Algorithm Configuration:
How to boost performance of your SAT solver?

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\[ \text{ML4AAD} \]

\footnote{Thanks to Frank Hutter!}
Ever looked into --help?

MiniSat (10 parameters)

CORE OPTIONS:
- \texttt{rnd-init, -no-rnd-init} \hspace{1cm} (default: off)
- \texttt{luby, -no-luby} \hspace{1cm} (default: on)
- \texttt{rnd-freq} = \texttt{<double>} [0 .. 1] (default: 0)
- \texttt{rnd-seed} = \texttt{<double>} (0 .. inf) (default: 9.16483e+07)
- \texttt{var-decay} = \texttt{<double>} (0 .. 1) (default: 0.95)
- \texttt{cla-decay} = \texttt{<double>} (0 .. 1) (default: 0.999)
- \texttt{rinc} = \texttt{<double>} (1 .. inf) (default: 2)
- \texttt{gc-frac} = \texttt{<double>} (0 .. inf) (default: 0.2)
- \texttt{rfirst} = \texttt{<int32>} [1 .. imax] (default: 100)
- \texttt{ccmin-mode} = \texttt{<int32>} [0 .. 2] (default: 2)
- \texttt{phase-saving} = \texttt{<int32>} [0 .. 2] (default: 2)

MAIN OPTIONS:
- \texttt{verb} = \texttt{<int32>} [0 .. 2] (default: 1)
- \texttt{cpu-lin} = \texttt{<int32>} [0 .. imax] (default: 2147483647)
- \texttt{mem-lin} = \texttt{<int32>} [0 .. imax] (default: 2147483647)

HELP OPTIONS:
- \texttt{--help} Print help message.
- \texttt{--help-verb} Print verbose help message.
Ever looked into --help?

Glucose (20 parameters)
Ever looked into --help?

lingeling (> 300 parameters)
Importance of Algorithm Configuration?

SAT Competition

- Submission of a solver
- Same parameter configuration on all instances

→ Robust performance across instances
Importance of Algorithm Configuration?

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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
Importance of Algorithm Configuration? (Example from CSSC)

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

![Graph showing the comparison between default and configured times with timeout values.](image-url)
Importance of Algorithm Configuration? (Example from CSSC)

Clasp on Rooks (\#TOs: 81 → 0)

![Graph showing the relationship between default and configured times with various timeout settings.]

- Default in sec.: $10^{-2}$, $10^{-1}$, 1, 10, 100
- Configured in sec.: 2x, 2x, 10x, 10x, 100x, 100x, 300
- Timeout: 2x, 10x, 100x
Importance of Algorithm Configuration? (Example from CSSC)

ProbSAT on 5SAT500 (#TOs: 250 → 0)

![Graph showing the importance of algorithm configuration with ProbSAT on 5SAT500. The graph compares the default and configured times for solving the problem with different timeouts. The x-axis represents the default time in seconds, and the y-axis represents the configured time in seconds. The graph includes lines for different timeouts (2x, 10x, 100x), indicating the improvement in performance when configuring the algorithm.]
In a Nutshell: Algorithm Configuration

How to *automatically* determine a well-performing parameter configuration?
## In a Nutshell: Algorithm Configuration

How to **automatically** determine a well-performing parameter configuration?

## Focus on basics

1. State-of-the-art in algorithm configuration
2. Parameter importance
3. Pitfalls and best practices in algorithm configuration
In a Nutshell: Algorithm Configuration

How to automatically determine a well-performing parameter configuration?

Focus on basics

1. State-of-the-art in algorithm configuration
2. Parameter importance
3. Pitfalls and best practices in algorithm configuration

- Please ask questions
- No special background assumed
- All literature references are hyperlinks

Slides at: www.ml4aad.org
1. The Algorithm Configuration Problem
   - Problem Statement
   - Motivation: a Success Stories
   - Overview of Methods

2. Using AC Systems

3. Importance of Parameters

4. Pitfalls and Best Practices

5. Final Remarks
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Algorithm Parameters

Parameter Types

- Continuous, integer, ordinal
- Categorical: finite domain, unordered, e.g., \{apple, tomato, pepper\}

Parameter space has structure

E.g., parameter $\theta_2$ of heuristic $H$ is only active if $H$ is used ($\theta_1 = H$)

In this case, we say $\theta_2$ is a conditional parameter with parent $\theta_1$

Sometimes, some combinations of parameter settings are forbidden

e.g., the combination of $\theta_3 = 1$ and $\theta_4 = 2$ is forbidden

Parameters give rise to a structured space of configurations

Many configurations (e.g., SAT solver lingeling with $10^{947}$)

