error-prone)
- Costs only computational time (after a short setup phase)
- Expensive human-time can be used for more creative tasks

Why Automated Algorithm Configuration?

Manual Tuning

- Requires a lot of expert knowledge about the solver and the instances
- Tedious and time-intensive task for a human
- Error-prone to human bias
- 1 week of a software developer costs: $\approx 1000-2000~{\rm EURO}$

Automatic Tuning

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- Costs only computational time (after a short setup phase)
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- $1~\mathrm{CPU}$ week costs in the cloud: $\approx 2-5~\mathrm{EURO}$

- Automatic algorithm configuration tool
- Combining cutting-edge optimization and machine learning methods

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Advantages by using SMAC

- Real algorithm configuration (opposed to "parameter tuning")
 - Handles different types of parameters
 - Considers instances

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Advantages by using SMAC

• Real algorithm configuration (opposed to "parameter tuning")

- Handles different types of parameters
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- 2 Efficient in the number of function evaluations
- Very efficient for runtime optimization

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Parameters of *MiniSAT*

MiniSAT

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-rnd-init, -nd -luby, -no-lu	o-rnd-init by					(default: (default:	off) on)	
-rnd-freq -rnd-seed -var-decay -cla-decay -rinc -gc-frac	= <double> = <double> = <double> = <double> = <double> = <double></double></double></double></double></double></double>		0 0 0 1 0		1] inf) 1) inf) inf)	(default: (default: (default: (default: (default: (default:	0) 9.16483e+07) 0.95) 0.999) 2) 0.2)	
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help help-verb	Print help Print verbo	mess ose l	sag hel	e. pr	nessage	2.		

Algorithm Parameters

Parameter Types

• Continuous, integer, ordinal

• Categorical: finite domain, unordered, e.g., {apple, tomato, pepper}

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Parameter space has structure

- E.g., parameter θ_2 of heuristic H is only active if H is used $(\theta_1 = H)$
- In this case, we say $heta_2$ is a conditional parameter with parent $heta_1$
- Sometimes, some combinations of parameter settings are forbidden e.g., the combination of $\theta_3=1$ and $\theta_4=2$ is forbidden

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Parameters give rise to a structured space of configurations

- \bullet Many configurations (e.g., SAT solver $\it lingeling$ with 10^{947})
- Configurations often yield qualitatively different behaviour
- $\rightarrow\,$ Algorithm Configuration (as opposed to "parameter tuning")



Algorithm Configuration - in More Detail



Definition: algorithm configuration

Given:

- a parameterized algorithm \mathcal{A} with possible parameter settings Θ ;
- \bullet a distribution ${\cal D}$ over problem instances with domain ${\cal I};$ and

Algorithm Configuration - in More Detail



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- a parameterized algorithm ${\mathcal A}$ with possible parameter settings $\Theta;$
- \bullet a distribution ${\cal D}$ over problem instances with domain ${\cal I};$ and
- a cost metric $m : \Theta \times \mathcal{I} \to \mathbb{R}$ (wrt a runtime cutoff).

Algorithm Configuration - in More Detail



Definition: algorithm configuration

Given:

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- \bullet a distribution ${\cal D}$ over problem instances with domain ${\cal I};$ and
- a cost metric $m : \Theta \times \mathcal{I} \to \mathbb{R}$ (wrt a runtime cutoff).

Find: $\theta^* \in \arg\min_{\theta \in \Theta} \mathbb{E}_{\pi \sim \mathcal{D}}(m(\theta, \pi)).$

Challenges of Algorithm Configuration

Expensive Algorithm Runs

- Evaluation of 1 configuration on 1 instance is already expensive (SAT: solving a \mathcal{NP} -complete problem)
- $\bullet\,$ Evaluation of n>1000 configurations on m>100 instances can be infeasible in practice

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Structured high-dimensional parameter space

- Categorical vs. continuous parameters
- Conditionals between parameters

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Structured high-dimensional parameter space

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Stochastic optimization

- Randomized algorithms: optimization across various seeds
- Distribution of benchmark instances (often wide range of hardness)
- Subsumes so-called *multi-armed bandit problem*

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Algorithm Configuration: Components



Algorithm Configuration: Components



Required Components of an Algorithm Configurator

- Which configuration to choose?
- 2 How to evaluate a configuration?

