Programming by Optimisation:

A Practical Paradigm for Computer-Aided Algorithm Design

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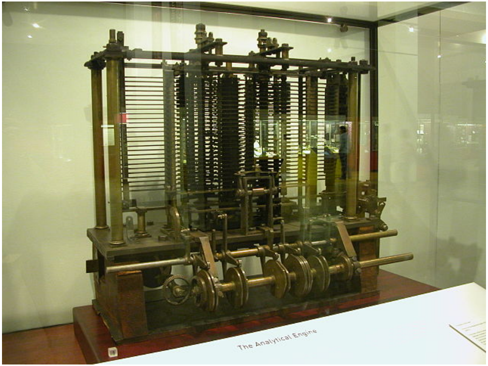
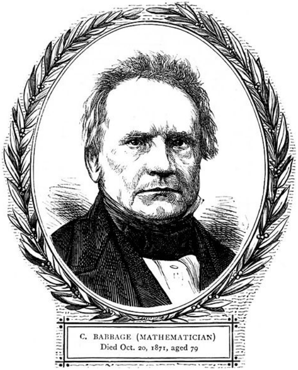
The age of machines





"As soon as an Analytical Engine exists, it will necessarily guide the future course of the science. Whenever any result is sought by its aid, the question will then arise – by what course of calculation can these results be arrived at by the machine in the shortest time?"

(Charles Babbage, 1864)

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When algorithms control the world

By Jane Wakefield
Technology reporter

If you were expecting some kind of warning when computers finally get smarter than us, then think again.

There will be no soothing HAL 9000-type voice informing us that our human services are now surplus to requirements.

In reality, our electronic overlords are already taking control, and they are doing it in a far more subtle way than science fiction would have us believe.

Their weapon of choice - the algorithm.

Behind every smart web service is some even smarter web code. From the web retailers - calculating what books and films we might be interested in, to Facebook's friend finding and image tagging services, to the search engines that guide us around the net.

Algorithms are spreading their influence around the globe

It is these invisible computations that increasingly control how we interact with our electronic world.

At last month's TEDGlobal conference, algorithm expert Kevin Slavin delivered one of the tech show's most "sit up and take notice" speeches where he warned that the "maths that computers use to decide stuff" was infiltrating every aspect of our lives.

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Are search engines skewing objectivity?

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"The maths[!] that computers use to decide stuff [is] infiltrating every aspect of our lives."

- financial markets
- social interactions
- cultural preferences
- artistic production
- ...

Performance matters ...

- computation speed (time is money!)
- energy consumption (battery life, ...)
- quality of results (cost, profit, weight, ...)

... increasingly:

- globalised markets
- just-in-time production & services
- tighter resource constraints

Example: Resource allocation

- resources $>$ demands $\rightsquigarrow$ many solutions, easy to find

  economically wasteful

  $\rightsquigarrow$ reduction of resources / increase of demand

- resources $<$ demands $\rightsquigarrow$ no solution, easy to demonstrate

  lost market opportunity, strain within organisation

  $\rightsquigarrow$ increase of resources / reduction of demand

- resources $\approx$ demands

  $\rightsquigarrow$ difficult to find solution / show infeasibilityresources $\approx$ demands

  $\rightsquigarrow$ difficult to find solution / show infeasibility

This tutorial:

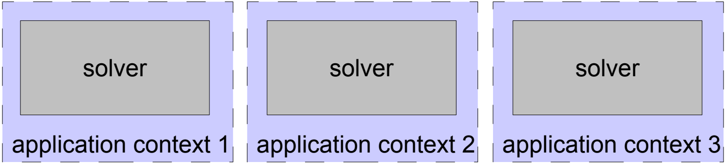
new approach to software development, leveraging ...

- human creativity
- optimisation & machine learning
- large amounts of computation / data

Key idea:

- program $\rightsquigarrow$ (large) space of programs
- encourage software developers to
  - avoid premature commitment to design choices
  - seek & maintain design alternatives
- automatically find performance-optimising designs for given use context(s)

$\Rightarrow$ Programming by Optimization (PbO)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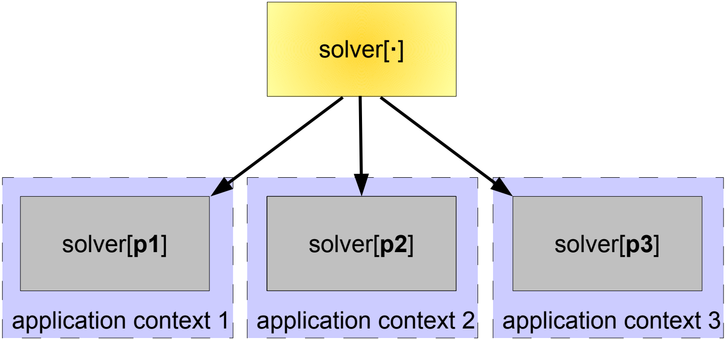
application context 1
application context 2
application context 3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application context 2
application context 3

Outline

1. Programming by Optimization: Motivation & Introduction
2. Algorithm Configuration (incl. Coffee Break)
3. Portfolio-based Algorithm Selection
4. Software Development Support & Further Directions

Programming by Optimization: Motivation & Introduction

Example: SAT-based software verification

Hutter, Babić, Hoos, Hu (2007)

- **Goal:** Solve SAT-encoded software verification problems as fast as possible
- new DPLL-style SAT solver SPEAR (by Domagoj Babić)
  = highly parameterised heuristic algorithm
  (26 parameters, $\approx 8.3 \times 10^{17}$ configurations)
- manual configuration by algorithm designer
- automated configuration using ParamILS, a generic algorithm configuration procedure
  Hutter, Hoos, Stützle (2007)

SPEAR: Performance on software verification benchmarks

solver	num. solved	mean run-time
MiniSAT 2.0	302/302	161.3 CPU sec
SPEAR original	298/302	787.1 CPU sec
SPEAR generic. opt. config.	302/302	35.9 CPU sec
SPEAR specific. opt. config.	302/302	1.5 CPU sec

- $\approx$ 500-fold speedup through use automated algorithm configuration procedure (ParamILS)
- new state of the art
  (winner of 2007 SMT Competition, QF_BV category)

Levels of PbO:

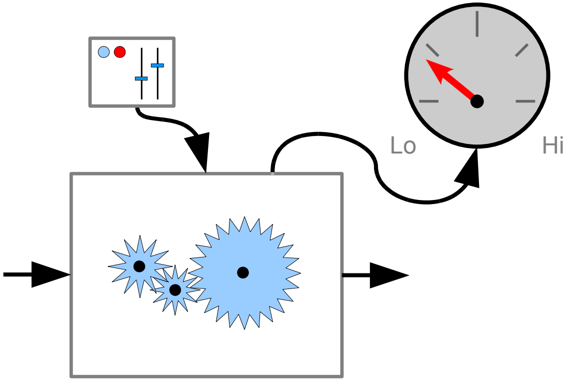
Level 4: Make no design choice prematurely that cannot be justified compellingly.

Level 3: Strive to provide design choices and alternatives.

Level 2: Keep and expose design choices considered during software development.

Level 1: Expose design choices hardwired into existing code (magic constants, hidden parameters, abandoned design alternatives).

Level 0: Optimise settings of parameters exposed by existing software.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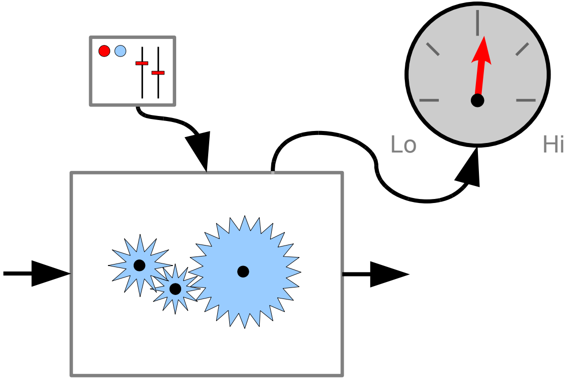
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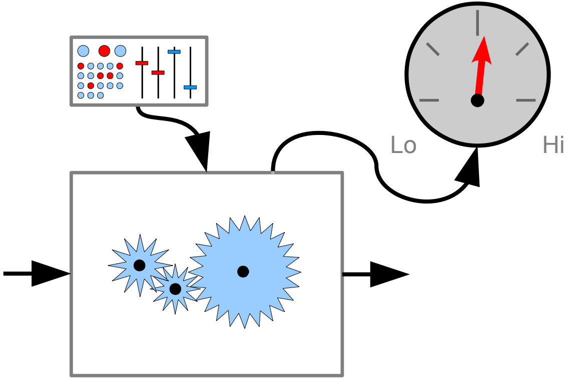
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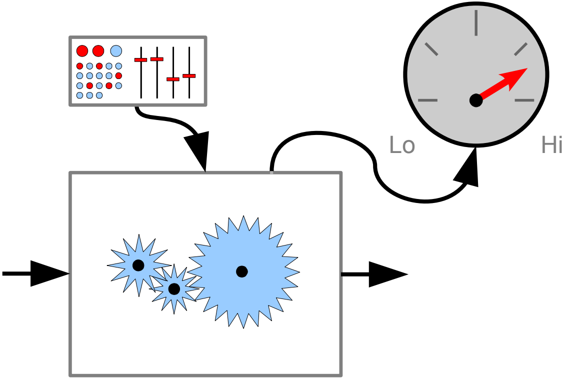

Lo
Hi

Success in optimising speed:

Application, Design choices	Speedup	PbO level
SAT-based software verification (SPEAR), 26 Hutter, Babić, Hoos, Hu (2007)	4.5–500 ×	2–3
AI Planning (LPG), 62 Vallati, Fawcett, Gerevini, Hoos, Saetti (2011)	3–118 ×	1
Mixed integer programming (CPLEX), 76 Hutter, Hoos, Leyton-Brown (2010)	2–52 ×	0

... and solution quality:

University timetabling, 18 design choices, PbO level 2–3
⇝ new state of the art; UBC exam scheduling
Fawcett, Chiarandini, Hoos (2009)

Machine learning / Classification, 786 design choices, PbO level 0–1
⇝ outperforms specialised model selection & hyper-parameter optimisation methods from machine learning
Thornton, Hutter, Hoos, Leyton-Brown (2012–13)

PbO enables ...

- performance optimisation for different use contexts
  (some details later)

- adaptation to changing use contexts
  (see, *e.g.*, life-long learning – Thrun 1996)

- self-adaptation while solving given problem instance
  (*e.g.*, Battiti *et al.* 2008; Carchrae & Beck 2005; Da Costa *et al.* 2008)

- automated generation of instance-based solver selectors
  (*e.g.*, SATzilla – Leyton-Brown *et al.* 2003, Xu *et al.* 2008;
  Hydra – Xu *et al.* 2010; ISAC – Kadioglu *et al.* 2010;
  AutoFolio – Lindaue 2015)

- automated generation of parallel solver portfolios
  (*e.g.*, Huberman *et al.* 1997; Gomes & Selman 2001;
  Hoos *et al.* 2012; Lindauer *et al.* 2017)

Cost & concerns

But what about ...

- Computational complexity?
- Cost of development?
- Limitations of scope?

Computationally too expensive?

Spear revisited:

- total configuration time on software verification benchmarks: $\approx$ 20 CPU days
- wall-clock time on 10 CPU cluster: $\approx$ 2 days
- cost on Amazon Elastic Compute Cloud (EC2): 60.23 AUD (= 48 USD)
- 60.23 AUD pays for ...
  - 1h42 of typical software engineer in Australia
  - 3h33 at minimum wage in Australia

Too expensive in terms of development?

Design and coding:

- tradeoff between performance/flexibility and overhead
- overhead depends on level of PbO
- traditional approach: cost from manual exploration of design choices!

Testing and debugging:

- design alternatives for individual mechanisms and components can be tested separately

$\rightsquigarrow$ effort linear (rather than exponential) in the number of design choices

Limited to the “niche” of NP-hard problem solving?

Some PbO-flavoured work in the literature:

- computing-platform-specific performance optimisation of linear algebra routines
  (Whaley *et al.* 2001)
- optimisation of sorting algorithms using genetic programming
  (Li *et al.* 2005)
- compiler optimisation
  (Pan & Eigenmann 2006; Cavazos *et al.* 2007; Fawcett *et al.* 2017)
- database server configuration
  (Diao *et al.* 2003)

Algorithm Configuration: Methods

Overview

- Programming by Optimization (PbO): Motivation and Introduction

- Algorithm Configuration
  - Methods (components of algorithm configuration)
  - Systems (that instantiate these components)
  - Demo & practical issues

  [coffee]
  - Case Studies

- Portfolio-Based Algorithm Selection

- Software Development Support & Further Directions

Algorithm Configuration

- In a nutshell: **optimization of free parameters**
  - Which parameters? The ones you'd otherwise tune manually & more

- Examples of free parameters in various subfields of AI
  - **Tree search** (in particular for SAT): pre-processing, branching heuristics, clause learning & deletion, restarts, data structures, ...
  - **Local search**: neighbourhoods, perturbations, tabu length, annealing...
  - **Genetic algorithms**: population size, mating scheme, crossover operators, mutation rate, local improvement stages, hybridizations, ...
  - **Machine Learning**: pre-processing, regularization (type & strength), minibatch size, learning rate schedules, optimizer & its parameters, ...
  - **Deep learning** (in addition): #layers (& layer types), #units/layer, dropout constants, weight initialization and decay, non-linearities, ...

Algorithm Parameters

Parameter types

- Continuous, integer, ordinal
- **Categorical**: finite domain, unordered, e.g. {a,b,c}

Parameter space has **structure**

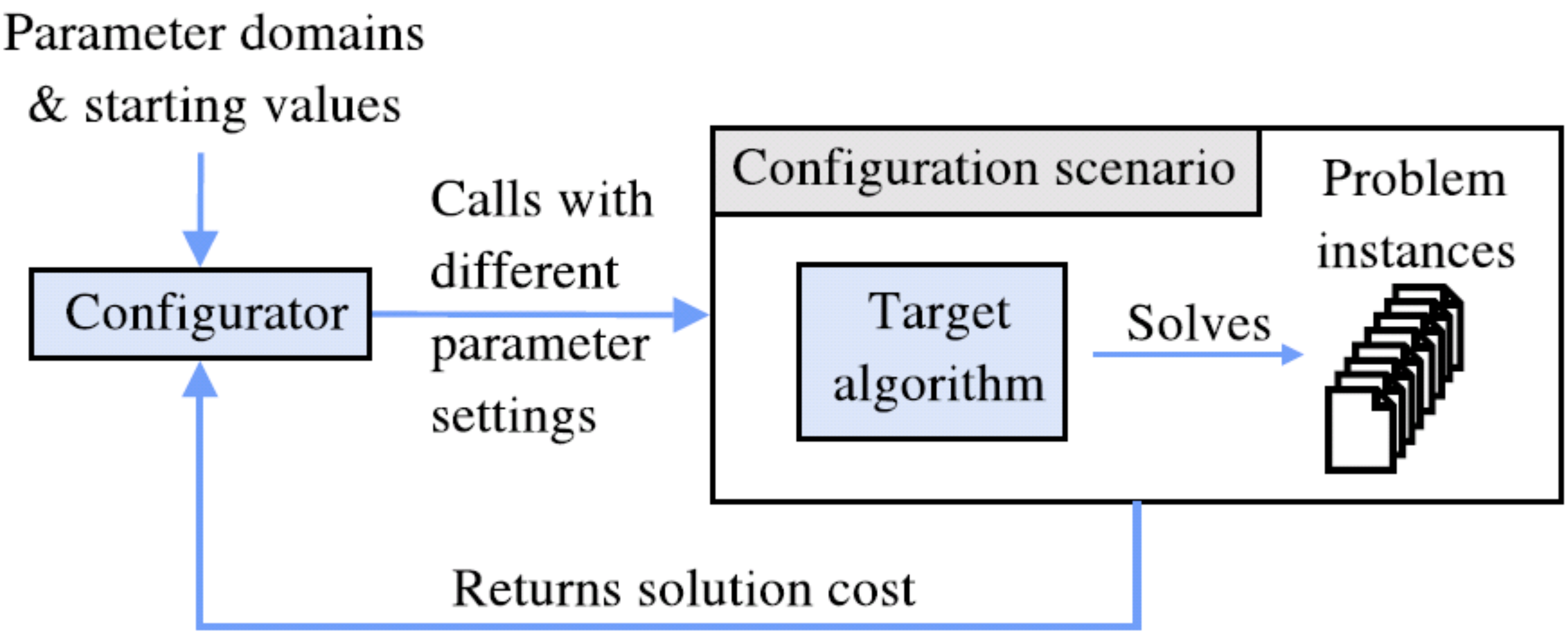
- E.g. parameter C is only active if heuristic H=h is used
- In this case, we say C is a **conditional parameter** with parent H

Parameters give rise to a **structured space of algorithms**

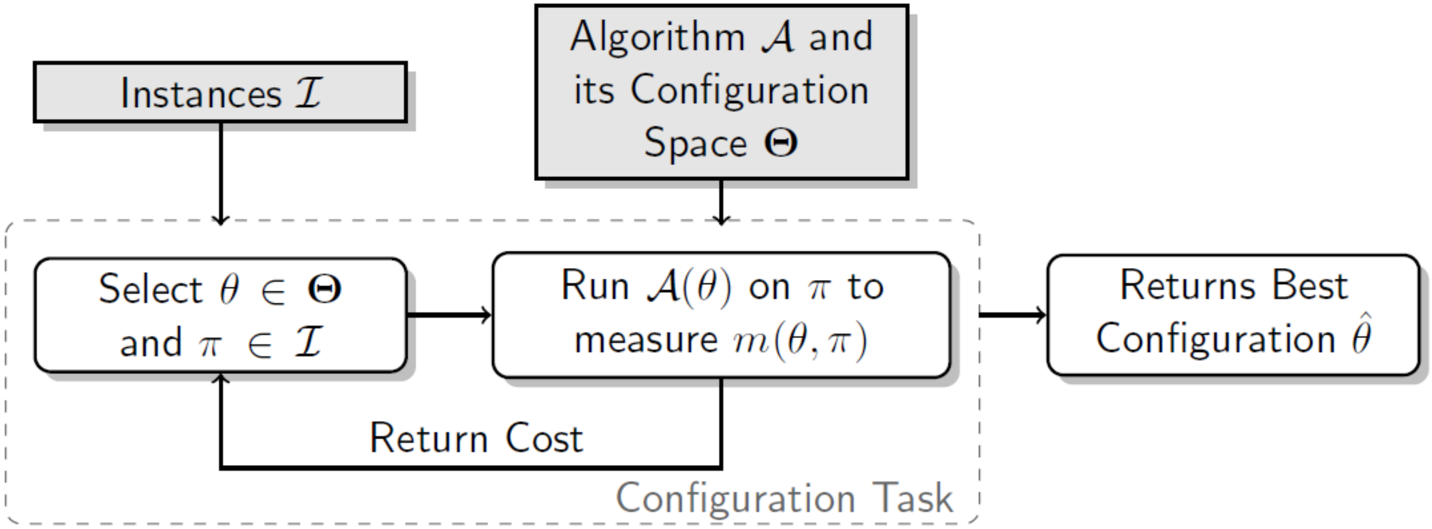
- Many **configurations** (e.g. 10^{47})
- Configurations often yield qualitatively different behaviour

→ Algorithm configuration (as opposed to "parameter tuning")

The Algorithm Configuration Process



Algorithm Configuration – in More Detail



Definition: algorithm configuration

Given:

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

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

Algorithm Configuration – Full Formal Definition

Definition: algorithm configuration

An instance of the algorithm configuration problem is a 5-tuple $(\mathcal{A}, \mathbf{\Theta}, \mathcal{D}, \kappa, m)$ where:

- $\mathcal{A}$ is a parameterized algorithm;
- $\mathbf{\Theta}$ is the parameter configuration space of $\mathcal{A}$;
- $\mathcal{D}$ is a distribution over problem instances with domain $\mathcal{I}$;
- $\kappa < \infty$ is a cutoff time, after which each run of $\mathcal{A}$ will be terminated if still running
- $m : \mathbf{\Theta} \times \mathcal{I} \rightarrow \mathbb{R}$ is a function that measures the observed cost of running $\mathcal{A}(\theta)$ on an instance $\pi \in \mathcal{I}$ with cutoff time κ

The cost of a candidate solution $\theta \in \mathbf{\Theta}$ is $c(\theta) = \mathbb{E}_{\pi \sim \mathcal{D}}(m(\theta, \pi))$.
The goal is to find $\theta^* \in \arg\min_{\theta \in \mathbf{\Theta}} c(\theta)$.

Distribution *vs* Set of Instances

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

Special case: distribution with finite support

- We often only have N instances from a given application
- In that case: split N instances into training and test set
- Find $\theta^* \in \arg\min_{\theta \in \boldsymbol{\Theta}} \frac{1}{N_{train}} \sum_{i=1}^{N_{train}} (m(\theta, \pi_i))$.