Configurations often yield qualitatively different behaviour

→ Algorithm Configuration (as opposed to “parameter tuning”)
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Parameters of MiniSAT

**MiniSAT**

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Algorithm Configuration Visualized

Parameter domains & starting values

Configurator

Calls with different parameter settings

Configuration scenario

Target algorithm

Solves

Problem instances

Returns solution cost
Algorithm Configuration – in More Detail

Definition: algorithm configuration

Given:

- a parameterized algorithm $A$ with possible parameter settings $\Theta$;
- a distribution $D$ over problem instances with domain $\mathcal{I}$; and
Definition: algorithm configuration

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- a cost metric $m : \Theta \times \mathcal{I} \to \mathbb{R}$,
Definition: algorithm configuration

Given:

- a parameterized algorithm $\mathcal{A}$ with possible parameter settings $\Theta$;
- a distribution $\mathcal{D}$ over problem instances with domain $\mathcal{I}$; and
- a cost metric $m : \Theta \times \mathcal{I} \to \mathbb{R}$,

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

Algorithm Configuration – in More Detail

Instances $\mathcal{I}$

Algorithm $\mathcal{A}$ and its Configuration Space $\Theta$

Select $\theta \in \Theta$ and $\pi \in \mathcal{I}$

Run $\mathcal{A}(\theta)$ on $\pi$ to measure $m(\theta, \pi)$

Returns Best Configuration $\hat{\theta}$

Configuration Task
1 The Algorithm Configuration Problem
   • Problem Statement
   • Motivation: a Success Stories
   • Overview of Methods

2 Using AC Systems

3 Importance of Parameters

4 Pitfalls and Best Practices

5 Final Remarks
Configuration of a SAT Solver for Verification [Hutter et al, 2007]

Formal verification

- Software verification [Babić & Hu; CAV ’07]
- Hardware verification (Bounded model checking) [Zarpas; SAT ’05]
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Tree search solver for SAT-based verification
- SPEAR, developed by Domagoj Babić at UBC
- 26 parameters, $8.34 \times 10^{17}$ configurations
Ran *ParamILS*, 2 days × 10 machines
  - On a training set from each benchmark
Ran *ParamILS*, 2 days \( \times \) 10 machines
- On a training set from each benchmark

Compared to manually-engineered configuration
- 1 week of performance tuning
- Competitive with the state of the art
- Comparison on unseen test instances
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4.5-fold speedup on hardware verification
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4.5-fold speedup on hardware verification

500-fold speedup $\leadsto$ won category QF_BV in 2007 SMT competition
Algorithm Configuration is Widely Applicable

- Hard combinatorial problems
  - SAT, MIP, TSP, AI planning, ASP, Time-tableting, ...
  - UBC exam time-tableling 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
Outline

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Challenges of Algorithm Configuration

Expensive Algorithm Runs

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

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**Structured high-dimensional parameter space**
- Categorical vs. continuous parameters
- Conditionals between parameters
Challenges of Algorithm Configuration

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Structured high-dimensional parameter space
- Categorical vs. continuous parameters
- Conditionals between parameters

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

1. 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 \( \theta \in \Theta \)

\[
\theta \rightarrow \text{black box} \rightarrow f(\theta)
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\[ \theta \rightarrow \text{Blackbox} \rightarrow f(\theta) \]

- Abstracts away the complexity of evaluating multiple instances
- A query is expensive
- \( \Theta \) is still a structured space
  - Mixed continuous/discrete
  - Conditional parameters
Component 1: Which Configuration to Evaluate?

- Trade-off between diversification and intensification
- The extremes
  - Random search
  - Gradient Descent
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How would you solve this problem?
Component 1: Which Configuration to Evaluate?

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

How would you solve this problem?

- Stochastic local search (SLS)
- Population-based methods
- Model-based Optimization (e.g. Bayesian Optimization)
- ...
Back to the general algorithm configuration problem

- Distribution over problem instances with domain $\mathcal{I}$;
- Performance metric $m : \Theta \times \mathcal{I} \rightarrow \mathbb{R}$
- $c(\theta) = \mathbb{E}_{\pi \sim D}(m(\theta, \pi))$
Component 2: How to Evaluate a Configuration?