Component 1: Which Configuration to Choose?

For this component, we can consider a simpler problem: Blackbox function optimization: $\min_{\theta \in \Theta} f(\theta)$

• Only mode of interaction: query $f(\theta)$ at arbitrary $\theta \in {old O}$

$$\theta \rightarrow f(\theta)$$
Component 1: Which Configuration to Choose?

For this component, we can consider a simpler problem: Blackbox function optimization: $\min_{\theta \in \Theta} f(\theta)$

• Only mode of interaction: query $f(\theta)$ at arbitrary $\theta \in {old O}$

$$\theta \rightarrow f(\theta)$$

- Abstracts away the complexity of evaluating multiple instances
- A query is expensive
- Θ is still a structured space
 - Mixed continuous/discrete
 - Conditional parameters

- Trade-off between diversification and intensification
- The extremes
 - Random search
 - Gradient Descent

- Trade-off between diversification and intensification
- The extremes
 - Random search
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- Stochastic local search (SLS)
- Population-based methods
- SMAC \rightarrow Model-based Optimization (e.g. Bayesian Optimization)

• . . .

Popular approach in the statistics literature since [Mockus, 1978]

- Efficient in # function evaluations
- Works when objective is nonconvex, noisy, has unknown derivatives, etc
- Recent convergence results

[Srinivas et al, 2010; Bull 2011; de Freitas et al, 2012; Kawaguchi et al, 2015]

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General approach

- Fit a probabilistic model to the collected function samples $\langle \theta, f(\theta) \rangle$
- Use the model to guide optimization, trading off exploration vs exploitation

Bayesian Optimization – Detour into Machine Learning





Bayesian Optimization - Detour into Machine Learning

t = 3



Bayesian Optimization – Detour into Machine Learning





Empirical Performance Models

Given:

- Configuration space $\Theta = \Theta_1 \times \cdots \times \Theta_n$
- For each problem instance π_i : $\mathbf{f_i}$, a vector of feature values
- Observed algorithm runtime data: $\langle (heta_i, \mathbf{f}_i, y_i)
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Find: a mapping $\hat{m} : [\theta, \mathbf{f}] \mapsto y$ predicting performance (regression model)

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Which type of regression model?

- Rich literature on performance prediction (overview: [Hutter et al, AIJ 2014])
- \bullet Here: we use a model \hat{m} based on random forests

Instance Features

Instance features are numerical representations of instances.

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Static Features

- Problem size features
- Variable-Clause graph features
- Variable graph features
- Clause graph features
- Balance features

Probing Features

- DPLL probing
- LP-based Probing
- SLS Probing
- CDCL Probing
- Survey Propagation

Also used in algorithm selection.

Component 2: How to Evaluate a Configuration?

Back to the general algorithm configuration problem

- Distribution over problem instances with domain \mathcal{I} ;
- Performance metric $m: \Theta \times \mathcal{I} \to \mathbb{R}$
- $c(\theta) = \mathbb{E}_{\pi \sim \mathcal{D}}(m(\theta, \pi))$
- Algorithm runs are expensive!

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Simplest, suboptimal solution: use N runs for each evaluation

- Treats the problem as a blackbox function optimization problem
- Issue: how large to choose N?
 - too small: overtuning
 - too large: every function evaluation is slow

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General principle to strive for

- Don't waste time on bad configurations
- Evaluate good configurations more thoroughly

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Algorithm Configuration

Problem: which one of N candidate algorithms is best?