Evaluation on new test instances

Same approach as in machine learning

- We configure algorithms on the training instances
- We only use test instances to assess generalization performance

  $\rightarrow$ unbiased estimate of generalization performance for unseen instances

Algorithm Configuration is a Useful Abstraction

Two different instantiations:

Minimize the runtime of a SAT solver for a benchmark set

- Optimize on training set:

$$\theta^* \in \arg\min_{\theta \in \mathbf{\Theta}} \frac{1}{N_{train}} \sum_{i=1}^{N_{train}} (m(\theta, \pi_i))$$

Minimize K-fold cross-validation error of a machine learning algorithm

- A cross-validation fold k plays the role of an instance

$$\theta^* \in \arg\min_{\theta \in \mathbf{\Theta}} \frac{1}{K} \sum_{k=1}^{K} (m(\theta, k))$$

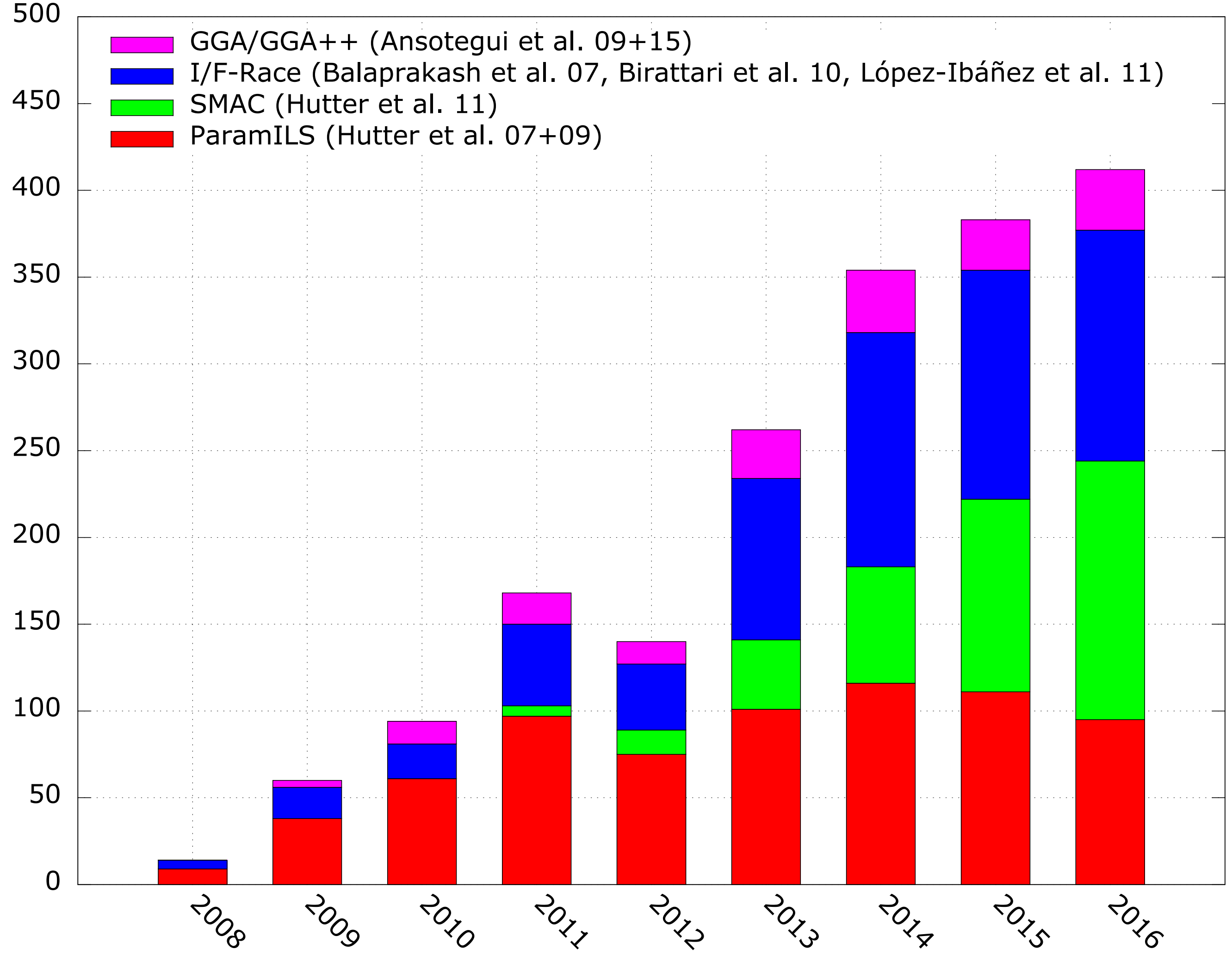
Large improvements to solvers for
many hard combinatorial problems

SAT, Max-SAT, MIP, SMT, TSP, ASP, time-tabling, AI planning, …

Competition winners for all of these rely on configuration tools

Algorithm Configuration is a Useful Abstraction

Increasingly popular (citation numbers: Google Scholar)



Overview

- Programming by Optimization (PbO): Motivation and Introduction

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  - Demo & practical issues
  - Case studies

- Portfolio-Based Algorithm Selection

- Software Development Support & Further Directions

Configurators have Two Key Components

- Component 1: **which configuration to evaluate** next?
  - Out of a large combinatorial search space
  - E.g., CPLEX: 76 parameters, 10^{47} configurations
- Component 2: **how to evaluate that configuration**?
  - Evaluating performance of a configuration is expensive
  - E.g., CPLEX: budget of 10000s per instance
  - Instances vary in hardness
    - Some take milliseconds, other days (for the default)
    - Improvement on a few instances might not mean much

Component 1: Which Configuration to Choose?

- For this component, we can consider a simpler problem:

  Blackbox function optimization $\boxed{\min_{\theta \in \Theta} f(\theta)}$

  – **Only mode of interaction: query $f(\theta)$ at arbitrary $\theta \in \Theta$**

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

  – Abstracts away the complexity of multiple instances

  – Θ is still a structured space

    - Mixed continuous/discrete
    - Conditional parameters
    - Still more general than “standard” continuous BBO [e.g., Hansen et al.]

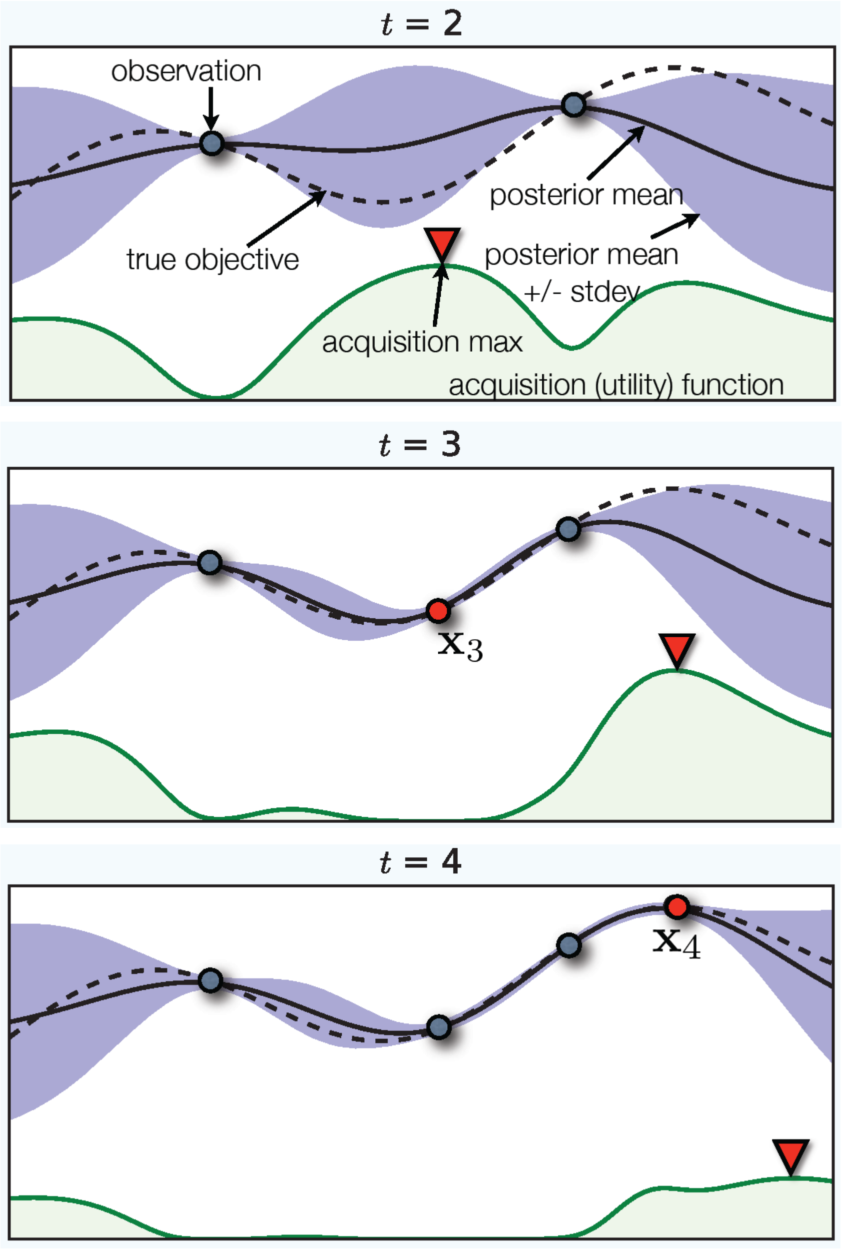
Component 1: Which Configuration to Choose?

- Need to balance diversification and intensification
- The extremes
  - Random search
  - Hill-climbing
- Stochastic local search (SLS)
- Population-based methods
- Model-Based Optimization

Sequential Model-Based Optimization

- Fit a (probabilistic) model of function *f*
- Use that model to trade off exploitation *vs* exploration

- In machine learning literature known as **Bayesian Optimization**



Component 2: How to Evaluate a Configuration?

Back to general algorithm configuration

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- **General principle**
  - Don't waste too much time on bad configurations
  - Evaluate good configurations more thoroughly

Simplest Solution: Use Fixed N Instances

- Effectively treats the problem as black-box function optimization
- **Issue: how large to choose N?**
  - Too small: over-tuning to those instances
  - Too large: every function evaluation is slow

Racing Algorithms

[Maron & Moore, NIPS 1994]

[Birattari, Stützle, Paquete & Varrentrapp, GECCO 2002]

- Compare two or more algorithms against each other
  - Perform one run for each configuration at a time
  - **Discard configurations when dominated**

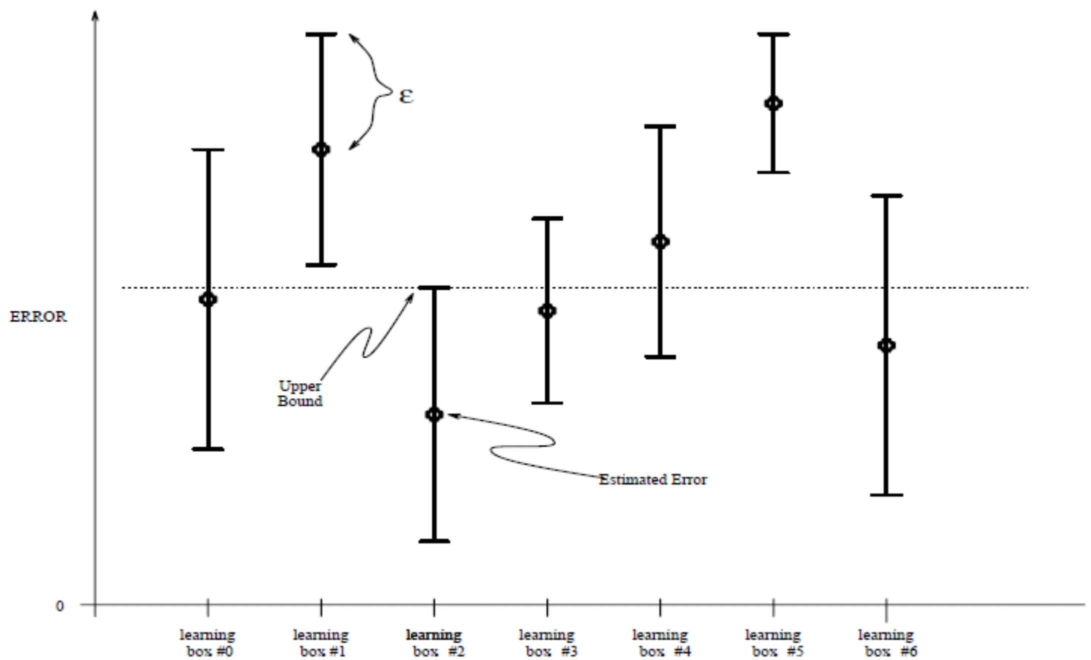


Image source: Maron & Moore, Hoeffding Races, NIPS 1994

Saving Time: Aggressive Racing

[Hutter, Hoos & Stützle, AAAI 2007]

- Race new configurations against the best known
  - Discard poor new configurations quickly
  - **No requirement for statistical domination**

- Search component should allow to return to configurations discarded because they were “unlucky”

Saving More Time: Adaptive Capping

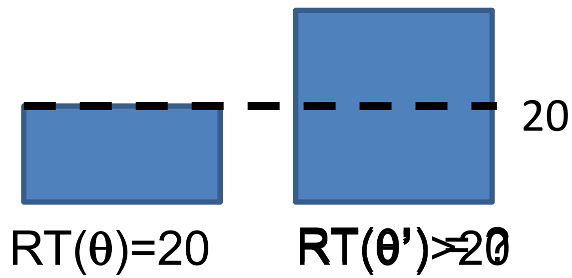
[Hutter, Hoos, Leyton-Brown & Stützle, JAIR 2009]

(only when minimizing algorithm runtime)

Can terminate runs for poor configurations θ' early:

– Is θ' better than θ?

- Example:



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

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Overview: Algorithm Configuration Systems

- Continuous parameters, single instances (**black-box function optimization**)
  - Covariance adaptation evolutionary strategy (CMA-ES) [Hansen *et al.* 2006-17]
  - Sequential Parameter Optimization (SPO) [Bartz-Beielstein *et al.* 2006]

- **General algorithm configuration** methods
  - ParamILS [Hutter *et al.* 2007, 2009; Blot *et al.* 2016]
  - Gender-based Genetic Algorithm (GGA) [Ansotegui *et al.* 2009, 2015]
  - Iterated F-Race [Birattari *et al.* 2002, 2010]
  - Sequential Model-based Algorithm Configuration (SMAC) [Hutter *et al.* 2011-17]
  - Distributed SMAC [Hutter *et al.* 2012-17]

The Baseline: Graduate Student Descent

Start with some configuration

repeat

Modify a single parameter

if *performance on a benchmark set degrades* **then**

undo modification

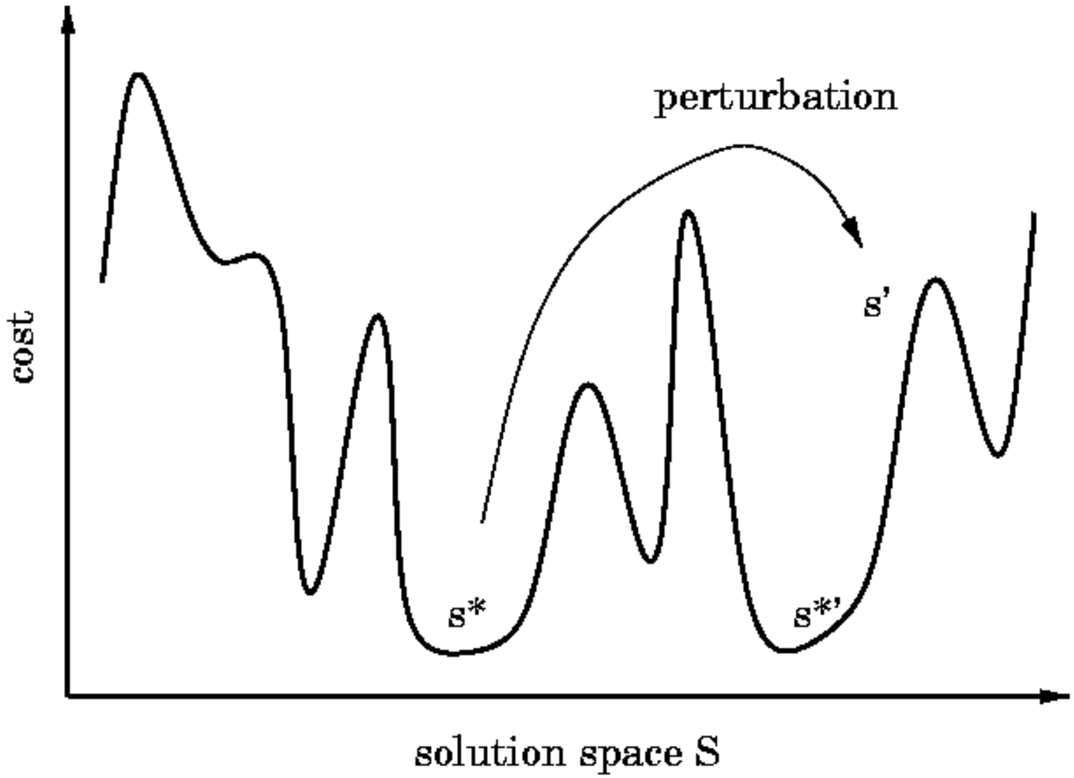
until *no more improvement possible*

(or "good enough")

The ParamILS Framework

[Hutter, Hoos, Leyton-Brown & Stützle, AAAI 2007 & JAIR 2009]

Iterated Local Search in parameter configuration space:



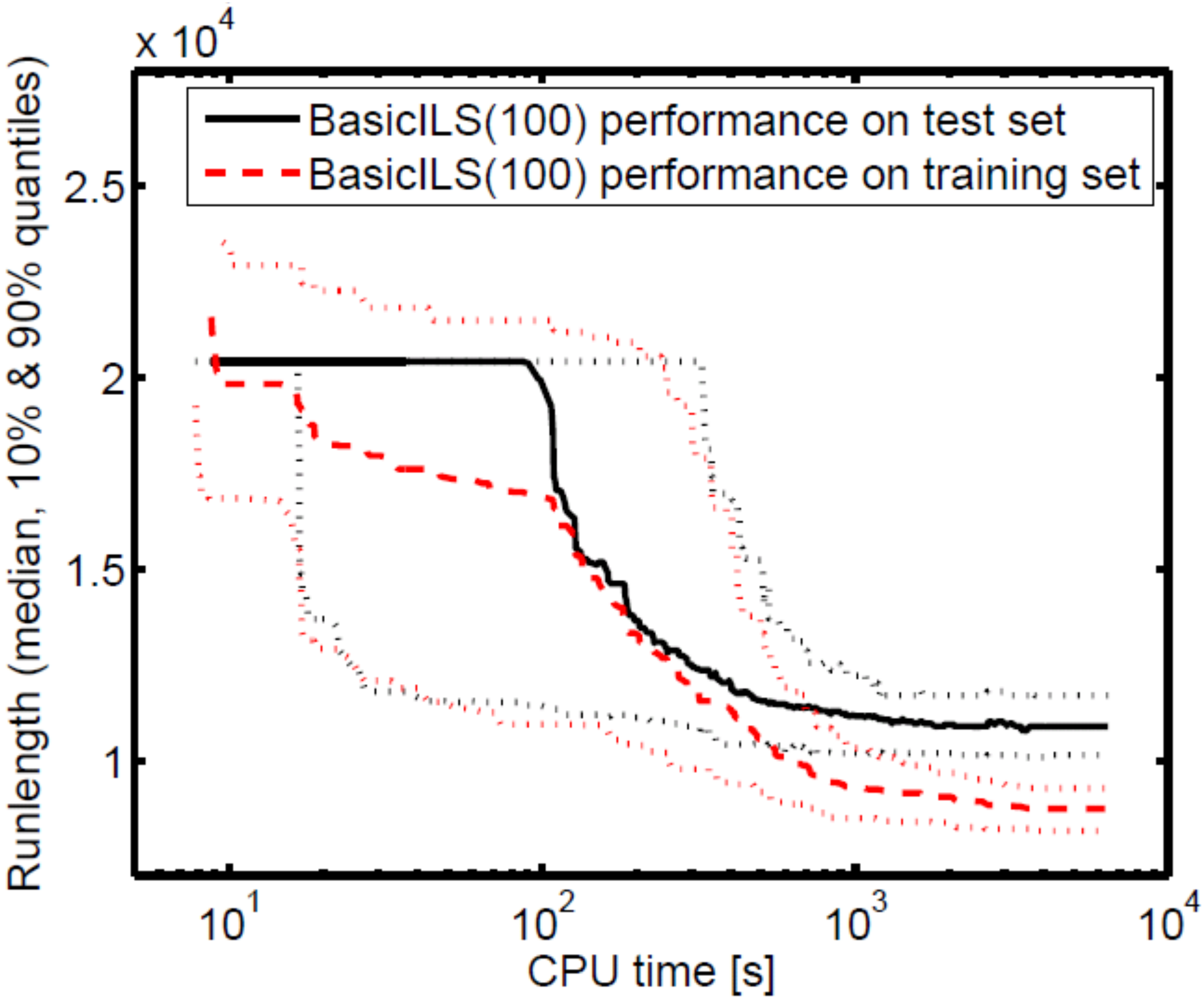
→ Performs **biased random walk over local optima**