Back to the general algorithm configuration problem

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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
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
Saving Time: Aggressive Racing

- Race new configurations against the best known
  - Discard poor new configurations quickly
  - No requirement for statistical domination
  - Evaluate best configurations with many runs
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- Search component should allow to return to configurations discarded because they were “unlucky”
Saving More Time: Adaptive Capping

When minimizing algorithm runtime, we can terminate runs for poor configurations $\theta'$ early:

- Is $\theta'$ better than $\theta$?
  - Example:

![Diagram showing comparison of runtime for configurations $\theta$ and $\theta'$]

RT$(\theta)=20$  RT$(\theta')>20$
When minimizing algorithm runtime, we can terminate runs for poor configurations $\theta'$ early:

- Is $\theta'$ better than $\theta$?
  - Example:

  ![Diagram](image)

  - RT($\theta$) = 20
  - RT($\theta'$) > 20

- Can terminate evaluation of $\theta'$ once guaranteed to be worse than $\theta$
General algorithm configuration systems

- **ParamILS** [Hutter et al, 2007 & 2009]
- **Gender-based Genetic Algorithm (GGA)** [Ansotegui et al, 2009]
- **Iterated F-Race** [López-Ibáñez et al, 2011]
- **Sequential Model-based Algorithm Configuration (SMAC)** [Hutter et al, since 2011]
Algorithm 1: Manual Greedy Algorithm Configuration

Start with some configuration $\theta$
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Modify a single parameter
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if results on benchmark set improve then
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Start with some configuration $\theta$

repeat
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until no more improvement possible (or “good enough”)
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$\leadsto$ Manually-executed first-improvement local search
Going Beyond Local Optima: Iterated Local Search

Animation credit: Holger Hoos
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Initialization

Animation credit: Holger Hoos
Going Beyond Local Optima: Iterated Local Search

Local Search

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Perturbation

Animation credit: Holger Hoos
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Animation credit: Holger Hoos
Selection (using Acceptance Criterion)

Animation credit: Holger Hoos
Going Beyond Local Optima: Iterated Local Search

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The *ParamILS* Framework [Hutter et al, 2007 & 2009]

ParamILS = Iterated Local Search in parameter configuration space

Appears: biased random walk over local optima
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*ParamILS* = Iterated Local Search in parameter configuration space

〜 Performs *biased random walk over local optima*

---

**How to evaluate a configuration’s quality?**

- **BasicILS**(N): use $N$ fixed instances
- **FocusedILS**: increase #instances for good configurations over time
The *ParamILS* Framework [Hutter et al, 2007 & 2009]

**Advantages**

- Theoretically shown to converge
- Often quickly finds local improvements over default (can exploit a good default)
- Very randomized $\rightarrow$ almost $k$-fold speedup for $k$ parallel runs

**Disadvantages**

- Very randomized $\rightarrow$ unreliable when only run once for a short time
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Genetic algorithm for algorithm configuration

- Genes = parameter values
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### Genetic algorithm for algorithm configuration

- **Genes** = parameter values
- **Population**: trades of exploration and exploitation
- Use $N$ instances to evaluate configurations in each generation
  - Increase $N$ in each generation: linearly from $N_{\text{start}}$ to $N_{\text{end}}$
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Disadvantages

- User has to specify \#generations ahead of time
- Not recommended for small budgets and categorical parameters
Iterated F-race [López-Ibáñez et al, 2011]

**Basic Idea**
- Use F-Race as a building block
- Iteratively sample configurations to race

**Advantages**
- Can parallelize easily: runs of each racing iteration are independent
- Well-supported software package (for the community that uses R)

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SMAC in a Nutshell [Hutter et al, since 2011]

SMAC = Sequential Model-based Algorithm Configuration

- Use a predictive model of algorithm performance to guide the search
- Combine this search strategy with aggressive racing & adaptive capping
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**One SMAC iteration**
- Construct a model to predict performance
- Use that model to select promising configurations
- Compare each of the selected configurations against the best known
  - Using a similar procedure as FocusedILS
Bayesian Optimization – Detour into Machine Learning

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
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**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]
Empirical Performance Models

Given:

- Configuration space \( \Theta = \Theta_1 \times \cdots \times \Theta_n \)
- For each problem instance \( \pi_i: f_i \), a vector of feature values
- Observed algorithm runtime data: \( \langle (\theta_i, f_i, y_i) \rangle_{i=1}^N \)

Find: a mapping \( \hat{m} : [\theta, f] \mapsto y \) predicting performance
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Which type of regression model?
- Rich literature on performance prediction (overview: [Hutter et al, AIJ 2014])
- Here: we use a model $\hat{m}$ based on random forests
Instance Features for SAT [Hutter et al, 2014]

Instance Features

Instance features are numerical representations of instances.
Instance Features for SAT

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What could be instance features for CNFs?
Instance Features for SAT

Instance Features

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What could be instance features for CNFs?