- Start with empty set of runs for each algorithm
- Iteratively:
 - Perform one run each
 - Discard inferior candidates
 - E.g., as judged by a statistical test (e.g., F-race uses an F-test)

• Stop when a single candidate remains or configuration budget expires

Toy Example

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Only importance: Is a challenger better than the best known

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Race new configurations against the best known

- Discard poor new configurations quickly
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Race new configurations against the best known

- Discard poor new configurations quickly
 - If challenger is worse on the first instance, discard it.
- Evaluate best configurations with many runs
- No requirement for statistical domination

Search component should allow to return to configurations discarded because they were "unlucky"

When minimizing algorithm runtime,

we can terminate runs for poor configurations θ' early:

• Is θ' better than θ ?



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we can terminate runs for poor configurations θ' early:

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• Can terminate evaluation of θ' once guaranteed to be worse than θ

Algorithm 2: SMAC

Initialize with a single run for the default

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Learn a RF model from data so far: $\hat{m}: \boldsymbol{\Theta} \times \mathcal{I} \rightarrow \mathbb{R}$

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Algorithm 2: SMAC

Initialize with a single run for the default

repeat

 $\begin{array}{|c|c|c|c|} \mbox{Learn a RF model from data so far: } \hat{m}: \Theta \times \mathcal{I} \to \mathbb{R} \\ \mbox{Aggregate over instances: } \hat{f}(\theta) = \mathbb{E}_{\pi \sim \mathcal{D}}(\hat{m}(\theta, \pi)) \\ \mbox{Use model } \hat{f} \mbox{ to select promising configurations} \\ \mbox{Race selected configurations against best known} \\ \mbox{until time budget exhausted} \end{array}$



Overview on algorithm configuration systems

- Sequential Model-based Algorithm Configuration (SMAC) [Hutter et al, since 2011]
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 - Parameters are genes and populations consists of parameter settings
 - + already parallelized
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- Parameters are genes and populations consists of parameter settings
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 - Requires adaption of GGA settings
- Iterated F-Race [López-Ibáñez et al, 2011]
 - Sampling of configurations and racing them
 - + Well maintained package in R
 - Not suited for runtime optimization

The Algorithm Configuration Problem

2 Using AC Systems

3 Importance of Parameters

Advanced Topics



SMAC Configurator implemented in JAVA

• Flexible but harder to setup



SMAC Configurator implemented in JAVA

- Flexible but harder to setup
- pySMAC Python Interface to SMAC
 - Very easy if you want to optimize a Python function



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 pySMAC Python Interface to SMAC

 Very easy if you want to optimize a Python function

 SpySMAC SAT-pySMAC: an easy-to-use AC framework for SAT-solvers

 Less flexibility, but adapted to SAT solving



SMAC Configurator implemented in JAVA

 Flexible but harder to setup

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Example: MiniSAT [Een et al, '03-'07]

MiniSAT (http://minisat.se/) is a SAT solver that is

- minimalistic,
- open-source,
- and developed to help researchers and developers alike to get started

Example: MiniSAT [Een et al, '03-'07]

MiniSAT (http://minisat.se/) is a SAT solver that is

- minimalistic,
- open-source,
- and developed to help researchers and developers alike to get started
- MiniSAT has 8 (performance-relevant) parameters

CORE OPTIONS:						
-rnd-init, -nd -luby, -no-lub	o-rnd-init by				(default: (default:	off) on)
-rnd-freq -rnd-seed -var-decay -cla-decay -rinc -gc-frac	<pre>= <double> = <double> = <double> = <double> = <double> = <double> = <double></double></double></double></double></double></double></double></pre>		0 0 0 1 0	1] inf) 1) inf) inf)	(default: (default: (default: (default: (default: (default:	0) 9.16483e+07) 0.95) 0.999) 2) 0.2)
-rfirst -ccmin-mode -phase-saving	= <int32> = <int32> = <int32></int32></int32></int32>	[[]	1 0 0	imax] 2] 2]	(default: (default: (default:	100) 2) 2)

Determine optimized configuration

- \$ python SpySMAC_run.py
- -i swv-inst/SWV-GZIP/
- -b minisat/core/minisat
- -p minisat/pcs.txt
- -o minisat-logs