The BasicILS(N) algorithm

- Instantiates the ParamILS framework
- **Uses a fixed number of N runs for each evaluation**
  - Sample N instance from given set (with repetitions)
  - Same instances (and seeds) for evaluating all configurations
  - Essentially treats the problem as blackbox optimization

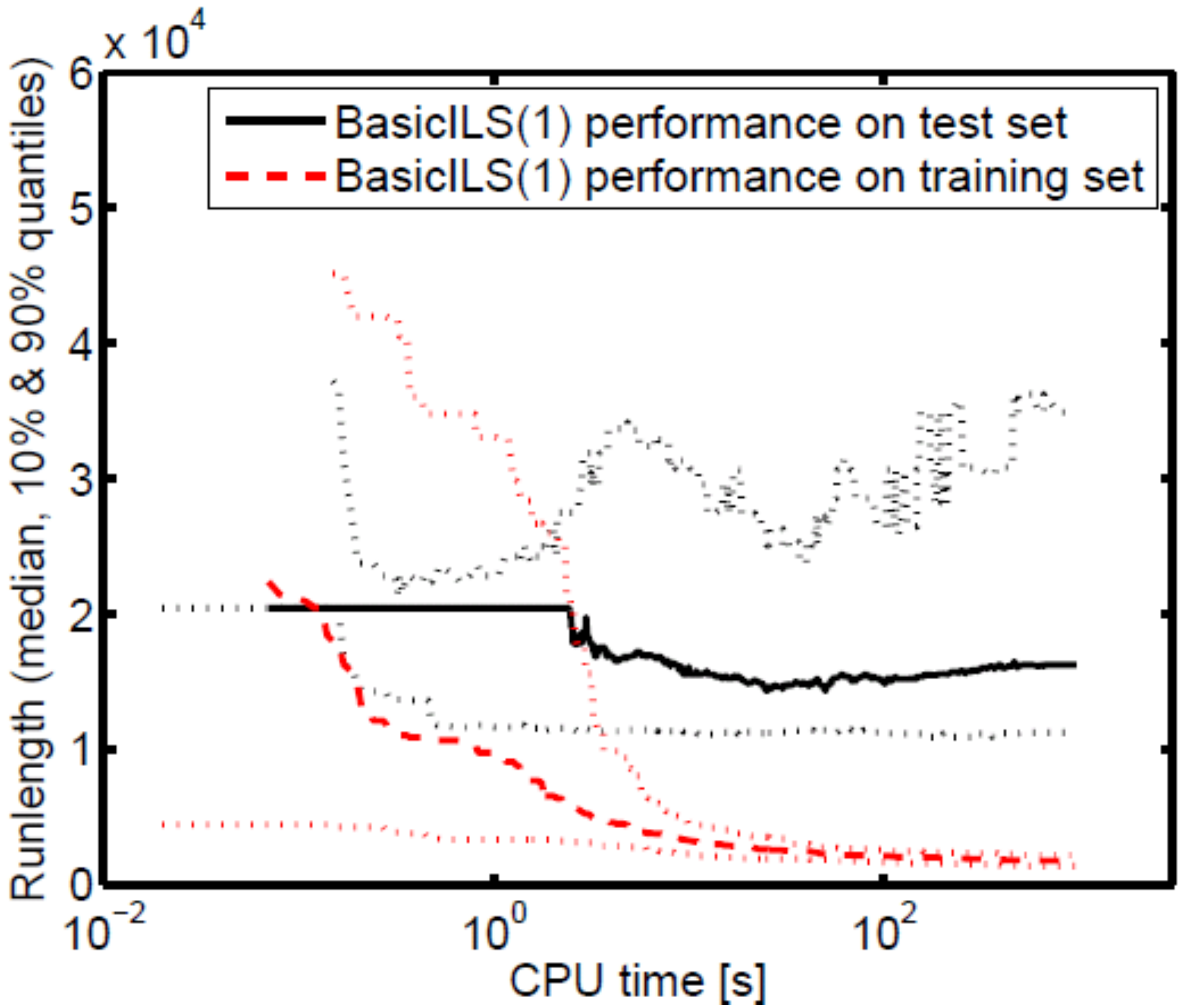
- **How to choose N?**
  - Too high: evaluating a configuration is expensive
    - $\rightarrow$ Optimization process is slow
  - Too low: noisy approximations of true cost
    - $\rightarrow$ Poor generalization to test instances / seeds

Generalization to Test set, Large N (N=100)



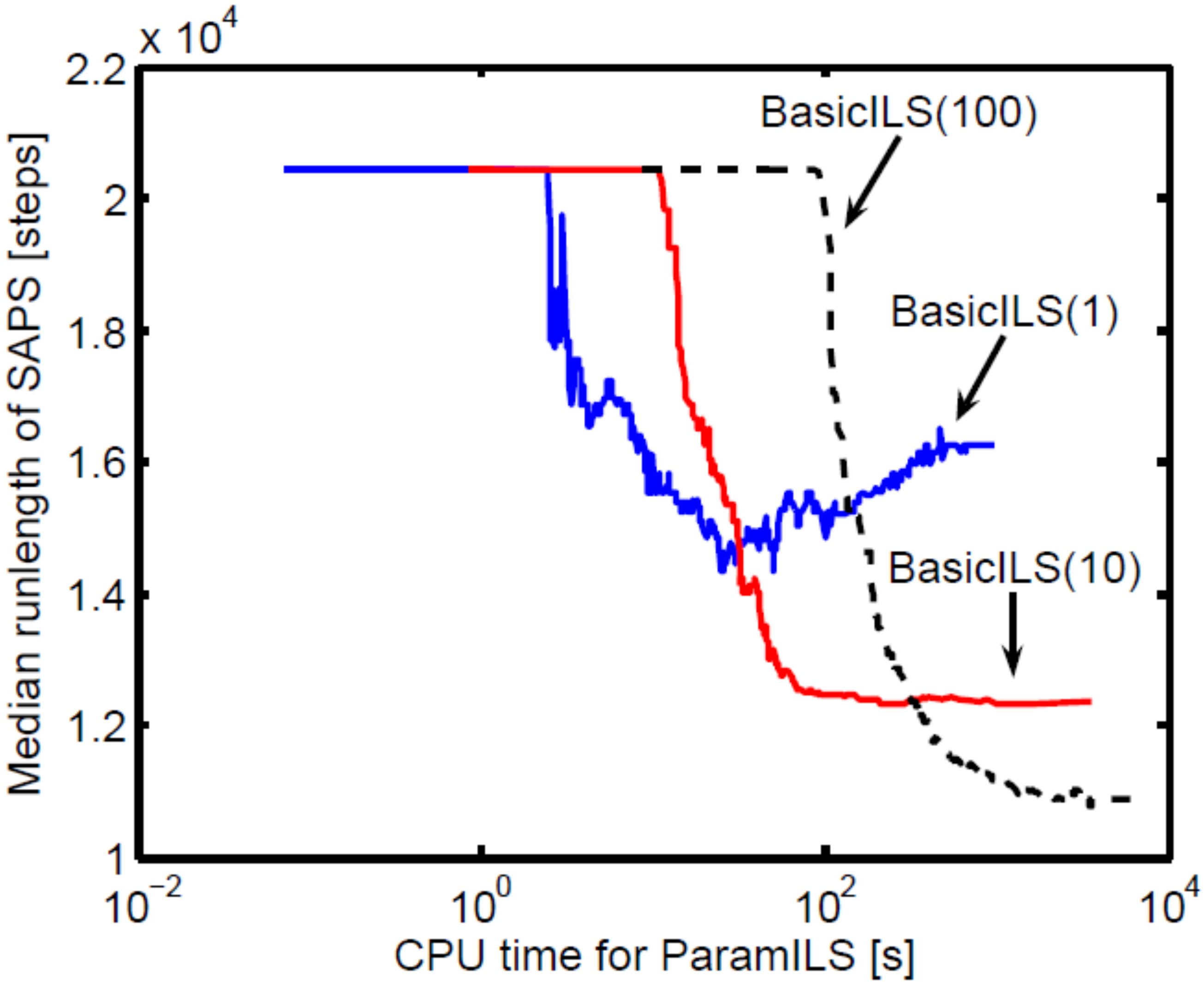
SAPS on a single QWH instance
(same instance for training & test; only difference: seeds)

Generalization to Test Set, Small N (N=1)



SAPS on a single QWH instance
(same instance for training & test; only difference: seeds)

BasicILS: Speed/Generalization Tradeoff



Test performance of SAPS on a single QWH instance

The FocusedILS Algorithm

Aggressive racing: more runs for good configurations

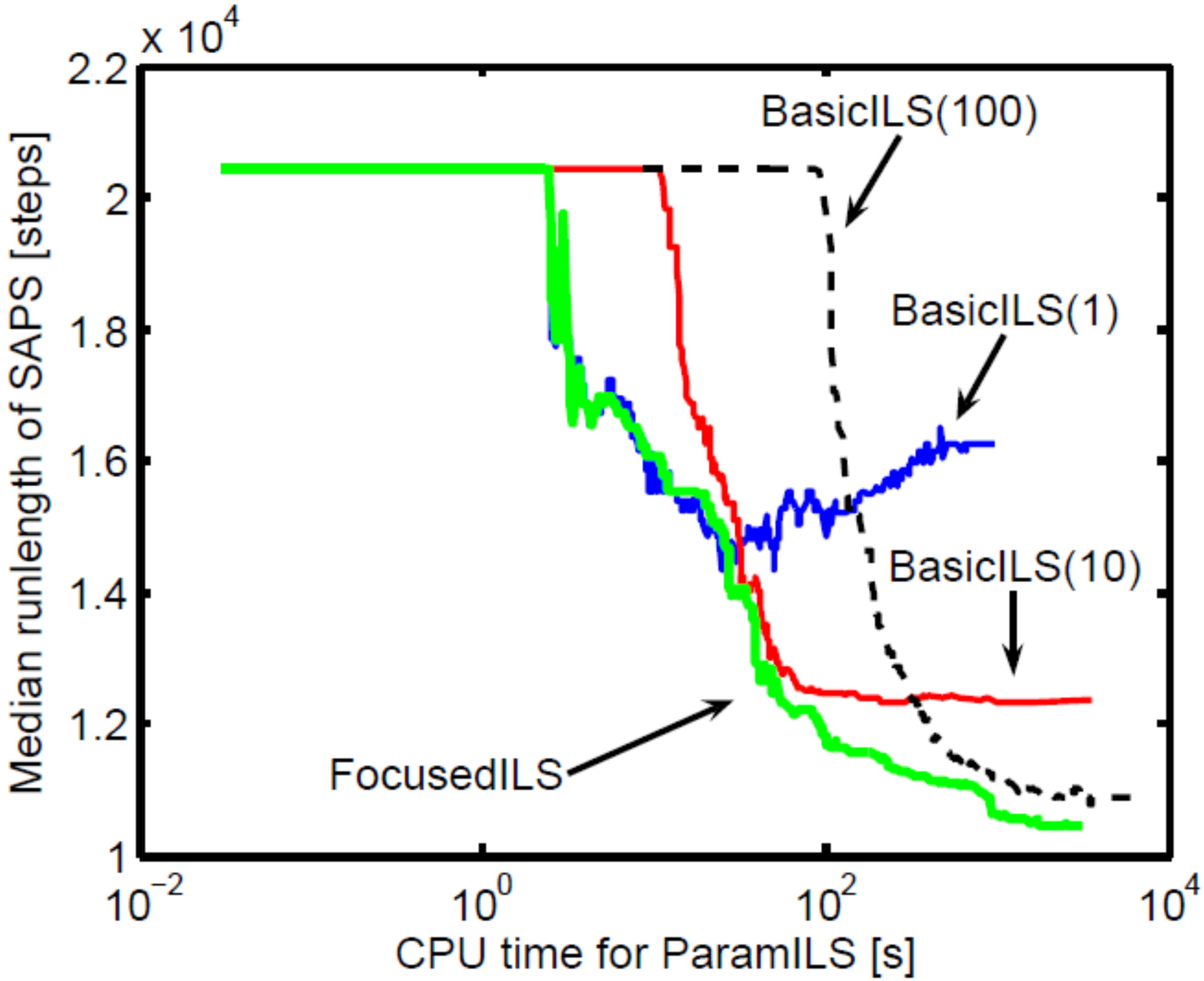
- Start with $N(\theta) = 0$ for all configurations
- Increment $N(\theta)$ whenever the search visits θ
- "Bonus" runs for configurations that win many comparisons

Theorem

As number of FocusedILS iterations $\rightarrow \infty$, convergence to optimal configuration

- Key ideas in proof:
  1. The underlying ILS eventually reaches any configuration
  2. For $N(\theta) \rightarrow \infty$, the error in cost approximations vanishes

FocusedILS: Speed/Generalization Tradeoff



Test performance of SAPS on a single QWH instance

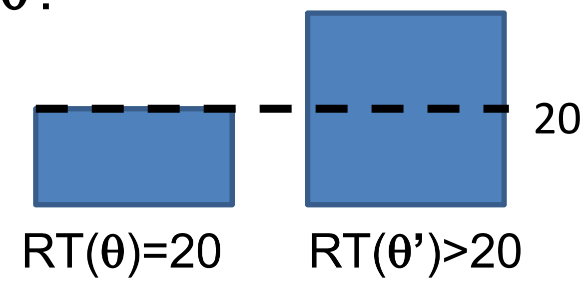
Speeding up ParamILS

[Hutter , Hoos, Leyton-Brown, and Stützle, JAIR 2009]

Standard adaptive capping

– Is θ' better than θ?

- Example:



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

Theorem

Early termination of poor configurations does not change ParamILS trajectory

– Often yields substantial speedups
– Especially when best configuration is much faster than worst

Gender-based Genetic Algorithm (GGA)

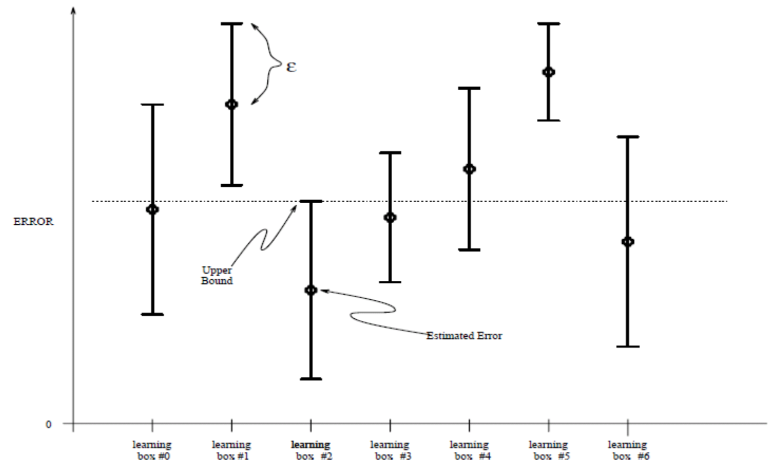
[Ansotegui, Sellmann & Tierney, CP 2009 & IJCAI 2015]

- Genetic algorithm
  - **Genome = parameter configuration**
  - Combine genomes of 2 parents to form an offspring
- **Supports adaptive capping**
  - Evaluate population members in parallel
  - Adaptive capping: can stop when the first k succeed
- Use N instances to evaluate configurations
  - Increase N in each generation
  - **Linear increase from N_{start} to N_{end}**
    - Not recommended for small budgets
    - User has to specify #generations ahead of time

F-Race and Iterated F-Race

[Birattari *et al.*, GECCO 2002 & OR Perspectives 2016;
Pérez Cáceres *et al.*, LION 2017]

- **F-Race**
  - Standard racing framework
  - F-test to establish that some configuration is dominated
  - Followed by pairwise *t* tests if F-test succeeds



- **Iterated F-Race**
  - Maintain a probability distribution over which configurations are good
  - Sample *k* configurations from that distribution & race them
  - Update distributions with the results of the race

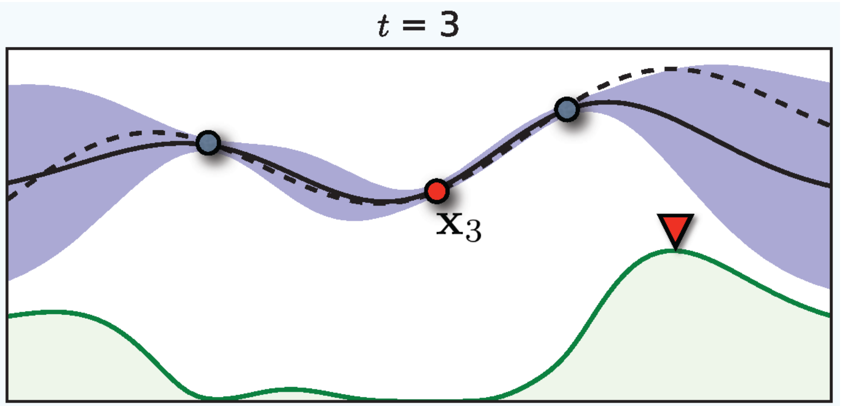
- **Well-supported software package in R**

Model-Based Algorithm Configuration

[Hutter, Hoos & Leyton-Brown, LION 2011]

SMAC: Sequential Model-Based Algorithm Configuration

– Sequential Model-Based Optimization
  & aggressive racing



repeat

- construct model to predict performance
- use that model to select promising configurations
- compare each selected configuration against the best known

until time budget exhausted

SMAC: Aggressive Racing

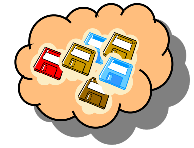
- Similar racing component as FocusedILS
  - More runs for good configurations
  - Increase #runs for incumbent over time

- **Theorem** for discrete configuration spaces:

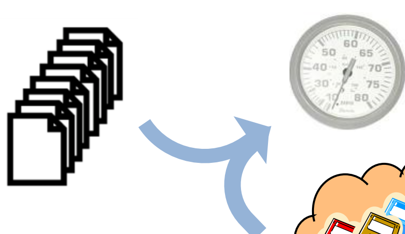
  As overall time budget for SMAC $\rightarrow \infty$,
  convergence to optimal configuration

Powering SMAC: Empirical Performance Models

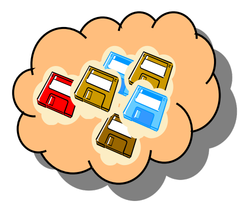
Given:

- Configuration space $\boldsymbol{\Theta} = \Theta_1 \times \cdots \times \Theta_n$ 
- For each problem instance i: vector $\mathbf{x}_i$ of feature values 
- Observed algorithm runtime data: $(\theta_1, \mathbf{x}_1, y_1), \ldots, (\theta_n, \mathbf{x}_n, y_n)$ 

Find: **mapping** $m: [\theta, x] \mapsto y$ predicting A's performance



$\approx m\,(\boldsymbol{\theta}, x)$



- Rich literature on such performance prediction problems
  [see, *e.g.*, Hutter, Xu, Hoos, Leyton-Brown, AIJ 2014, for overview]
- Here: use model m based on **random forests**

Regression Trees: Fitting to Data

- In each internal criterion used
- In each leaf: sto

param 1	feature 2	param 3	runtime
false	2	red	3.7
false	2.5	blue	20
true	5.5	red	2.1
false	5.5	blue	25
false	5	red	1.2
true	4.5	green	19
true	4	blue	12
true	3.5	green	17

$param_3 \in \{red\}$

param 1	feature 2	param 3	runtime
false	2	red	3.7
true	5.5	red	2.1
false	5	red	1.2

$feature_2 \leq 3.5$

param 1	feature 2	param 3	runtime
false	2	red	3.7

$feature_2 > 3.5$

param 1	feature 2	param 3	runtime
true	5.5	red	2.1
false	5	red	1.2

$param_3 \in \{blue, green\}$

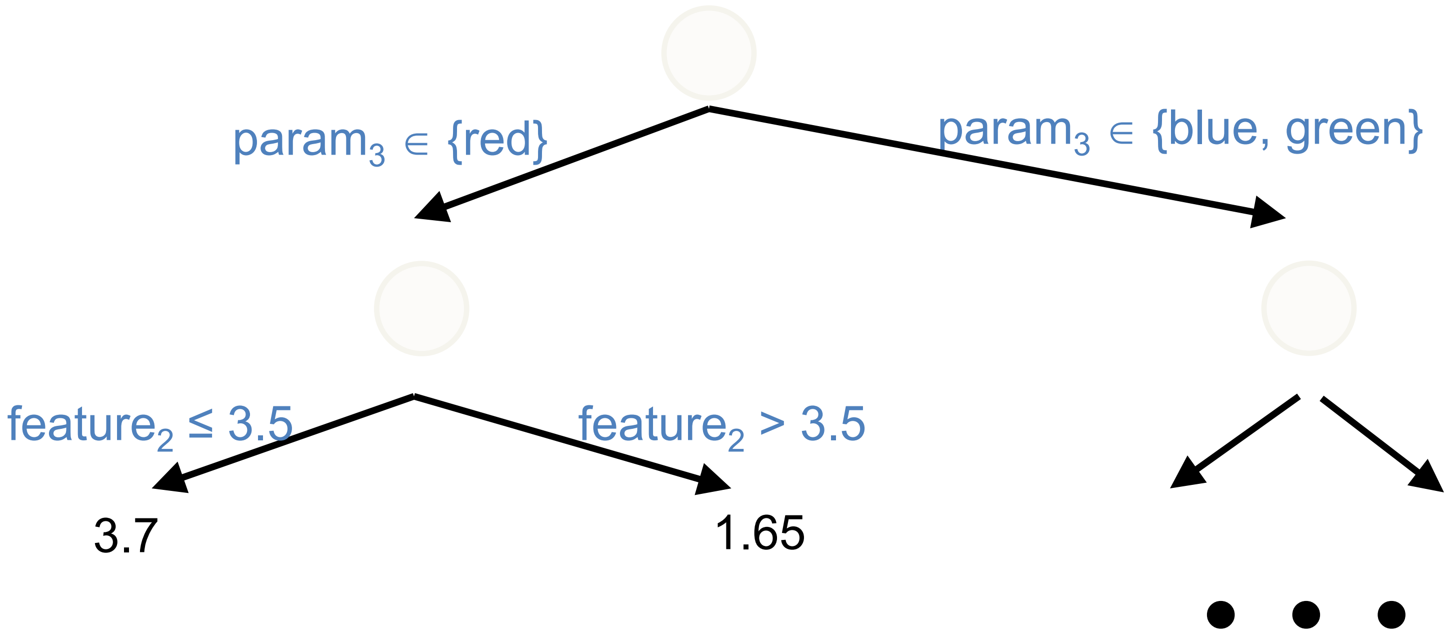
param 1	feature 2	param 3	runtime
false	2.5	blue	20
false	5.5	blue	25
true	4.5	green	19
true	4	blue	12
true	3.5	green	17