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
Algorithm 2: SMAC

Initialize with a single run for the default
Algorithm 2: SMAC

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Learn a RF model from data so far: $\hat{m}: \Theta \times \mathcal{I} \rightarrow \mathbb{R}$
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Use model $\hat{f}$ to select promising configurations

Race selected configurations against best known
Algorithm 2: SMAC

Initialize with a single run for the default

repeat

- Learn a RF model from data so far: \( \hat{m} : \Theta \times \mathcal{I} \rightarrow \mathbb{R} \)
- Aggregate over instances: \( \hat{f}(\theta) = \mathbb{E}_{\pi \sim D}(\hat{m}(\theta, \pi)) \)
- Use model \( \hat{f} \) to select promising configurations
- Race selected configurations against best known

until time budget exhausted
Outline

1 The Algorithm Configuration Problem
2 Using AC Systems
3 Importance of Parameters
4 Pitfalls and Best Practices
5 Final Remarks
**SMAC** Configurator implemented in JAVA

**pySMAC** Python Interface to **SMAC**

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

- **SMAC** Configurator implemented in JAVA
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Future: One tool in Python.
Example: *MiniSAT* \cite{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 on SAT.
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*MiniSAT* has 8 (performance-relevant) 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: 0.999)
-rinc      = <double> ( 1 ..  inf) (default: 2)
-gc-frac   = <double> ( 0 ..  inf) (default: 0.2)
-rfirs    = <int32> [ 1 ..  imax] (default: 100)
-ccmn-mode = <int32> [ 0 ..  2] (default: 2)
-phase-saving = <int32> [ 0 ..  2] (default: 2)
```
Hands-on: SpySMAC

Determine optimized configuration

```
$ python SpySMAC_run.py
-i swv-inst/SWV-GZIP/
-b minisat/core/minisat
-p minisat/pcs.txt
-o minisat-logs
--prefix "-"
-c 2
-B 60
```

← Call
← Instances
← Binary
← Configuration Space
← log-files
← parameter prefix
← cutoff
← budget [sec]
There are many different types of parameter

- 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
PCS Example: *MiniSAT*