- -c 2
- -B 60

- $\leftarrow \mathsf{Call}$
- $\leftarrow \mathsf{Instances}$
- $\leftarrow \mathsf{Binary}$
- $\leftarrow \text{Configuration Space}$
- $\leftarrow \mathsf{log-files}$
- \leftarrow parameter prefix
- $\leftarrow \mathsf{cutoff}$
- \leftarrow budget [sec]

Different Types of Parameters

• As for other combinatorial problems, there is a standard representation that different configuration procedures can read

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The simple standard format: PCS

- PCS (short for "parameter configuration space")
- human readable/writable
- allows to express a wide range of parameter types

```
rnd-freq [0,1][0]
var-decay [0.001,1][0.95]1
cla-decay [0.001,1][0.999]1
rinc [1.00001,1024][2]1
gc-frac [0,1][0.2]
rfirst [1,10000000][100]i1
ccmin-mode {0,1,2}[2]
phase-saving {0,1,2}[2]
```

CORE OPTIONS:

```
-rnd-init, -no-rnd-init
                                      (default: off)
 -luby. -no-luby
                                      (default: on)
 -rnd-freg
              = <double> [
                            0 .. 1] (default: 0)
 -rnd-seed
                            0 .. inf) (default: 9.16483e+07)
              = <double> (
 -var-decay
              = <double> (
                            0 .. 1) (default: 0.95)
 -cla-decay
              = <double> (
                            0 .. 1) (default: 0.999)
 -rinc
              = < double> (
                            1 .. inf) (default: 2)
 -gc-frac
              = <double> (
                            0 .. inf) (default: 0.2)
 -rfirst
              = <int32> [
                            1 .. imaxl (default: 100)
 -ccmin-mode
              = <int32> [
                            0.. 21 (default: 2)
 -phase-saving = <int32> [
                                   21 (default: 2)
MAIN OPTIONS:
                           0 .. 21 (default: 1)
 -verb
              = <int32> [
 -verb
-cpu-lim
              = <int32> [
                           0 .. imax] (default: 2147483647)
 -mem-lim
                            0 .. imax] (default: 2147483647)
              = <int32> [
HELP OPTIONS:
 --help
              Print help message.
 --help-verb
              Print verbose help message.
```

Configuration Budget

- Dictated by your resources and needs
 - E.g., start configuration before leaving work on Friday
- The longer the better (but diminishing returns)
 - Rough rule of thumb: at least enough time for $1000 \ {\rm target} \ {\rm runs}$
 - $\bullet\,$ But have also achieved good results with 50 target runs in some cases

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Maximal cutoff time per target run

- Dictated by your needs (typical instance hardness, etc.)
- Too high: slow progress
- Too low: possible overtuning to easy instances
- $\bullet\,$ For SAT etc, often use at least 300 CPU seconds

Live Demo of a SpySMAC Report

The Algorithm Configuration Problem

2 Using AC Systems

3 Importance of Parameters

- Ablation
- fANOVA

4 Advanced Topics

Recommendations & Observation

- Configure all parameters that could influence performance
- Dependent on the instance set, different parameters matter
- How to determine the important parameters?

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Example

- SAT-solver *lingeling* has more than 300 parameters
- Often, less than 10 are important to optimize performance

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Idea

- Comparison of two parameter configurations
- Starting from the default, we change the value of the parameters
- Which of these changes were important?
- $\rightarrow\,$ Ablation compares parameter flips between default and optimized configuration

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Basic Approach

- Iterate over all non-flipped parameters
- Flip the parameter with the largest influence on the performance in each iteration



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4 Advanced Topics

Using an EPM $\hat{m}: \Theta \to \mathbb{R}$, predict the performance of configurations θ .