• • •

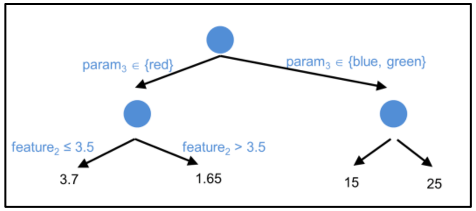
Regression Trees: Predictions for New Inputs

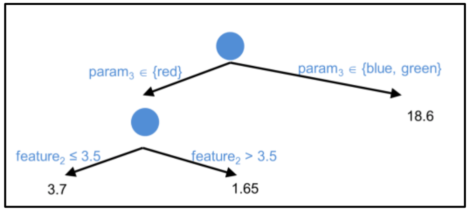
E.g. x_{n+1} = (true, 4.7, red)

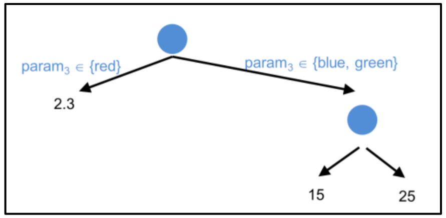
- Walk down tree, return mean runtime stored in leaf $\Rightarrow$ 1.65



Random Forests: Sets of Regression Trees







Training

- Draw T **bootstrap samples** of the data
- For each bootstrap sample, fit a **randomized** regression tree

Prediction

- Predict with each of the T trees
- Return empirical **mean and variance** across these T predictions

Complexity for N data points

- Training: $O(TN \log^2 N)$
- Prediction: $O(T \log N)$

Advantages of Random Forests

Automated selection of important input dimensions

- Continuous, integer, and categorical inputs
- Up to 138 features, 76 parameters
- Can identify important feature and parameter subsets
  - Sometimes 1 feature, 2 parameters sufficient!

[Hutter, Hoos, Leyton-Brown, LION 2013]

Robustness

- No need to optimize hyperparameters
- Already good predictions with few training data points

SMAC: Averaging Across Multiple Instances

- Fit random forest model $m : \mathbf{\Theta} \times \Pi \to \mathbb{R}$

- Aggregate over instances by marginalization

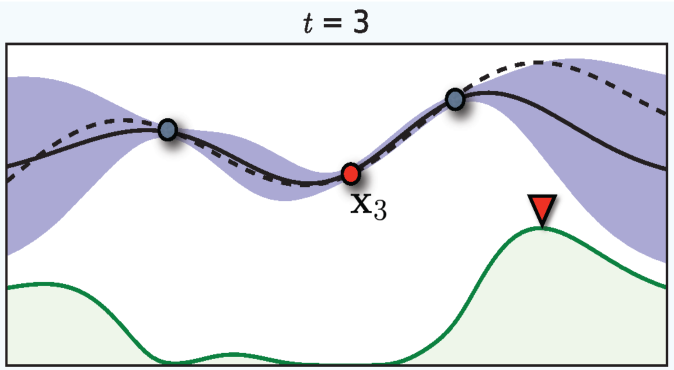
$$f(\boldsymbol{\theta}) := \mathbb{E}_{\pi \sim D}[m(\boldsymbol{\theta}, \pi)]$$

  – **Intuition: predict for each instance and then average**
  – More efficient implementation in random forests

SMAC: Putting it all Together

Initialize with single run for default configuration

repeat



1. Learn RF model from data so far:
$$m : \boldsymbol{\Theta} \times \Pi \to \mathbb{R}$$
2. Aggregate over instances:
$$f(\boldsymbol{\theta}) := \mathbb{E}_{\pi \sim D}[m(\boldsymbol{\theta}, \pi)]$$
3. Use model f to select promising configurations
4. Race each selected configuration against the best known

until time budget exhausted

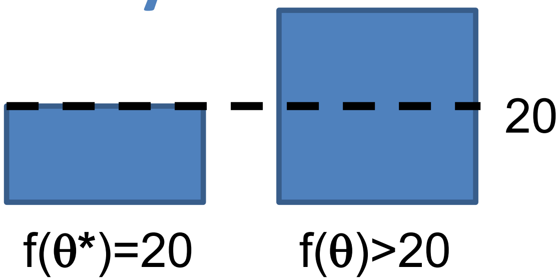
- **Distributed SMAC** [Hutter, Hoos & Leyton-Brown, 2012]
  - Maintain queue of promising configurations
  - Race these against best known on distributed worker cores

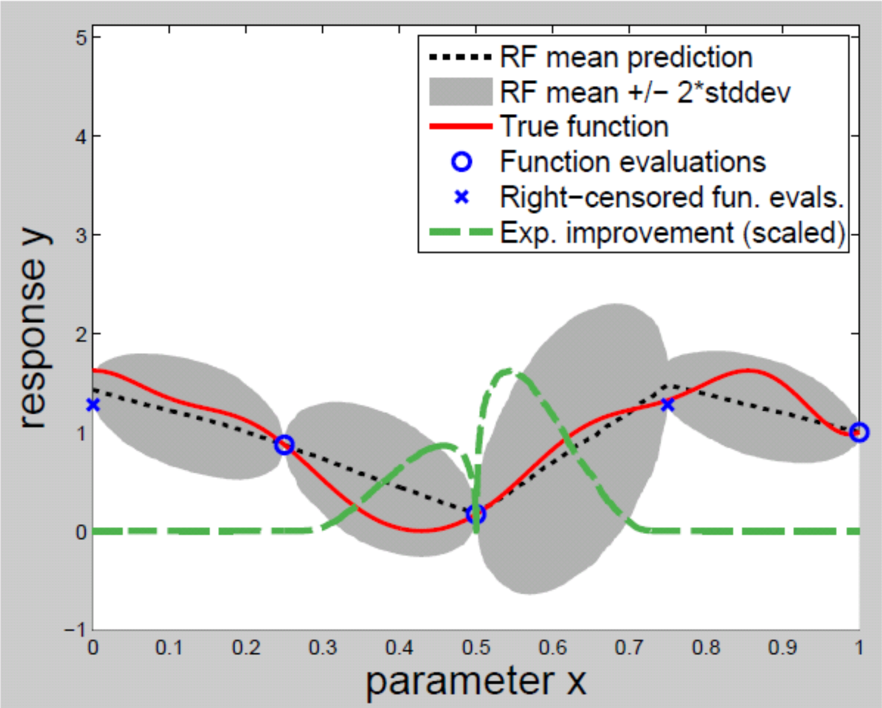
SMAC: Adaptive Capping

[Hutter, Hoos & Leyton-Brown, BayesOpt 2011]

Terminate runs for poor configurations θ early:

– Lower bound on runtime
  → right-censored data point





Experimental Evaluation

[Hutter, Hoos & Leyton-Brown, LION 2011]

Compared SMAC to ParamILS, GGA

– On 17 SAT and MIP configuration scenarios, same time budget




SMAC performed best

– Improvements in test performance of configurations returned
  - *vs* ParamILS: 0.93× – 2.25× (11/17 cases significantly better)
  - *vs* GGA: 1.01× – 2.76× (13/17 cases significantly better)

Wall-clock speedups in distributed SMAC

– Almost perfect with up to 16 parallel workers

– Up to 50-fold with 64 workers
  - Reductions in wall clock time: 5h → 6 min -15 min
    2 days → 40min - 2h

Overview

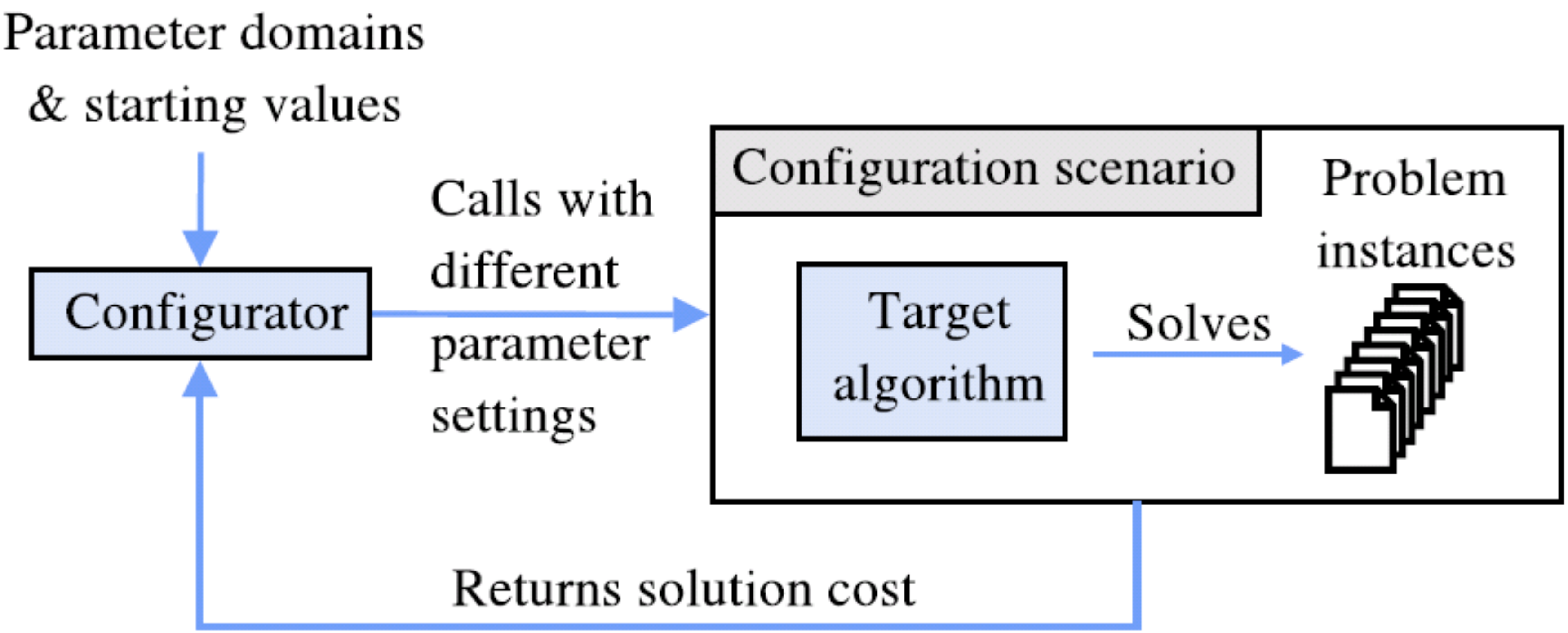
- Programming by Optimization (PbO):
  Motivation and Introduction

- Algorithm Configuration
  - Methods (components of algorithm configuration)
  - Systems (that instantiate these components)
  - Demo & practical issues
  - Case studies

- Portfolio-Based Algorithm Selection

- Software Development Support & Further Directions

The Algorithm Configuration Process



What the user has to provide

Parameter space declaration file

preproc {none, simple, expensive} [simple]
alpha [1,5] [2]
beta [0.1,1] [0.5]

Wrapper for command line call

./wrapper –inst X –timeout 30
-preproc none -alpha 3 -beta 0.7
→ e.g. "successful after 3.4 seconds"

Example: Running SMAC

```
wget http://www.cs.ubc.ca/labs/beta/Projects/SMAC/smac-v2.10.03-master-778.tar.gz

tar xzvf smac-v2.10.03-master-778.tar.gz

cd smac-v2.10.03-master-778

./smac

./smac --seed 0 --scenarioFile example_scenarios/spear/spear-scenario.txt
```

For a usage screen

Scenario file holds:

- Location of parameter file, wrapper & instances
- Objective function (here: minimize avg. runtime)
- Configuration budget (here: 30s)
- Maximal captime per target run (here: 5s)

Output of a SMAC run

```
[…]

[INFO ] *****Runtime Statistics*****
 Incumbent ID: 12 (0x22BB8)
 Number of Runs for Incumbent: 43
 Number of Instances for Incumbent: 5
 Number of Configurations Run: 42
 Performance of the Incumbent: 0.01255555555555556
 Configuration Time Budget used: 30.589647351000067 s (101%)
 Sum of Target Algorithm Execution Times (treating minimum value as 0.1): 24.70000s
 CPU time of Configurator: 5.889042742 s
[INFO ] ******************************************

[INFO ] Total Objective of Final Incumbent 12 (0x22BB8) on training set:
0.01255555555555556; on test set: 0.014499999999999999

[INFO ] Sample Call for Final Incumbent 12 (0x22BB8)
cd /ubc/cs/home/h/hutter/tmp/smac-v2.06.00-master-615/example_scenarios/spear; ruby spear_wrapper.rb
instances/qcplin2006.10408.cnf 0 5.0 2147483647 3282095 -sp-update-dec-queue '0' -sp-rand-var-dec-scaling
'0.3528466348383826' -sp-clause-decay '1.713857938112484' -sp-variable-decay '1.461422623379798' -sp-orig-
clause-sort-heur '7' -sp-rand-phase-dec-freq '0.05' -sp-clause-del-heur '0' -sp-learned-clauses-inc
'1.452683835620401' -sp-restart-inc '1.6481745669620091' -sp-resolution '0' -sp-clause-activity-inc
'0.7121640599232154' -sp-learned-clause-sort-heur '12' -sp-var-activity-inc '0.9358501810374242' -sp-rand-var-dec-
freq '0.0001' -sp-use-pure-literal-rule '1' -sp-learned-size-factor '0.27995062371127827' -sp-var-dec-heur '16' -sp-
phase-dec-heur '6' -sp-rand-phase-scaling '1.0424648235977578' -sp-first-restart '31'
```

Decision #1: Configuration Budget & Captime

- **Configuration budget**
  - Dictated by your resources & needs
    - *E.g.*, start configuration before leaving work on Friday
  - The longer the better (but diminishing returns)
    - Rough rule of thumb: typically time for at least 1000 target runs
    - But have also achieved good results with 50 target runs in some cases

- **Maximal captime 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 300 CPU seconds

Decision #2: Choosing the Training Instances

- **Representative instances, moderately hard**
  - Too hard: won't solve many instances, no traction
  - Too easy: will results generalize to harder instances?
  - Rule of thumb: mix of hardness ranges
    - Roughly 75% instances solvable by default in maximal captime
- **Enough instances**
  - The more training instances, the better
  - Very homogeneous instance sets: 50 instances might suffice
  - Preferably $\geq$ 300 instances, better even $\geq$ 1000 instances

Decision #2: Choosing the Training Instances

- **Split instance set into training and test sets**
  - Configure on the training instances $\rightarrow$ configuration θ^*
  - Run (only) θ^* on test instances
    - Unbiased estimate of performance

Pitfall: configuring on your test instances

That's from the dark ages

Fine practice: do multiple configuration runs and pick the θ^* with best training performance

Not (!!) best on test set

Decision #2: Choosing the Training Instances

- **Works much better on homogeneous benchmarks**
  - Instances that 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

Pitfall: configuration on too heterogeneous sets

There often is no single great overall configuration
(but see algorithm selection *etc.*, later in the tutorial)

Decision #3: How Many Parameters to Expose?

- Suggestion: all parameters you don't know to be useless
  - More parameters $\rightarrow$ larger gains possible
  - More parameters $\rightarrow$ harder problem
  - Max. #parameters tackled so far: 768
    [Thornton, Hutter, Hoos & Leyton-Brown, KDD'13]
    - With more time you can search a larger space

Pitfall: including parameters that change the problem

E.g., optimality threshold in MIP solving
E.g., how much memory to allow the target algorithm

Decision #4: How to Wrap the Target Algorithm

- Do not trust any target algorithm
  - Will it terminate in the time you specify?
  - Will it correctly report its time?
  - Will it never use more memory than specified?
  - Will it be correct with all parameter settings?

Good practice: wrap target runs with tool controlling time and memory (*e.g.*, runsolver [Roussel et al, '11]**)**

Good practice: verify correctness of target runs

Detect crashes & penalize them

Pitfall: blindly minimizing target algorithm runtime

Typically, you will minimize the time to crash

Further Best Practices and Pitfalls to Avoid

[Eggensperger, Lindauer & Hutter, arXiv 2017]

- Pitfalls
  - Using different wrappers for comparing different configurators
    - Often causes subtle bugs that completely invalidate the comparison
  - Not terminating algorithm runs properly
    - Use generic wrapper to handle this for you (we provide one in Python)
  - File system issues when running many parallel experiments
- Best practices
  - Choose configuration spaces dependent on budget
    - If you have time for 10 evaluations, don‘t configure 100s of parameters
  - Realistic and/or reproducible running time metrics
    - CPU *vs* wall-clock time *vs* MEMS
  - Compare configurators on existing, open-source benchmarks
    - *E.g.*, use AClib (in version 2: https://bitbucket.org/mlindauer/aclib2)

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Applications of Algorithm Configuration

Helped win Competitions

SAT: since 2009

ASP: since 2009

IPC: since 2011

Time-tabling: 2007

SMT: 2007

Other Academic Applications

Mixed integer programming (MIP)

TSP & Quadratic Assignment Problem

Game Theory: Kidney Exchange

Linear algebra subroutines

Improving Java Garbage Collection

ML Hyperparameter Optimization

Deep learning

FCC spectrum auction

[Auction]omics

IBM ILOG **Mixed integer programming**

Analytics & Optimization

ORTEC OPTIMIZE YOUR WORLD

Social gaming

zynga

Scheduling and Resource Allocation

actenum

Back to the Spear Example

[Hutter, Babic, Hu & Hoos, FMCAD 2007]

Spear [Babic, 2007]

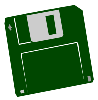
- 26 parameters
- 8.34×10^{17} configurations

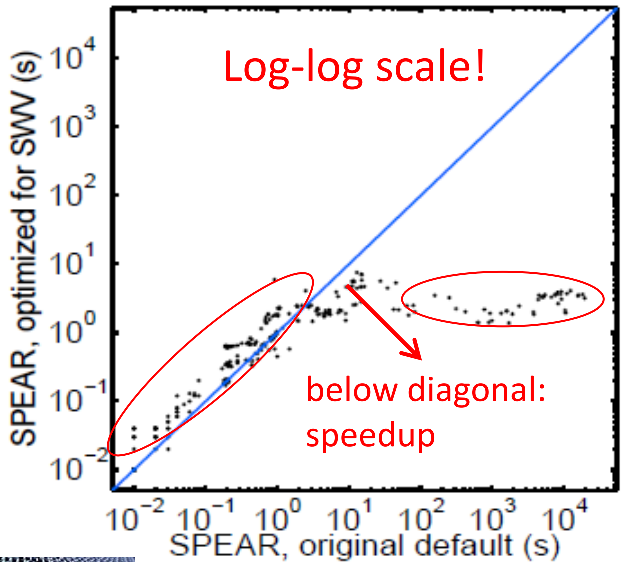
Ran ParamILS, 2 to 3 days × 10 machines

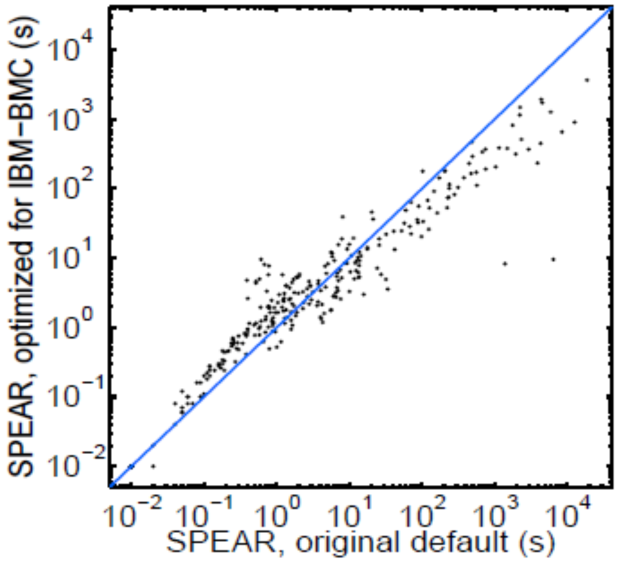
- On a training set from each of 2 distributions