```plaintext
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] 1
rfirst [1,10000000] [100] 1
ccmin-mode {0,1,2} [2] 1
phase-saving {0,1,2} [2] 1
```
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: typically at least enough time for 1000 target runs
  - But have also achieved good results with 50 target runs in some cases
Decision: Configuration Budget and Cutoff

Configuration Budget

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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
- For SAT etc, often use at least 300 CPU seconds
Live Demo of a SpySMAC Report
Outline

1. The Algorithm Configuration Problem
2. Using AC Systems
3. Importance of Parameters
   - Ablation
   - fANOVA
4. Pitfalls and Best Practices
5. Final Remarks
Parameter Importance

Recommendations & Observation

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

Example

SAT-solver lingeling has more than 300 parameters. Often, less than 10 are important to optimize performance.
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Ablation [Fawcett et al. 2013]

Idea

- Starting from the default configuration, we change the value of the parameters
- Which of these changes were important?

→ Ablation compares parameter flips between default and incumbent configuration
Ablation  [Fawcett et al. 2013]

Idea
- Starting from the default configuration, we change the value of the parameters
- Which of these changes were important?
  → Ablation compares parameter flips between default and incumbent configuration

Basic Approach
- Iterate over all non-flipped parameters
- Flip the parameter with the largest influence on the performance in each iteration
Ablation Example: *Spear on SWV*

![Graph showing performance (PAR10, s) vs. number of parameters modified]

Source: [Fawcett et al. 2013]
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Reminder: Empirical Performance Model (EPM)

Using an EPM \( \hat{m} : \Theta \rightarrow \mathbb{R} \), predict the performance of configurations \( \theta \).
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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)
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Application to Parameter Importance

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

*lingeling on circuit fuzz*

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Importance</th>
</tr>
</thead>
<tbody>
<tr>
<td>score</td>
<td>24.95</td>
</tr>
<tr>
<td>minlocalgluelim</td>
<td>6.52</td>
</tr>
<tr>
<td>blkclslim</td>
<td>0.85</td>
</tr>
<tr>
<td>gaussreleff</td>
<td>0.85</td>
</tr>
<tr>
<td>blksuccesslim</td>
<td>0.79</td>
</tr>
<tr>
<td>seed</td>
<td>0.70</td>
</tr>
<tr>
<td>unhdlnpr</td>
<td>0.51</td>
</tr>
<tr>
<td>gluekeep</td>
<td>0.47</td>
</tr>
<tr>
<td>trnrmaxeff</td>
<td>0.47</td>
</tr>
<tr>
<td>blkboostvlim</td>
<td>0.47</td>
</tr>
</tbody>
</table>
probSAT on 3-SAT instances
Comparison Parameter Importance Procedures

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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4. Pitfalls and Best Practices
   - Overtuning
   - General Advice

5. Final Remarks
Outline

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Generalization of Performance

The dark ages

1. Student tweaks the parameters manually on 10 problems until it works
2. Supervisor may not even know about the tuning
3. Results get published without acknowledging the tuning
4. Of course, the approach *does not generalize*
Generalization of Performance

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How to do better?
## Generalization of Performance

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### A step further

- Optimize parameters on a **training set**
- Evaluate generalization on a **test set**
Generalization of Performance

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A step further

- Optimize parameters on a training set
- Evaluate generalization on a test set

Even better: avoid “peeking” at the test set

- Put test set into a vault (i.e., never look at it)
- Split training set again into training and validation set
- Only use test set in the end to generate results for publication
The concept of overtuning

Very related to overfitting in machine learning

- Performance improves on the training set
- Performance does not improve on the test set, and may even degrade
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More pronounced for more heterogeneous benchmark sets

- But it even happens for very homogeneous sets
- Indeed, one can even overfit on a single instance, to the seeds used for training
### Example: minimizing SLS solver runlengths for a single SAT instance

- **Training cost**, here based on $N=100$ runs with different seeds
- **Test cost** of $\hat{\theta}$ here based on 1000 new seeds
Example: minimizing SLS solver runlengths for a single SAT instance

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![Graph showing runlengths vs CPU time](image)
Overtuning is Stronger For Smaller Training Sets

Best Practice
Provide as many instances as possible, and we will take care to run only as many as necessary.
Overtuning is Stronger For Smaller Training Sets

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Provide as many instances as possible, and we will take care to run only as many as necessary.
Several communities dislike randomness

Key arguments: **reproducibility, tracking down bugs**

- I agree these are important
- But you can achieve them by keeping track of your seeds
- In fact: your tests will cover more cases when randomized
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Key arguments: **reproducibility, tracking down bugs**
- I agree these are important
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It’s much easier to get more seeds than more instances
- Performance should generalize to new seeds
- Otherwise, it’s less likely to generalize to new instances
Different Types of Overtuning

One can overtune to various specifics of the training setup:

- To the specific \textit{instances} used in the training set
- To the specific \textit{seeds} used in the training set
Different Types of Overtuning

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- To the (small) runtime cutoff used during training
- To a particular machine type
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- To the specific *instances* used in the training set
- To the specific *seeds* used in the training set
- To the (small) *runtime cutoff* used during training
- To a *particular machine type*
- To the *type of instances* in the training set
  - These should just be drawn according to the distribution of interest
  - But in practice, the distribution might change over time
Outline

1 The Algorithm Configuration Problem

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4 Pitfalls and Best Practices
   - Overtuning
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5 Final Remarks
Choosing the Training Instances #1

Split instance set into training and test sets

- Configure on the training instances $\rightarrow$ configuration $\hat{\theta}$
- Run (only) $\hat{\theta}$ on the test instances $\rightarrow$ unbiased performance estimate
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Configuring on your test instances

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Fine practice

Do multiple configuration runs and pick the $\hat{\theta}$ with the best training performance
AC works much better on homogeneous instance sets

- Instances have something in common
  - E.g., come from the same problem domain
  - E.g., use the same encoding
- One configuration likely to perform well on all instances
Choosing the Training Instances #2

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Pitfall

Configuration on too heterogeneous sets (e.g., SAT Competition)

→ There often is no single great overall configuration
Choosing the Training Instances: Recommendation

Representative instances

- Representative of the instances you want to solve later

<table>
<thead>
<tr>
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- Too easy: will results generalize to harder instances?
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**Simplest method: use multiple independent configurator runs**

This can work very well [Hutter et al, LION 2012]

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- SMAC: about 8-fold speedup with 16 runs
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### Parallel SMAC (p-SMAC) [unpublished]

Simple asynchronous scheme

- Simply execute $k$ different SMAC runs with different seeds
- Add `--shared-model-mode true`
Advanced Topics

Automatic Construction of Parallel Portfolios [Lindauer et al, AIJ 2016]

parallel portfolio of complementary parameter configurations
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**SpyBug: Automated Bug Detection** [Manthey et al, SAT 2016]
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**Per-Instance Algorithm Selection** [Xu et al, AAAI 2010]
selection of a well-performing configuration for an instance at hand
Further tips and tricks

Further Tools

- see www.ml4aad.org

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http://aclib.net/smac

Quickstart guide, FAQ, extensive manual

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

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Thank you!