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fANOVA [Sobol 1993]

Using *fANOVA*, write performance predictions \hat{y} as a sum of components:

$$\hat{y}(\theta_1,\ldots,\theta_n) = \hat{m}_0 + \sum_{i=1}^n \hat{m}_i(\theta_i) + \sum_{i\neq j} \hat{m}_{ij}(\theta_i,\theta_j) + \ldots$$

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With variance decomposition, compute the performance variance explained by a single parameter (or combinations of them)

Application to Parameter Importance

How much of the variance can be explained by a parameter (or combinations of parameters) marginalized over all other parameters?

lingeling on circuit fuzz

Parameter	Importance		
score	24.95		
minlocalgluelim	6.52		
blkclslim	0.85		
gaussreleff	0.85		
blksuccesslim	0.79		
seed	0.70		
unhdinpr	0.51		
gluekeep	0.47		
trnrmaxeff	0.47		
blkboostvlim	0.47		

fANOVA Example



Ablation

- + Only method to compare two configurations
 - Needs a lot of algorithm runs \rightarrow slow

fANOVA

- + EPM can be trained by the performance data collected during configuration
- + Considers the complete configuration space or only "interesting" areas
- Importance of interactions between parameters can be expensive

1 The Algorithm Configuration Problem

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Advanced Topics

- (Current) Algorithm configurators can only be effectively applied to homogeneous instance sets
 - there exists a configuration that performs well on all instances

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 - there exists a configuration that performs well on all instances
- Robustness on heterogeneous instance sets is also important
- How to deal with heterogeneous instance sets?
 - Parallel portfolios, i.e., running a set of complementary algorithms/configurations in parallel
 - Algorithm Selection

ACPP

Given sequential algorithm \mathcal{A} and configuration space Θ , automatically find a complementary portfolio of configurations running in parallel.

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	lingeling on industrial		clasp on hard combinatorial	
	# TOs	PAR1	#TOs	PAR1
Sequential Solver	S			
Default	72	373	137	481
Configured	68	368	140	473
Parallel Solvers w	ith 8 cores	5		
Default	64	345	96	358

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Default	64	345	96	358
parHydra	55	303	96	353

	<i>clasp</i> (hard combinatorial)	
Solver set	#TOs	PAR1
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Default	96	358
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Default+CS	90	333
parHydra	96	353
parHydra+default CS	90	347

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Solver set	#TOs	PAR1
Parallel Solvers with 8 cores		
Default	96	358
Default+CS	90	333
parHydra	96	353
parHydra+default CS	90	347
parHydra+tuned CS	88	346

Complementary Configurations via Algorithm Configuration

Hydra [Xu et al, AAAI 2010] iteratively build a complementary portfolio

ISAC [Kadioglu et al, ECAI 2010] use unsupervised clustering to get instance clusters and determine a configuration for each of them

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Algorithm Selection [Rice, 1976]

Using machine learning, predict the best performing algorithm (or parameter configuration) for a given instance.

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 \rightsquigarrow Riss BlackBox [Alfonso & Manthey, 2014] won 3 medals with such an approach in the SAT Competition 2014

Robust Benchmark Sets [Hoos et al., LION 2013]

Heterogenous vs. Homogeneous Instances

- Homogeneous: there is one configuration performing well on all
 - Similar properties, e.g., from the same encoding
- Heterogeneous: no configuration performing well on all
 - perfect for algorithm selection
 - hard to configure on such instances

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Heterogeneous Benchmark Sets for Robust Configuration

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 - Different properties should be uniformly represented

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 - Too easy: will results generalize to harder instances?
 - Rule of thumb: mix of hardness ranges

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- Free of duplicates

Further Tools & Material

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- E.g., resuming SMAC runs, warmstarting with previous runs, etc.

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Ask questions in the SMAC Forum

https://groups.google.com/forum/#!forum/smac-forum

• It can also help to read through others' issues and solutions

Algorithm Configuration is Widely Applicable

- Hard combinatorial problems
 - SAT, MIP, TSP, AI planning, ASP, Time-tabling, ...
 - UBC exam time-tabling since 2010
- Game Theory: Kidney Exchange
- Mobile Robotics
- Monte Carlo Localization
- Motion Capture
- Machine Learning
 - Automated Machine Learning
 - Deep Learning

Also popular in industry

- Better performance
- Increased productivity



Thank you!