Compared to default (1 week of manual tuning)

- On a disjoint test set from each distribution







500-fold speedup ⇒ won QF_BV category in 2007 SMT competition

4.5-fold speedup

Other Examples of PbO for SAT

- SATenstein [KhudaBukhsh, Xu, Hoos & Leyton-Brown, IJCAI 2009 & AIJ 2016]
  - Combined ingredients from existing solvers
  - 54 parameters, over 10^{12} configurations
  - Speedup factors: 1.6x to 218x

- Captain Jack [Tompkins & Hoos, SAT 2011]
  - Explored a completely new design space
  - 58 parameters, over 10^{50} configurations
  - After configuration: best known solver for 3sat10k and IL50k

Configurable SAT Solver Competition (CSSC)

[Hutter, Balint, Bayless, Hoos & Leyton-Brown 2013]

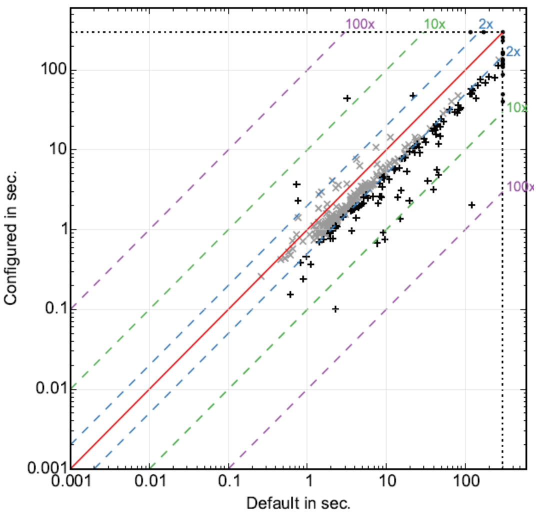
- Annual SAT competition
  - Scores SAT solvers by their performance across instances
  - Medals for best average performance with solver defaults
    - Misleading results: implicitly highlights solvers with good defaults

- CSSC 2013 & 2014
  - Better reflects an application setting: homogeneous instances
    $\rightarrow$ can automatically optimize parameters
  - Medals for best performance **after configuration**

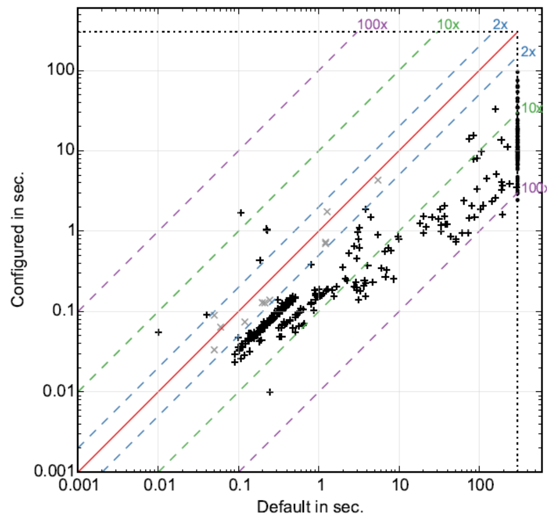
CSSC Result #1

[Hutter, Lindauer, Balint, Bayless, Hoos & Leyton-Brown 2014]

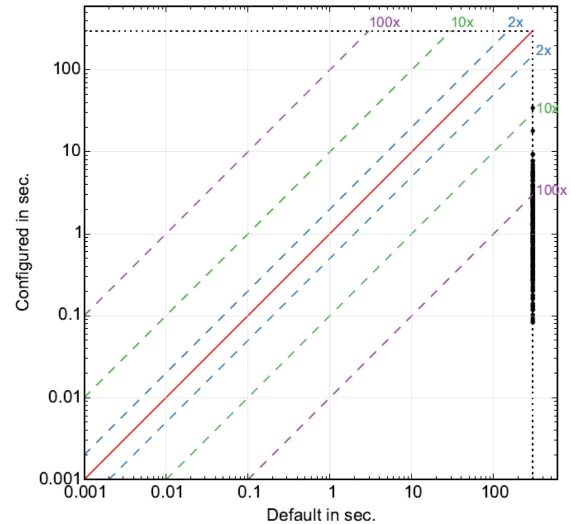
- Solver performance often improved a lot:



Lingeling on CircuitFuzz:
Timeouts: 119 → 107



Clasp on n-queens:
Timeouts: 211 → 102



probSAT on unif rnd 5-SAT:
Timeouts: 250 → 0

CSSC Result #2

[Hutter, Lindauer, Balint, Bayless, Hoos & Leyton-Brown 2014]

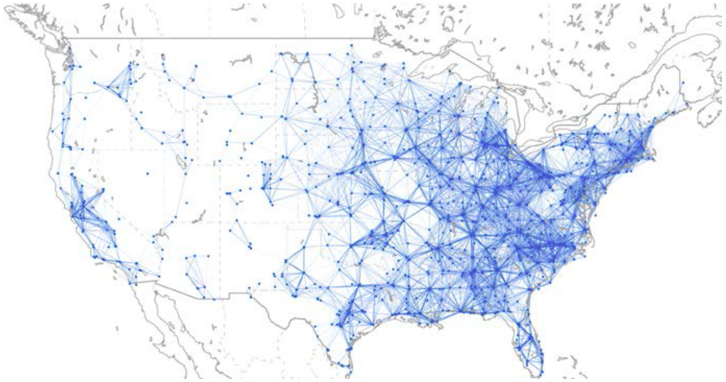
- Automated configuration changed algorithm rankings
  - Example: random SAT+UNSAT category in 2013

Solver	CSSC ranking	Default ranking
Clasp	1	6
Lingeling	2	4
Riss3g	3	5
Solver43	4	2
Simpsat	5	1
Sat4j	6	3
For1-nodrup	7	7
gNovelty+GCwa	8	8
gNovelty+Gca	9	9
gNovelty+PCL	10	10

Real-World Application: FCC Spectrum Auction

- Wireless frequency spectra: demand increases
  - US Federal Communications Commission (FCC) is currently holding an auction
  - **Expected net revenue: $10 billion to $40 billion**

- **Key computational problem:**
  feasibility testing based on interference constraints
  - A hard **graph colouring problem**
  - 2991 stations (nodes) &
    2.7 million interference constraints
  - Need to solve many different instances
  - More instances solved: higher revenue



- **Best solution: based on SAT solving & configuration with SMAC**
  - Improved #instances solved from 73% to 99.6%
    [Frechette, Newman & Leyton-Brown, AAAI 2016]

Configuration of a Commercial MIP solver

[Hutter, Hoos & Leyton-Brown, CPAIOR 2010]

Mixed Integer Programming (MIP)

$$\begin{aligned} \min \quad & c^{\mathsf{T}} x \\ \text{s. t.} \quad & Ax \le b \\ & x_i \in \mathbb{Z} \text{ for i} \in \text{I} \end{aligned}$$

Commercial MIP solver: IBM ILOG CPLEX

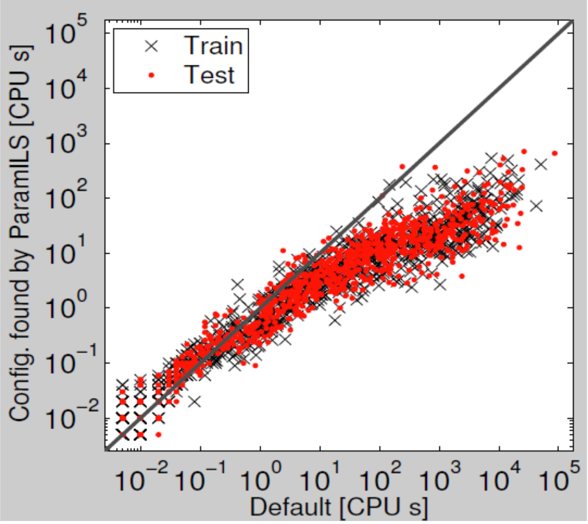
- Leading solver for 15 years
- Licensed by over 1 000 universities and 1 300 corporations
- 76 parameters, 10^{47} configurations

Minimizing runtime to optimal solution

- Speedup factor: 2× to 50×
- Later work: speedups up to 10,000×

Minimizing optimality gap reached

- Gap reduction factor: 1.3× to 8.6×



Comparison to CPLEX Tuning Tool

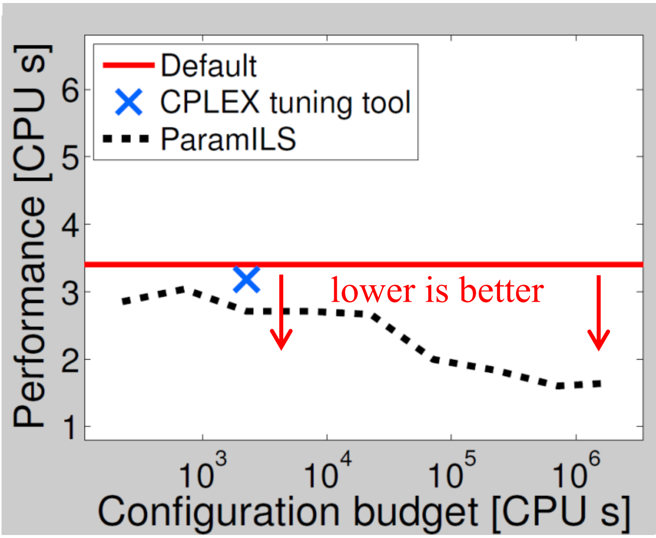
[Hutter, Hoos & Leyton-Brown, CPAIOR 2010]

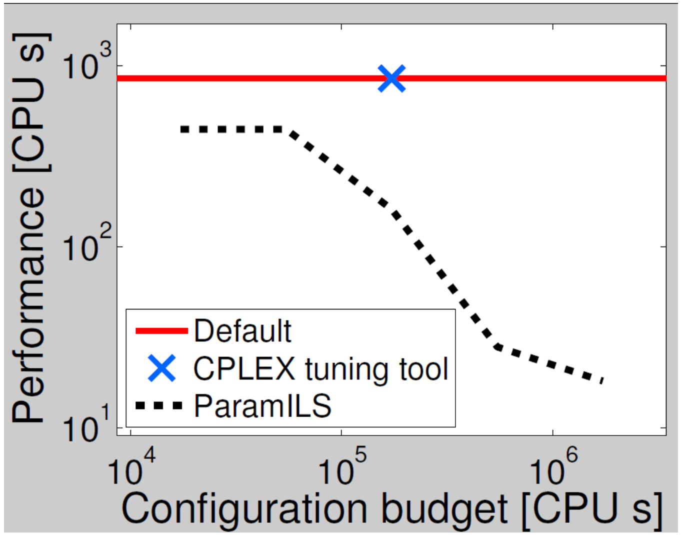
CPLEX tuning tool

- Introduced in version 11 (late 2007, after ParamILS)
- Evaluates predefined good configurations, returns best one
- Required runtime varies (from < 1h to weeks)

ParamILS: anytime algorithm

- At each time step, keeps track of its incumbent





2-fold speedup
(our worst result)

50-fold speedup
(our best result)

Configuration of Machine Learning Algorithms

- Machine Learning has celebrated **substantial successes**
- But it requires **human machine learning experts** to
  - Preprocess the data
  - Perform feature selection
  - Select a model family
  - Optimize hyperparameters
  - …
- **AutoML**: taking the human expert out of the inner loop
  - Yearly AutoML workshops at ICML since 2014
  - PbO applied to machine learning

Auto-WEKA

[Thornton, Hutter, Hoos & Leyton-Brown, KDD 2013]

WEKA [Witten et al, 1999-current]

- most widely used off-the-shelf machine learning package
- over 20 000 citations on Google Scholar

Java implementation of a **broad range of methods**

- 27 base classifiers (with up to 10 parameters each)
- 10 meta-methods
- 2 ensemble methods
- 3 feature search methods & 8 feature evaluators

Different methods work best on different data sets

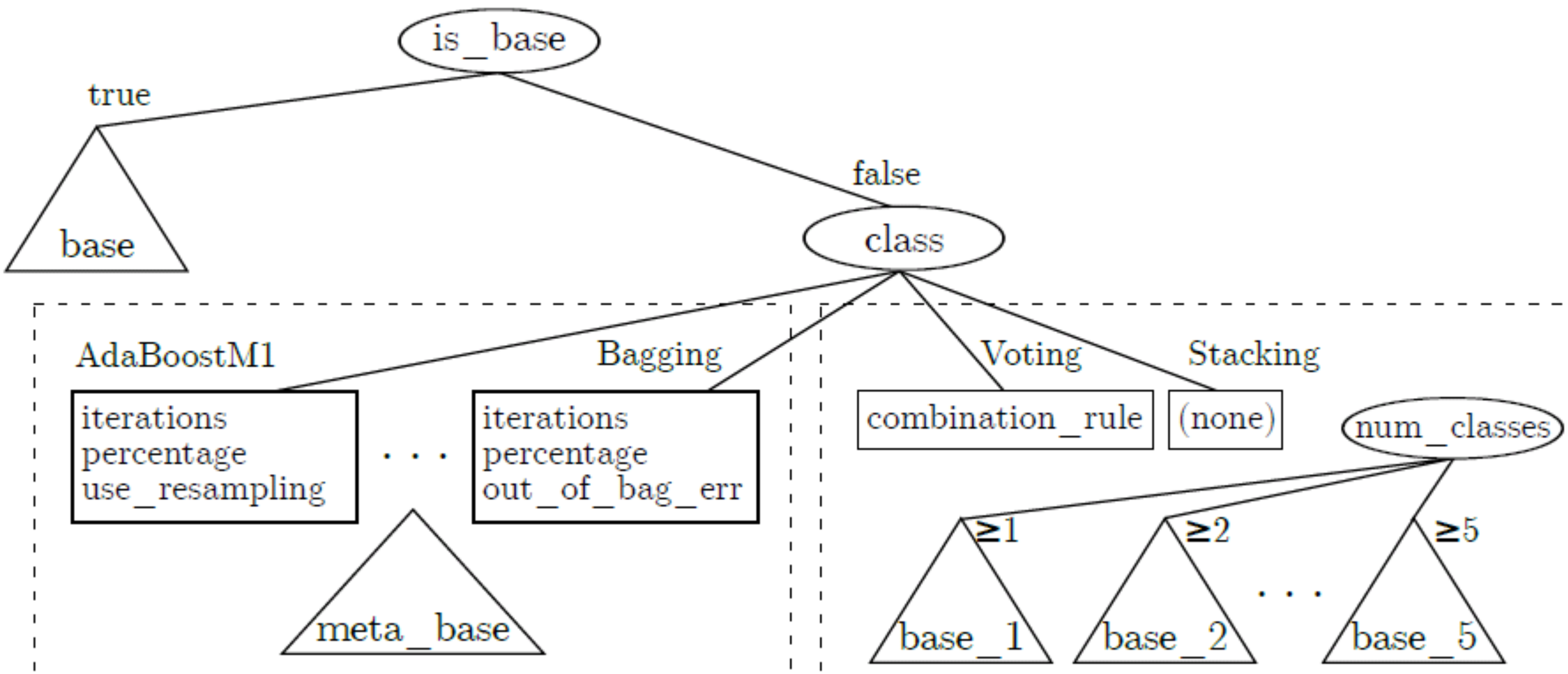
- Want a **true off-the-shelf solution**: Learn

WEKA's configuration space

Base classifiers

- 27 choices, each with up to 10 subparameters
- Coarse discretization: about **10^8 instantiations**

Hierarchical structure on top of base classifiers

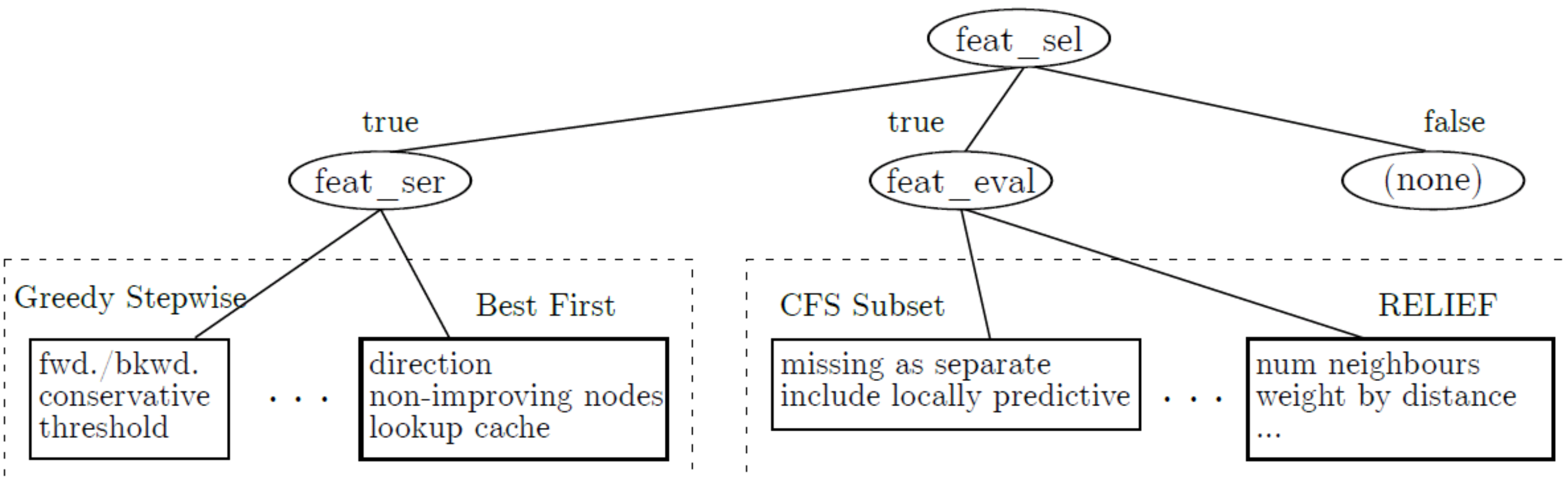


WEKA's configuration space (cont'd)

Feature selection

- **Search** method: which feature subsets to evaluate
- **Evaluation** method: how to evaluate feature subsets in search
- Both methods have **subparameters** → about **10^7 instantiations**

In total: **768 parameters, 10^{47} configurations**



Auto-WEKA: Results

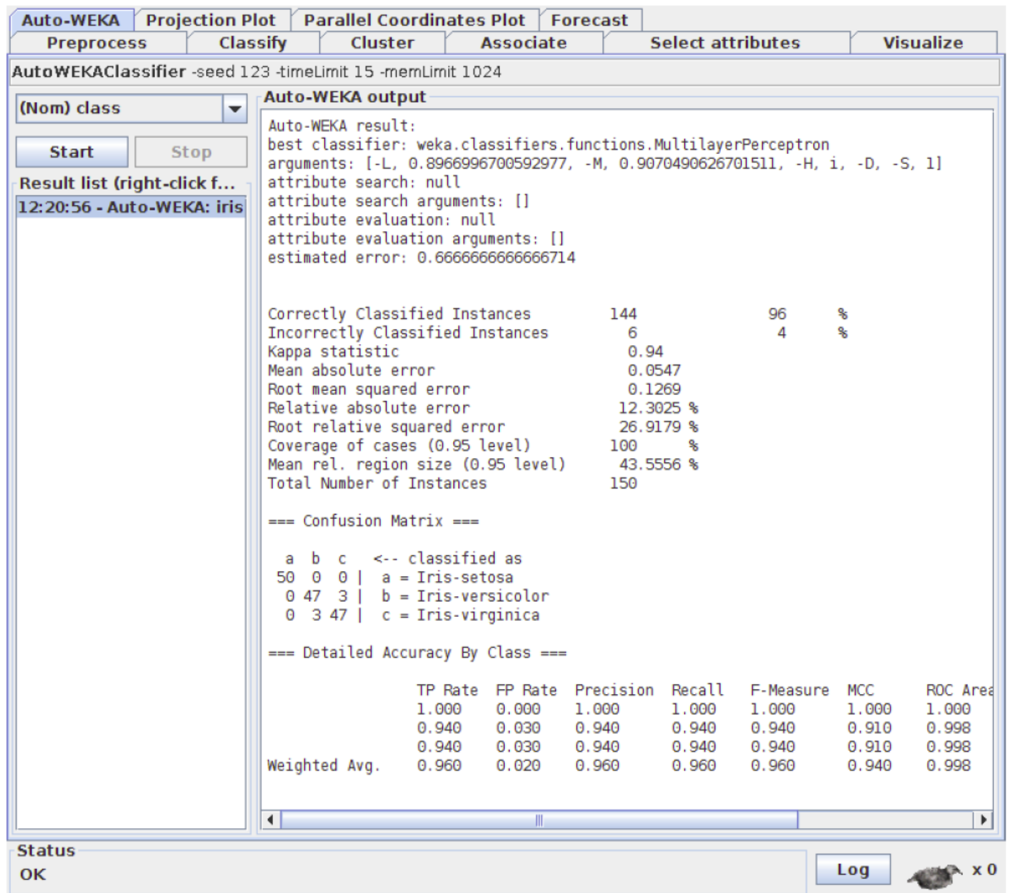
- **Auto-WEKA performed better than best base classifier**
  - Even when "best base classifier" determined by oracle
  - In 6/21 datasets more than 10% reductions in relative error
- Comparison to full grid search
  - Union of grids over parameters of all 27 base classifiers
  - **Auto-WEKA was 100 times faster**
  - **Auto-WEKA had better test performance in 15/21 cases**
- Auto-WEKA based on SMAC *vs* TPE [Bergstra *et al.*, NIPS 2011]
  - SMAC yielded **better CV performance in 19/21 cases**
  - SMAC yielded **better test performance in 14/21 cases**
  - Differences usually small, in 3 cases substantial (SMAC better)

Auto-WEKA as a WEKA plugin

- Command line example:

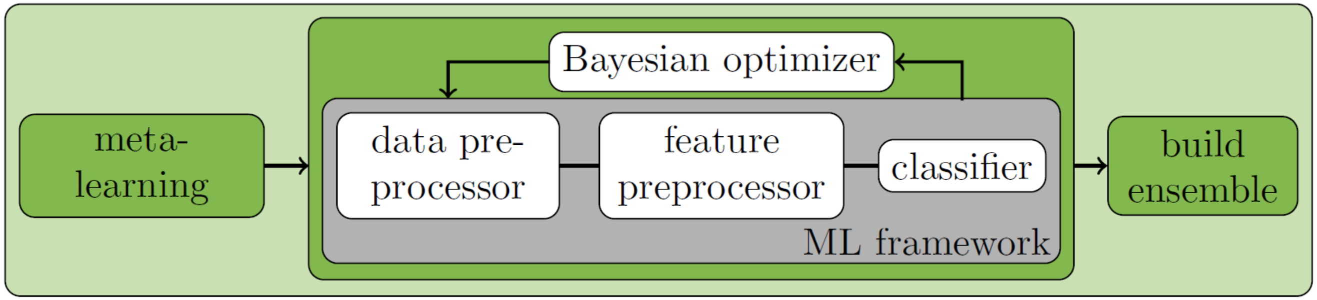
  java -cp autoweka.jar weka.classifiers.meta.AutoWEKAClassifier -t iris.arff -timeLimit 5 -no-cv

- GUI example:



Auto-sklearn

[Feuerer, Klein, Eggensperger, Springenberg, Blum, Hutter, NIPS 2015]



- Followed and extended Auto-WEKA's AutoML approach
- Scikit-learn optimized by SMAC, plus
  - Meta-learning to warmstart Bayesian optimization
  - Automated **posthoc ensemble construction** to combine the models Bayesian optimization evaluated

Auto-sklearn's configuration space

- Scikit-learn [Pedregosa *et al.*, 2011-current] instead of WEKA
  - 15 classifiers, (with a total of 59 hyperparameters)
  - 13 feature preprocessors (42 hyperparams)
  - 4 data preprocessors (5 hyperparams)
- 110 hyperparameters *vs* 768 in Auto-WEKA

name	$\#\lambda$
AdaBoost (AB)	4
Bernoulli naïve Bayes	2
decision tree (DT)	4
extreml. rand. trees	5
Gaussian naïve Bayes	-
gradient boosting (GB)	6
kNN	3
LDA	4
linear SVM	4
kernel SVM	7
multinomial naïve Bayes	2
passive aggressive	3
QDA	2
random forest (RF)	5
Linear Class. (SGD)	10

name	$\#\lambda$
extreml. rand. trees prepr.	5
fast ICA	4
feature agglomeration	4
kernel PCA	5
rand. kitchen sinks	2
linear SVM prepr.	3
no preprocessing	-
nystroem sampler	5
PCA	2
polynomial	3
random trees embed.	4
select percentile	2
select rates	3

one-hot encoding	2
imputation	1
balancing	1
rescaling	1

Auto-sklearn: Ready for Prime Time

- Winning approach in the 14-month AutoML challenge
  - **Best-performing approach in auto-track and human track**
  - Won both tracks in both final phases
  - ***Vs* 150 teams of human experts**

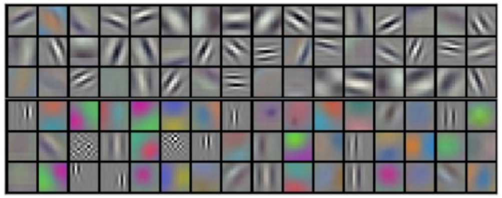
- Trivial to use:

```
import autosklearn.classification as cls
automl=cls.AutoSklearnClassifier(include_
    estimators = ['lda', 'decision_tree'])
automl.fit(X_train, y_train)
y_hat = automl.predict(X_test)
```

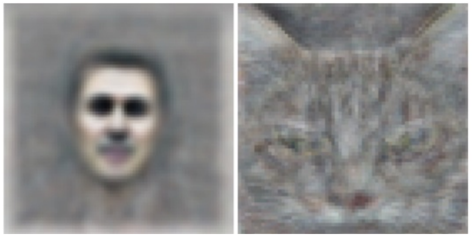
- Available online: https://github.com/automl/auto-sklearn

PbO for Deep Learning

- What is deep learning?
  - Neural networks with many layers
- Why is there so much excitement about it?
  - Dramatically improved the state-of-the-art in many areas, e.g.,
    - Speech recognition
    - Image recognition
  - Automatic learning of representations
    $\rightarrow$ no more manual feature engineering



Source: Krizhevsky *et al.*, 2012

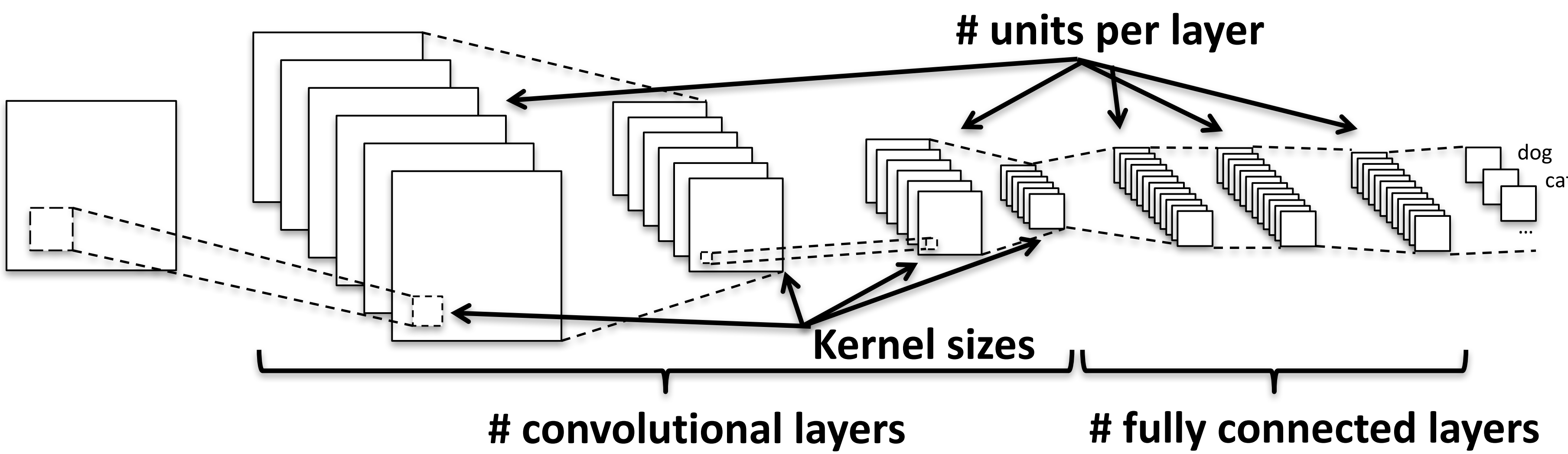


Source: Le *et al.*, 2012

- What changed?
  - Larger datasets
  - Better regularization methods, *e.g.*, dropout [Hinton *et al.*, 2012]
  - Fast GPU implementations [Krizhevsky *et al.*, 2012]

Deep Learning is Sensitive to Many Choices

Choice of network architecture …



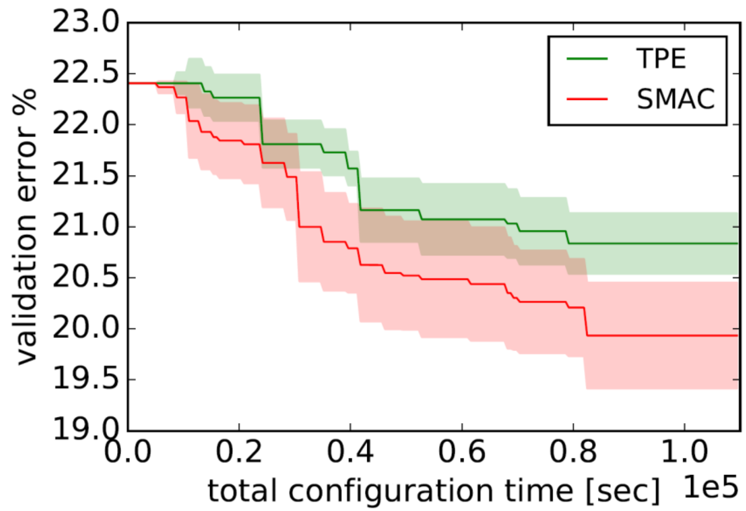
… and 20-30 other numerical choices

Learning rate schedule (initialization, decay, adaptation), momentum, batch normalization, batch size, #epochs, dropout rates, weight initializations, weight decay, …

Auto-Net for Computer Vision Data

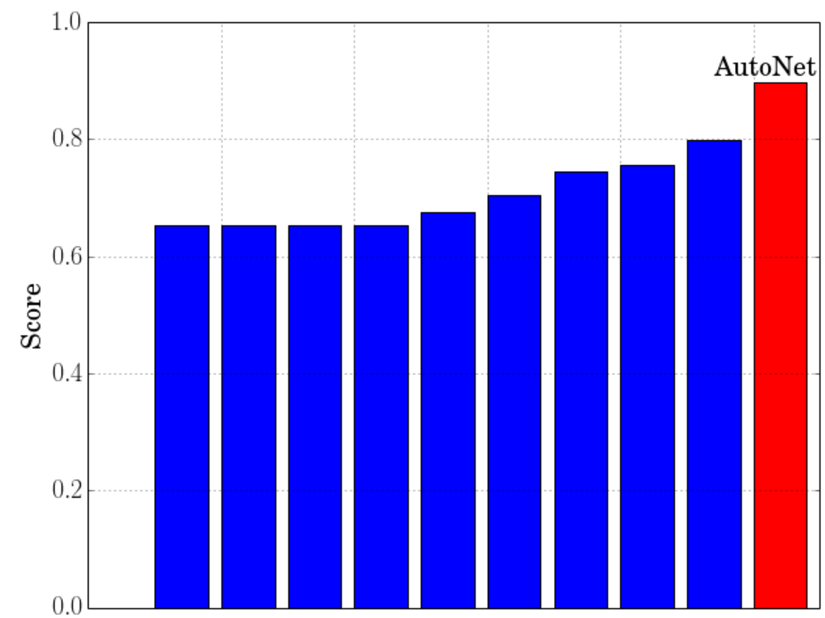
[Domhan, Springenberg, Hutter, IJCAI 2015]

- Application: object recognition
- Parameterized the Caffe framework [Jia, 2013]
  - Convolutional neural network
  - 9 network hyperparameters
  - 12 hyperparameters per layer, up to 6 layers
  - In total **81 hyperparameters**
- Results for CIFAR-10
  - **New best result for CIFAR-10 without data augmentation**
  - SMAC outperformed TPE (only other applicable hyperparameter optimizer)



Auto-Net in the AutoML Challenge

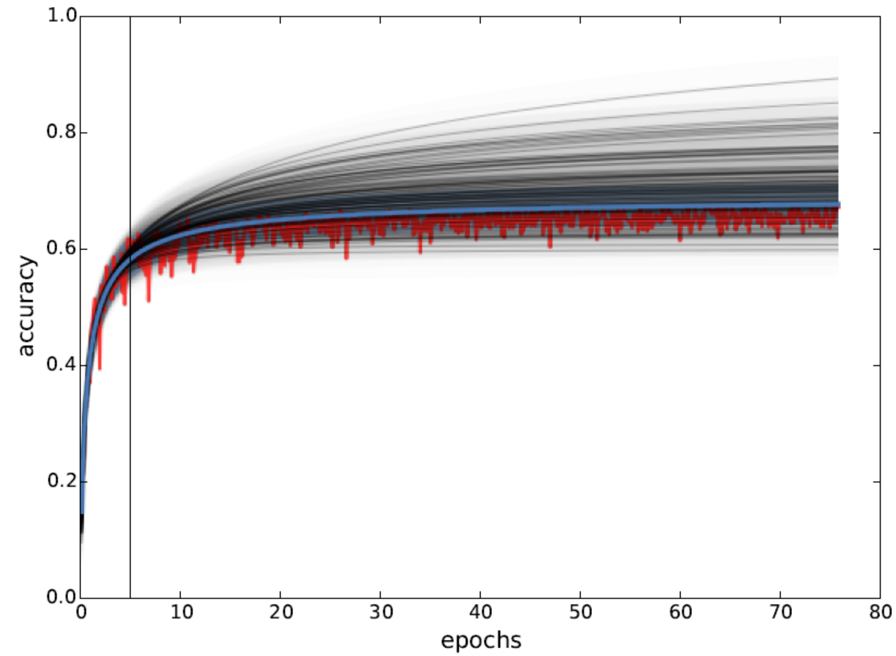
- **Clearly won a dataset of AutoML challenge**
  - 54 491 data points, 5000 features, 18 classes
- Unstructured data → fully-connected network
  - Up to 5 layers (with 3 layer hyperparameters each)
  - 14 network hyperparameters, in total **29 hyperparameters**
  - Optimized for 18h on 5GPUs
- Result (on private test set)
  - AUC 90%
  - All other (manual) approaches < 80%



Speedups by Prediction of Learning Curves

[Domhan, Springenberg & Hutter, IJCAI 2015]

- Humans can look inside the blackbox
  - They **can predict the final performance of a target algorithm run early**
  - After few epochs of stochastic gradient descent
  - **Stop if not promising**



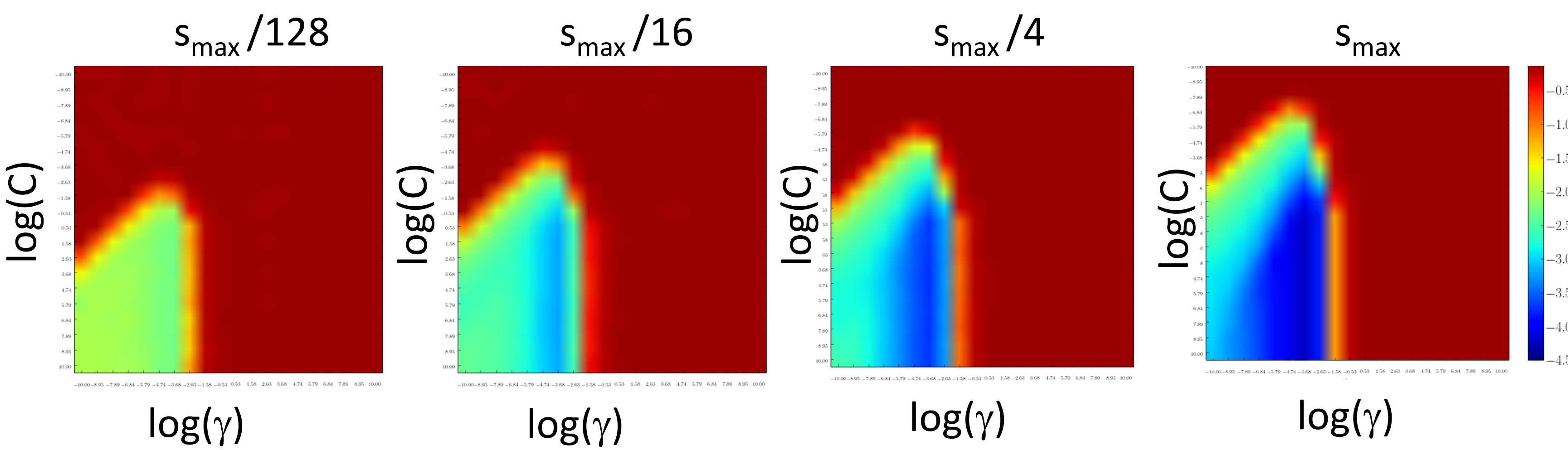
- We automated that heuristic
  - Fitted linear combination of 22 parametric models
  - MCMC to preserve uncertainty over model parameters
  - Stopped poor runs early: overall 2-fold speedup

Speedups by Reasoning over Data Subsets

[Klein, Bartels, Falkner, Hennig, Hutter, arXiv 2016]

- **Problem**: training is very slow for large datasets
- **Solution approach**:
  scaling up from subsets of given data

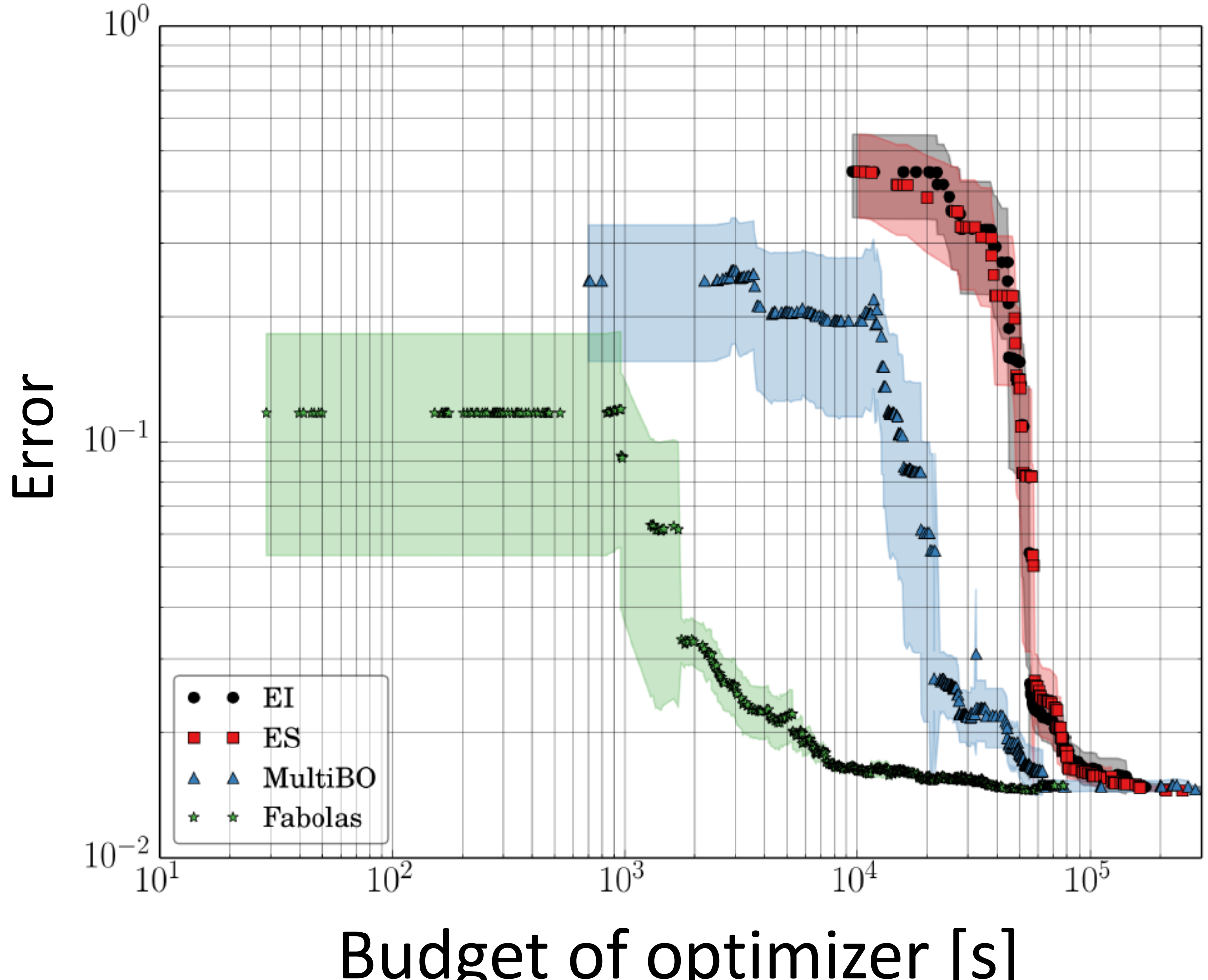
- **Example: SVM**
  - Computational cost grows quadratically in dataset size s
  - **Error shrinks smoothly with s**



Speedups by Reasoning over Data Subsets

[Klein, Bartels, Falkner, Hennig, Hutter, arXiv 2016]

- **10-100x speedup** for optimizing SVM hyperparameters
- **5-10x speedup** for convolutional neural networks



Summary of Algorithm Configuration

- Algorithm configuration
  - Methods (components of algorithm configuration)
  - Systems (that instantiate these components)
  - Demo & practical issues
  - Case studies

- Useful abstraction with many (!) applications
- Often better performance than human experts
- Much less human expert time required

Links to all our code: http://ml4aad.org

Overview

- Programming by Optimization (PbO): Motivation and Introduction

- Algorithm Configuration

- **Portfolio-Based Algorithm Selection**
  - **SATzilla: a framework for algorithm selection**
  - **Hydra: automatic portfolio construction**

- Software Development Tools and Further Directions

Motivation: no single great configuration exists

- Heterogeneous instance distributions
  - Even best overall configuration is not great; *e.g.:*

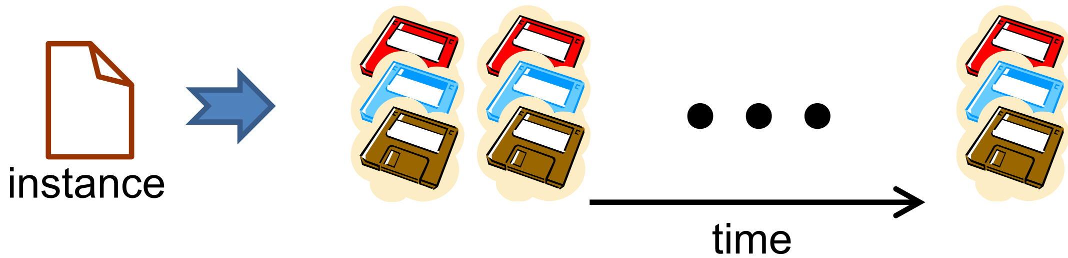
Configuration	Instance type 1	Instance type 2
#1	1s	1000s
#2	1000s	1s
#3	100s	100s

- No single best solver
  - *E.g.,* SAT solving:
    different solvers win different categories
  - **Virtual best solver (VBS) much better than single best solver (SBS)**

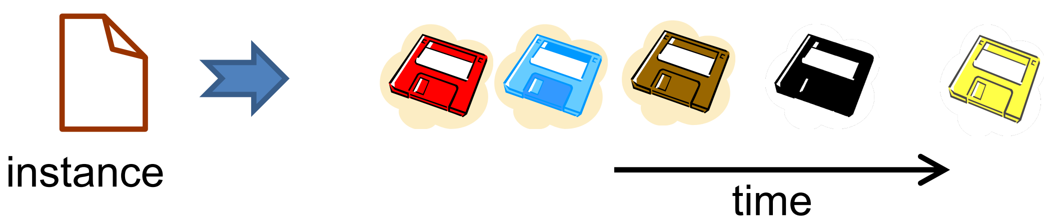
Algorithm portfolios

Exploiting complementary strengths of different algorithms

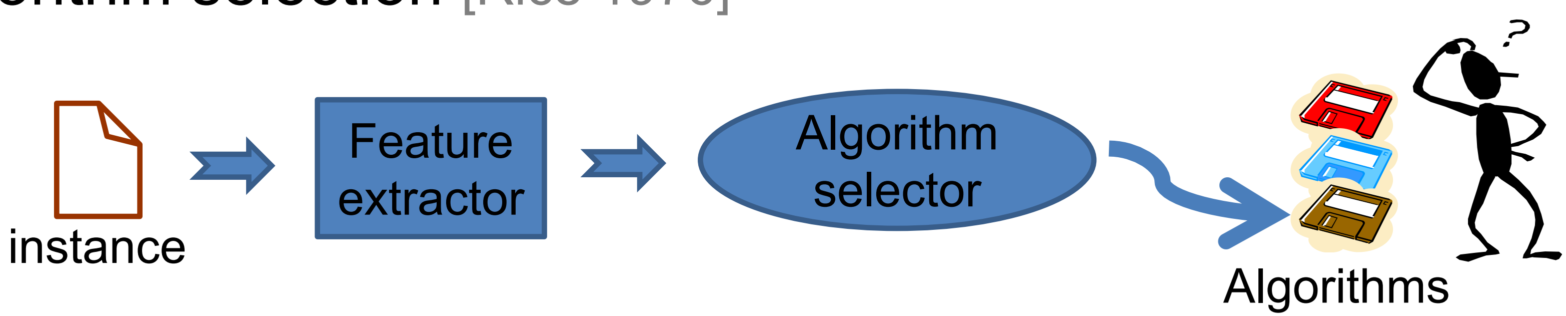
Parallel portfolios [Huberman *et al.* 1997]



Algorithm schedules [Sayag *et al.* 2006]



Algorithm selection [Rice 1976]



Portfolios have been successful in many areas

[*]Algorithm Selection   [†]Sequential Execution   [‡]Parallel Execution

- **Satisfiability:**
  - SATzilla[*†] [various coauthors, cited in the following slides; 2003-17]
  - 3S[*†] [Sellmann 2011]
  - ppfolio[‡] [Roussel 2011]
  - claspfolio[*] [Gebser, Kaminski, Kaufmann, Schaub, Schneider, Ziller 2011]
  - aspeed[†‡] [Kaminski, Hoos, Schaub, Schneider 2012]
- **Constraint Satisfaction:**
  - CPHydra[*†] [O'Mahony, Hebrard, Holland, Nugent, O'Sullivan 2008]

Portfolios have been successful in many areas

**Algorithm Selection* *†Sequential Execution* *‡Parallel Execution*

- **Planning:**
  – FD Stone Soup† [Helmert, Röger, Karpas 2011]
- **Mixed Integer Programming:**
  – ISAC* [Kadioglu, Malitsky, Sellmann, Tierney 2010]
  – MIPzilla*† [Xu, Hutter, Hoos, Leyton-Brown 2011]
- **..and this is just the tip of the iceberg:**
  – http://dl.acm.org/citation.cfm?id=1456656 [Smith-Miles 2008]
  – http://4c.ucc.ie/~larsko/assurvey [Kotthoff 2012]

Overview

- Programming by Optimization (PbO):
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  - **SATzilla: a framework for algorithm selection**
  - **Hydra: automatic portfolio construction**

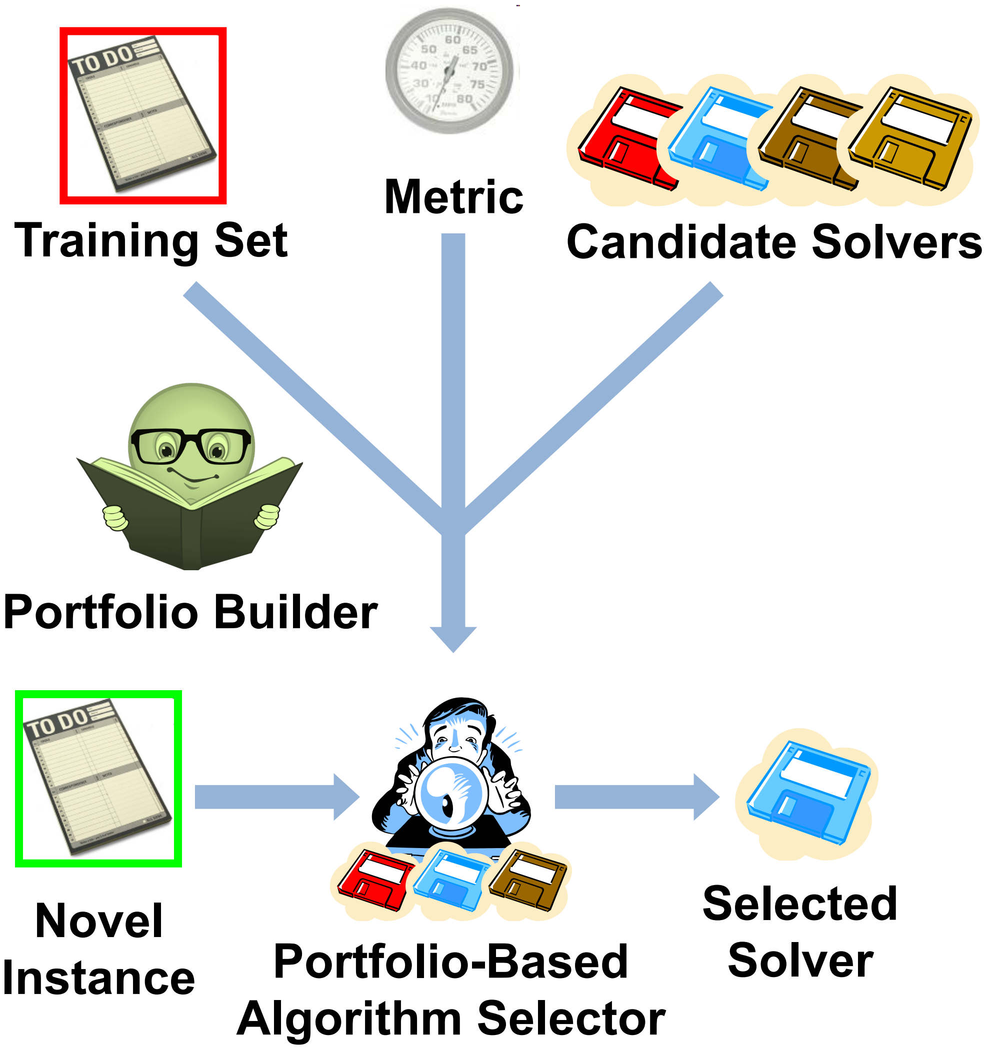
- Software Development Tools and Further Directions

SATzilla: the early core approach

[Leyton-Brown, Nudelman, Andrew, J. McFadden, Shoham 2003]
[Nudelman, Leyton-Brown, Devkar, Shoham, Hoos 2004]

- Training (part of algorithm development)
  - Build a statistical model to predict runtime for each component algorithm
- Test (for each new instance)
  - Predict performance for each algorithm
  - Pick the algorithm predicted to be best
- Good performance in SAT competitions
  - 2003: 2 silver, 1 bronze medals
  - 2004: 2 bronze medals

SATzilla (stylized version)

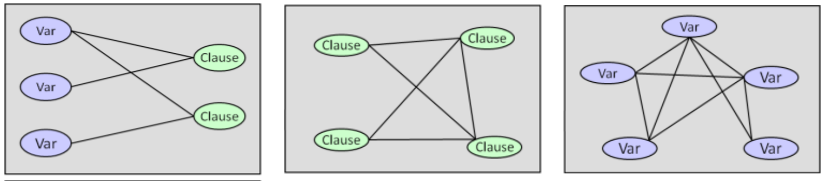


- **Given:**
  - **training set of instances**
  - **performance metric**
  - **candidate solvers**
  - **portfolio builder** ***(incl. instance features)***
- Training:
  - collect performance data
  - learn a model for selecting among solvers
- At Runtime:
  - evaluate model
  - run selected solver

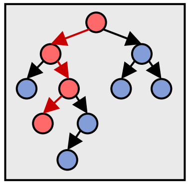
SAT Instance Features (2003-14)

Over 100 features, including:

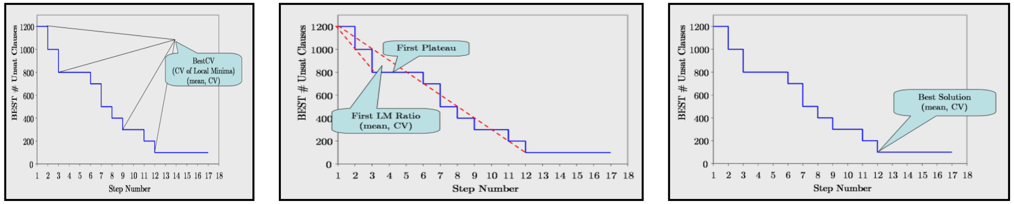
- Instance **size** (clauses, variables, clauses/variables, …)
- **Syntactic** properties (*e.g.*, positive/negative clause ratio)
- Statistics of various **constraint graphs**
  - factor graph
  - clause–clause graph
  - variable–variable graph



- Knuth's **search space size** estimate



- **Tree search probing**
- **Local search probing**



- **Linear programming** relaxation

maximize: $\sum_{k\in C}\left(\sum_{i\in L,\, i\in k} v_i + \sum_{j\in \overline{L},\, i\in k} (1-v_j)\right)$

subject to: $\sum_{i\in k,\, i\in L} v_i + \sum_{j\in k,\, j\in \overline{L}} (1-v_j) \geq 1 \quad \forall k \in C$

$v_i \in \{0,1\} \quad \forall i$

SATzilla 2007

[Xu, Hutter, Hoos & Leyton-Brown, CP 2007; JAIR 2008]

- Substantially extended features
- Early algorithm schedule: identify set of "**presolvers**" and a schedule for running them
  - For every choice of two presolvers + captimes, run entire SATzilla pipeline and evaluate overall performance
  - Keep choice that yields best performance
  - For later steps: Discard instances solved by this presolving schedule
- Identify a "**backup solver**": SBS on remaining data
  - Needed in case feature computation crashes
- 2007 SAT competition: **3 gold**, 1 silver, 1 bronze medals

SATzilla 2009

[Xu, Hutter, Hoos & Leyton-Brown, CP 2007; JAIR 2008]

- Robustness: selection of best subset of component solvers
  - Consider every subset of given solver set
    - omitting weak solvers prevents their accidental selection
    - conditioned on choice of presolvers
    - computationally cheap: models decompose across solvers
  - Keep subset that achieves best performance
- Fully automated procedure
  - optimizes loss on a validation set
- 2009 SAT competition: **3 gold**, 2 silver medals

SATzilla 2011 and later: cost-sensitive DFs

[Xu, Hutter, Hoos & Leyton-Brown, SAT 2012]

- How it works:
  - Build classifier to determine which algorithm to prefer between each pair of algorithms in given portfolio
  - Loss function: **cost of misclassification**
- Decision forests and support vector machines have **cost-sensitive variants**
- Classifiers vote for different algorithms; select algorithm with most votes
  - Advantage: selection is a classification problem
  - Advantage: big and small errors treated differently
- 2011 SAT competition: entered **Evaluation Track** (more later)

2012 SAT Challenge: Application

Rank	Solver	% solved	# solved
	VBS	**94.7**	**568**
1	SATzilla2012 APP	88.5	531
2	SATzilla2012 ALL	85.8	515
3	Industrial SAT Solver	83.2	499
4	interactSAT	80.0	480
5	glucose	79.2	475
6	SINN	78.7	472
7	ZENN	78.0	468
8	Lingeling	77.8	467

* Interacting multi-engine solvers: like portfolios, but richer interaction between solvers

2012 SAT Challenge: Hard Combinatorial

Rank	Solver	% solved	# solved
	VBS	**88.2**	**529**
1	SATzilla2012 COMB	79.3	476
2	SATzilla2012 ALL	78.8	473
3	ppfolio2012	70.3	422
4	interactSAT_c	79.5	417
5	pfolioUZK	66.8	401
6	aspeed-crafted	61.7	370
7	clasp-crafted	61.2	367
8	claspfolio-crafted	58.7	352

SAT Challenge 2012: Random

Rank	Solver	% solved	# solved
	VBS	**93.0**	**558**
1	CCASat	70.5	423
2	SATzilla2012 RAND	53.5	321
3	SATzilla2012 ALL	51.0	306
4	sattime2012	44.8	269
5	ppfolio2012	42.2	253
6	pfolioUZK	38.3	230
7	ssa	25.0	150
8	gNovelty+PCL	20.5	123

2012 SAT Challenge: Sequential Portfolio

Rank	Solver	% solved	# solved
	VBS	**80.7**	**484**
1	SATzilla2012 ALL	72.2	433
2	ppfolio2012	61.7	370
3	pfolioUZK	60.3	362

- 3S **deserves mentioning**, but didn't rank officially
  [Kadioglu, Malitsky, Sabharwal, Samulowitz, Sellmann, 2011]
  – Disqualified on a technicality
    - chose a buggy solver that returned an incorrect result
    - an occupational hazard for portfolios!
  – Overall performance **nearly as strong as SATzilla**

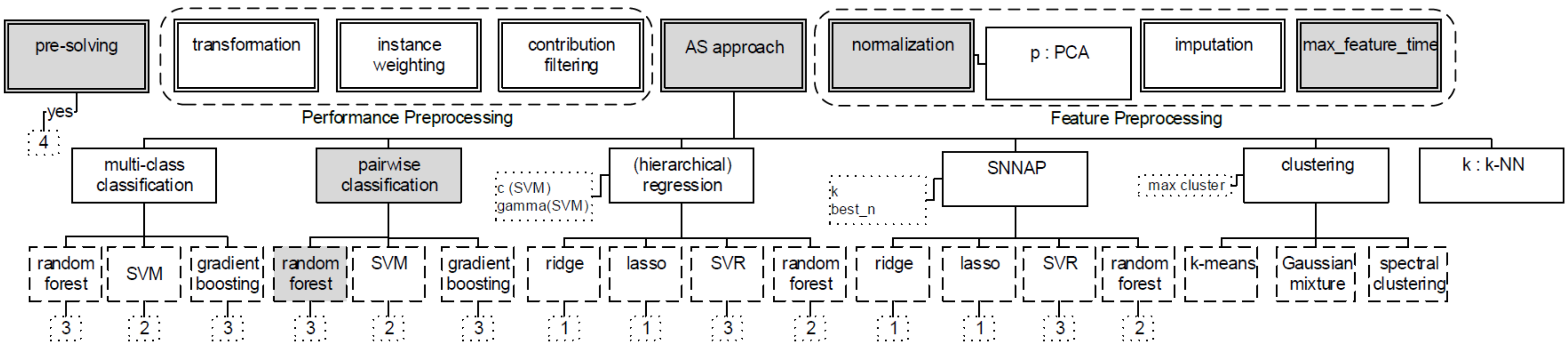
2013 onwards

- Algorithm selection a victim of its own success
- 2013: “The emphasis of SAT Competition 2013 is on evaluation of core solvers:”
  - Single-core portfolios of >2 solvers **not eligible**
  - One “open track” allowing parallel solvers, portfolios, etc
  - That open track was dominated by portfolios
- 2014 onwards
  - “SAT Competition 2014 **only allows submission of core solvers**”
  - Portfolio researchers started their own competition:
    the **ICON Algorithm Selection Challenge**

AutoFolio: PbO for Algorithm Selection

[Lindauer, Hoos, Hutter & Schaub, JAIR 2015]

- **Define a general space** of algorithm selection methods
  - AutoFolio's configuration space: 54 choices



- Use algorithm configuration to **select best instantiation**
  - Partition the training benchmark instances into 10 folds
  - Use SMAC to find algorithm selection approach & its hyperparameters that optimize CV performance

ICON Algorithm Selection Challenge 2015

- Ingredients of an algorithm selection (AS) benchmark
  - A set of solvers
  - A set of benchmark instances (split into training & test)
  - Measured performance of all solvers on all instances

- Algorithm selection competition:
  - 13 AS benchmarks from SAT, MaxSAT, CSP, ASP, QBF, Premarshalling
  - 9 competitors using regression, classification, clustering, k-NN, etc

- Winning algorithms in the 3 tracks:
  - Penalized average runtime: **AutoFolio**
  - Number of instances solved: **AutoFolio**
  - Frequency of selecting the best algorithm: **SATzilla**
  - **Overall winner SATzilla** (2nd in first two tracks)

Try it yourself!

- SATzilla and AutoFolio are **freely available online**

  http://www.cs.ubc.ca/labs/beta/Projects/SATzilla/

  http://ml4aad.org/autofolio

- You can try them for your problem
  - we have features for SAT, MIP, AI planning and TSP
  - you need to provide features for other domains
    - in many cases, the general ideas behind our features apply
    - can also make features by reducing your problem to e.g. SAT and computing the SAT features

Automatically Configuring Algorithms for Portfolio-Based Selection

Xu, Hoos, Leyton-Brown (2010); Kadioglu *et al.* (2010)

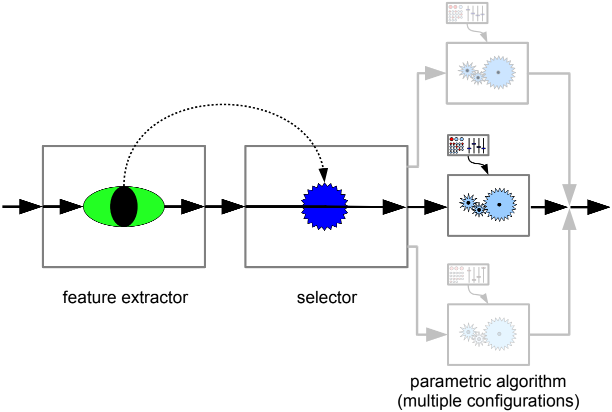
Note:

- SATzilla builds algorithm selector based on given set of SAT solvers
  but: success entirely depends on quality of given solvers

- Automated configuration produces solvers that work well *on average* on a given set of SAT instances
  (*e.g.*, SATenstein – KhudaBukhsh, Xu, Hoos, Leyton-Brown 2009)
  but: may have to settle for compromises
  for broad, heterogenous instance sets

Idea: Combine the two approaches $\rightsquigarrow$ portfolio-based selection
from set of automatically constructed solvers

Combined Configuration + Selection



Approach #1:

1. build solvers for various types of instances using automated algorithm configuration
2. construct portfolio-based selector from these

Problem: requires suitably defined sets of instances

Solution: automatically partition heterogenous instance set

Instance-specific algorithm configuration (ISAC)

Kadioglu, Malitsky, Sellmann, Tierney (2010); Malitky, Sellman (2012)

1. cluster training instances based on features (using G-means)
2. configure given parameterised algorithm independently for each cluster (using GGA)
3. construct portfolio-based selector from resulting configurations (using distance to cluster centroids)

Drawback: Instance features may not correlate well with impact of algorithm parameters on performance (*e.g.*, uninformative features)

Approach #2:

Key idea: Augment existing selector *AS* by targetting instances on which *AS* performs poorly

(*cf.* Leyton-Brown *et al.* 2003; Leyton-Brown *et al.* 2009)

- interleave configuration and selector construction
- in each iteration, determine configuration that complements current selector best

Advantages:

- any-time behaviour: iteratively adds configurations
- desirable theoretical guarantees (under idealising assumptions)

Hydra

Xu, Hoos, Leyton-Brown (2010); Xu, Hutter, Hoos, Leyton-Brown (2011)

1. configure given target algorithm A on complete instance set I
   $\rightsquigarrow$ configuration A_1 = selector AS_1 (always selects A_1)

2. configure a new copy of A on I such that performance of selector $AS := AS_1 + A_{new}$ is optimised
   $\rightsquigarrow$ configuration A_2
   $\rightsquigarrow$ selector $AS_2 := AS_1 + A_2$ (selects from $\{A_1, A_2\}$)

3. configure a new copy of A on I such that performance of selector $AS := AS_2 + A_{new}$ is optimised
   $\rightsquigarrow$ configuration A_3
   $\rightsquigarrow$ selector $AS_3 := AS_2 + A_3$ (selects from $\{A_1, A_2, A_3\}$)

...

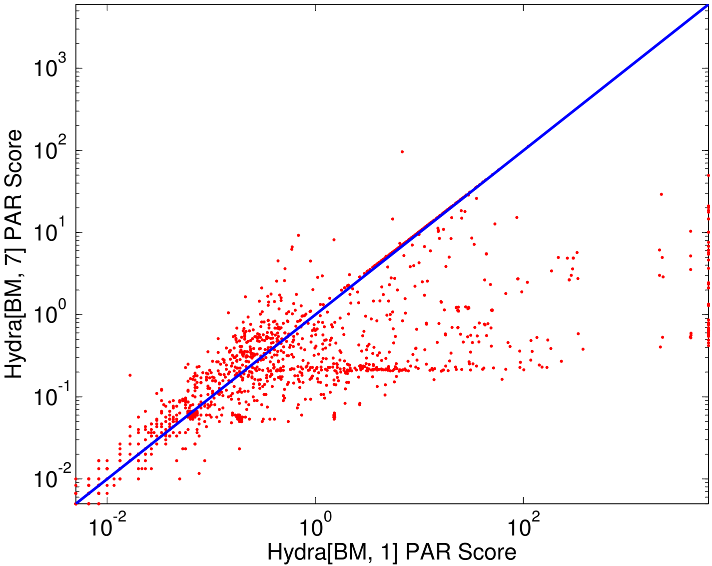
Note:

- effectively adds A with maximal marginal contribution in each iteration
- estimate marginal contribution using perfect selector (oracle) $\rightsquigarrow$ avoids costly construction of selectors during configuration
- works well using FocusedILS for configuration, *zilla for selection (but can use other configurators, selectors)
- can be further improved by adding multiple configurations per iteration; using performance estimates from configurator

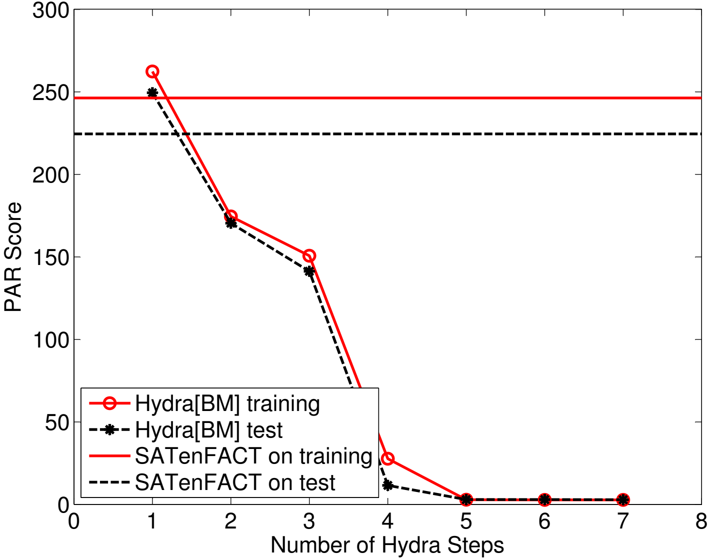
Results on SAT:

- target algorithm: SATenstein-LS (KhudaBukhsh *et al.* 2009)
- 6 well-known benchmark sets of SAT instances (application, crafted, random)
- 7 iterations of Hydra
- 10 configurator runs per iteration, 1 CPU day each

Results on mixture of 6 benchmark sets



Results on mixture of 6 benchmark sets

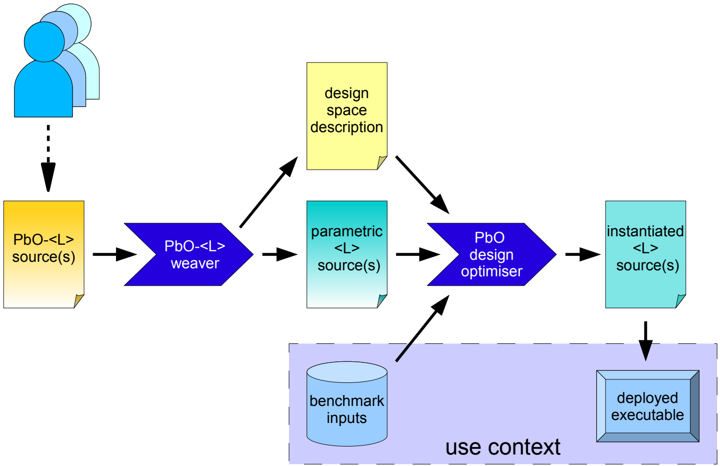


Note:

- good results also for MIP (CPLEX)
  (Xu, Hutter, Hoos, Leyton-Brown 2011)
- idea underlying Hydra can also be applied to automatically construct *parallel algorithm portfolios* from single parameterised target algorithm
  (Hoos, Leyton-Brown, Schaub, Schneider 2012–14)

Software Development Support and Further Directions

Software development in the PbO paradigm



Design space specification

Option 1: use language-specific mechanisms

- command-line parameters
- conditional execution
- conditional compilation (`ifdef`)

Option 2: generic programming language extension

Dedicated support for ...

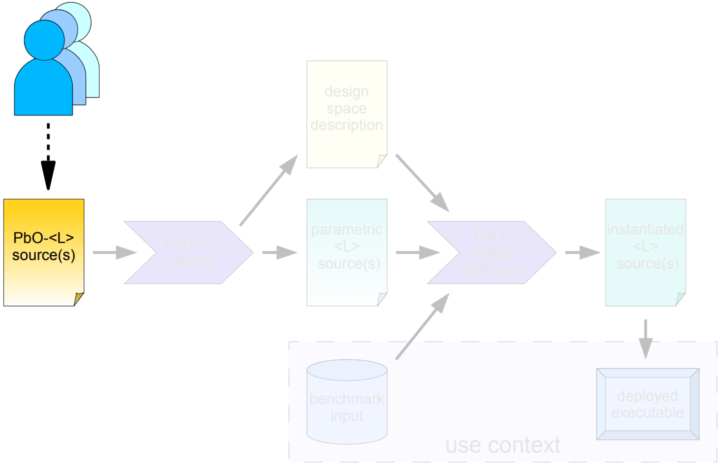
- exposing parameters
- specifying alternative blocks of code

Advantages of generic language extension:

- reduced overhead for programmer
- clean separation of design choices from other code
- dedicated PbO support in software development environments

Key idea:

- augmented sources: *PbO-Java* = Java + PbO constructs, ...
- tool to compile down into target language: *weaver*


PbO-<L> source(s)
PbO-<L> weaver
design space description
parametric <L> source(s)
PbO design optimiser
instantiated <L> source(s)
benchmark input
deployed executable
use context

Exposing parameters

```
...
numerator -= (int) (numerator / (adjfactor+1) * 1.4);
...      ...
##PARAM(float multiplier=1.4)
numerator -= (int) (numerator / (adjfactor+1) * ##multiplier);
...
```

- parameter declarations can appear at arbitrary places (before or after first use of parameter)
- access to parameters is read-only (values can only be set/changed via command-line or config file)

Specifying design alternatives

- **Choice:** set of interchangeable fragments of code that represent design alternatives (**instances of choice**)
- **Choice point:**
  location in a program at which a choice is available

```
##BEGIN CHOICE preProcessing
<block 1>
##END CHOICE preProcessing
```

Specifying design alternatives

- **Choice:** set of interchangeable fragments of code that represent design alternatives (**instances of choice**)
- **Choice point:** location in a program at which a choice is available

```
##BEGIN CHOICE preProcessing=standard
<block S>
##END CHOICE preProcessing

##BEGIN CHOICE preProcessing=enhanced
<block E>
##END CHOICE preProcessing
```

Specifying design alternatives

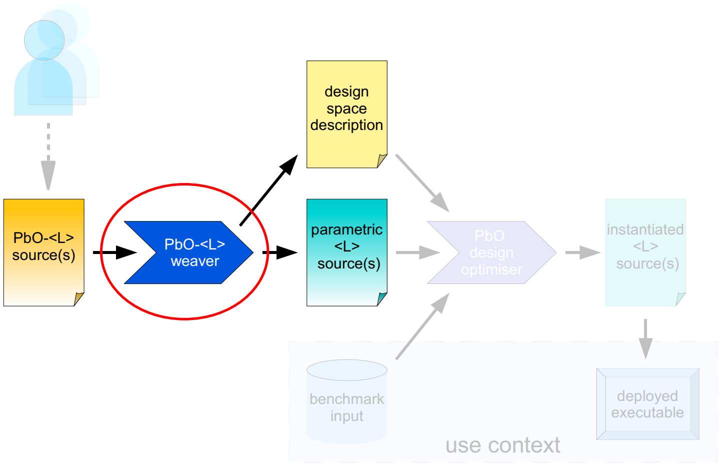
- **Choice:** set of interchangeable fragments of code that represent design alternatives (**instances of choice**)
- **Choice point:** location in a program at which a choice is available

```
##BEGIN CHOICE preProcessing
<block 1>
##END CHOICE preProcessing

...

##BEGIN CHOICE preProcessing
<block 2>
##END CHOICE preProcessing
```

Specifying design alternatives

- **Choice:** set of interchangeable fragments of code that represent design alternatives (**instances of choice**)
- **Choice point:**
  location in a program at which a choice is available

```
##BEGIN CHOICE preProcessing
<block 1a>
  ##BEGIN CHOICE extraPreProcessing
  <block 2>
  ##END CHOICE extraPreProcessing
<block 1b>
##END CHOICE preProcessing
```


design space description
PbO-<L> source(s)
PbO-<L> weaver
parametric <L> source(s)
PbO design optimiser
instantiated <L> source(s)
benchmark input
deployed executable
use context

The Weaver

transforms PbO-<L> code into <L> code
(<L> = Java, C++, ...)

- parametric mode:
  - expose parameters
  - make choices accessible via (conditional, categorical) parameters
- (partial) instantiation mode:
  - hardwire (some) parameters into code (expose others)
  - hardwire (some) choices into code (make others accessible via parameters)

The road ahead

- Support for PbO-based software development
  - Weavers for PbO-C, PbO-C++, PbO-Java
  - PbO-aware development platforms
  - Improved / integrated PbO design optimiser
  - Debugging and performance analysis tools
- Best practices
- Many further applications
- Scientific insights

Which choices matter?

Observation: Some design choices matter more than others

depending on ...

- algorithm under consideration
- given use context

Knowledge which choices / parameters matter may ...

- guide algorithm development
- facilitate configuration

3 recent approaches:

- Forward selection based on empirical performance models
  Hutter, Hoos, Leyton-Brown (2013)
- Functional ANOVA based on empirical performance models
  Hutter, Hoos, Leyton-Brown (2014)
- Ablation analysis
  Fawcett & Hoos (2013–16)

Functional ANOVA based on empirical performance models

Hutter, Hoos, Leyton-Brown (2014)

Key idea:

- build regression model of algorithm performance as a function of all input parameters (= design choices)

  $\leadsto$ empirical performance models (EPMs)

- analyse variance in model output (= predicted performance) due to each parameter, parameter interactions

- importance of parameter: fraction of performance variation over configuration space explained by it (main effect)

- analogous for sets of parameters (interaction effects)

Decomposition of variance in a nutshell

For parameters $p_1, \ldots, p_n$ and a function (performance model) y:

$$\begin{aligned}
y(p_1, \ldots, p_n) \quad = \quad & \mu \\
& + f_1(p_1) + f_2(p_2) + \cdots + f_n(p_n) \\
& + f_{1,2}(p_1, p_2) + f_{1,3}(p_1, p_3) + \cdots + f_{n-1,n}(p_{n-1}, p_n) \\
& + f_{1,2,3}(p_1, p_2, p_3) + \cdots \\
& + \cdots
\end{aligned}$$

Note:

- Straightforward computation of main and interaction effects is intractable.
  (integration over combinatorial spaces of configurations)
- For random forest models, marginal performance predictions and variance decomposition (up to constant-sized interactions) can be computed exactly and efficiently.

Empirical study:

- 8 high-performance solvers for SAT, ASP, MIP, TSP (4–85 parameters)
- 12 well-known sets of benchmark data (random + real-world structure)
- random forest models for performance prediction, trained on 10 000 randomly sampled configurations per solver + data from 25+ runs of SMAC configuration procedure

Fraction of variance explained by main effects:

CPLEX on RCW (comp sust)	70.3%
CPLEX on CORLAT (comp sust)	35.0%
Clasp on software verificatition	78.9%
Clasp on DB query optimisation	62.5%
CryptoMiniSAT on bounded model checking	35.5%
CryptoMiniSAT on software verification	31.9%

Fraction of variance explained by main + 2-interaction effects:

CPLEX on RCW (comp sust)	70.3% + 12.7%
CPLEX on CORLAT (comp sust)	35.0% + 8.3%
Clasp on software verificatition	78.9% + 14.3%
Clasp on DB query optimisation	62.5% + 11.7%
CryptoMiniSAT on bounded model checking	35.5% + 20.8%
CryptoMiniSAT on software verification	31.9% + 28.5%

Note:

may pick up variation caused by poorly performing configurations

Simple solution:

cap at default performance or quantile from distribution of randomly sampled configurations; build model from capped data.

Ablation analysis

Fawcett & Hoos (2013, 2016)

Key idea:

- given two configurations, A and B, change one parameter at a time to get from A to B

  $\rightsquigarrow$ ablation path

- in each step, change parameter to achieve maximal gain (or minimal loss) in performance

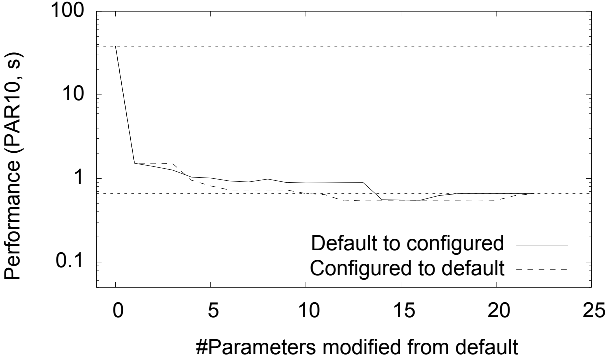
- for computational efficiency, use racing (F-race) for evaluating parameters considered in each step

Empirical study:

- high-performance solvers for SAT, MIP, AI Planning
  (26–76 parameters),
  well-known sets of benchmark data (real-world structure)

- optimised configurations obtained from ParamILS
  (minimisation of penalised average running time;
  10 runs per scenario, 48 CPU hours each)

Ablation between default and optimised configurations:



LPG on Depots planning domain

Which parameters are important?

LPG on `depots`:

- `cri_intermediate_levels` (43% of overall gain!)
- `triomemory`
- `donot_try_suspected_actions`
- `walkplan`
- `weight_mutex_in_relaxed_plan`

Note: Importance of parameters varies between planning domains

New development: Ablation based on surrogate models
(Biedenkapp, Lindauer, Eggensperger, Hutter, Fawcett, Hoos 2017)

Algorithm configuration: parameter importance
$\rightsquigarrow$ Algorithm selection: component contribution

Xu, Hutter, Hoos, Leyton-Brown (2012)

Consider:

portfolio-based algorithm selector AS
with candidate algorithms $A_1, A_2, \ldots A_k$

Question:

How much does each A_i contribute
to overall performance of AS?

Marginal contribution of A_i to portfolio-based selector AS

$=$ difference in performance of AS with and without A_i (trained separately)

- $\neq$ frequency of selecting A_i
- $\neq$ fraction of instances solved by A_i
- $\neq$ contribution of A_i to virtual best solver (VBS)

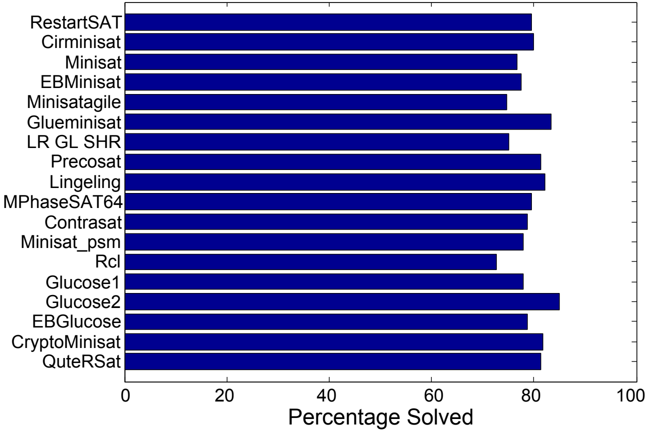
Application to SATzilla:

- all instances from 2011 SAT Competition:
  300 Application; 300 Crafted; 300 Random
- candidate solvers from 2011 SAT Competition:
  - for determining virtual best solver (VBS)
    and single best solver (SBS):
    all solvers from Phase 2 of competition:
    31 Application; 25 Crafted; 17 Random
  - for building SATzilla:
    all sequential, non-portfolio solvers from Phase 2:
    18 Application; 15 Crafted; 9 Random
- SATzilla assessed by 10-fold cross validation

SATzilla 2011 Performance (Inst. Solved)

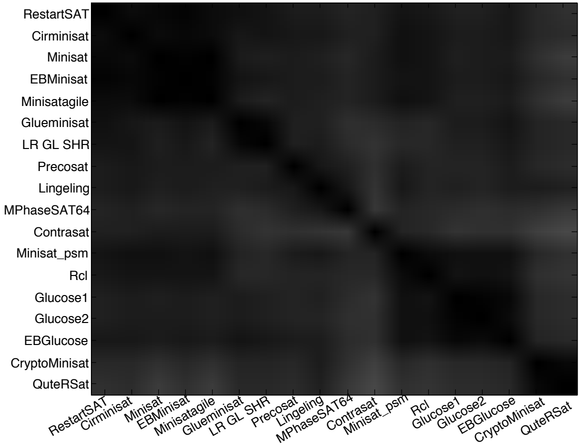
Solver	*Application*	*Crafted*	*Random*
VBS	84.7%	76.3%	82.2%
SATzilla 2011	75.3%	66.0%	80.8%
SATzilla 2009	70.3%	63.0%	80.3%
Gold medalist (SBS)	71.7%	54.3%	68.0%

Performance of Individual Solvers
Application



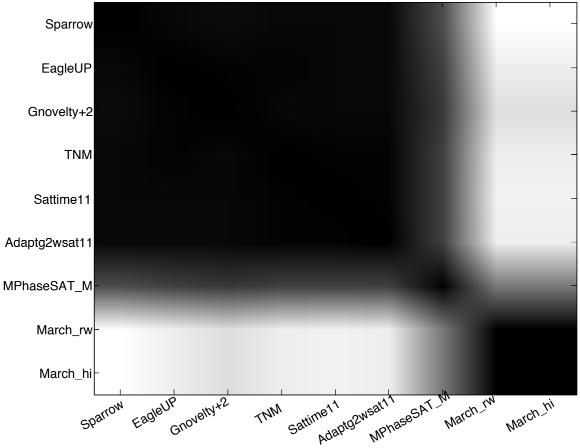
5000 CPU sec cutoff

Correlation of Solver Performance
Application



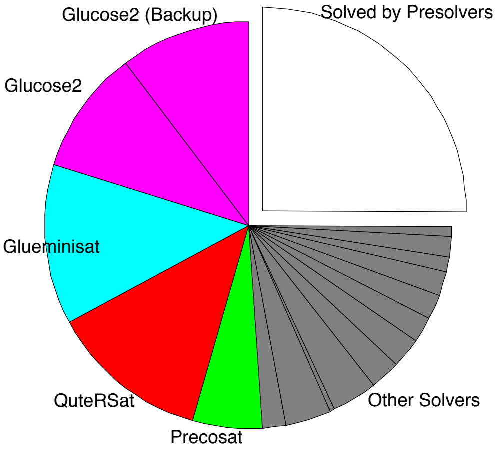
darker = higher Spearman correlation coefficient

Correlation of Solver Performance
Random

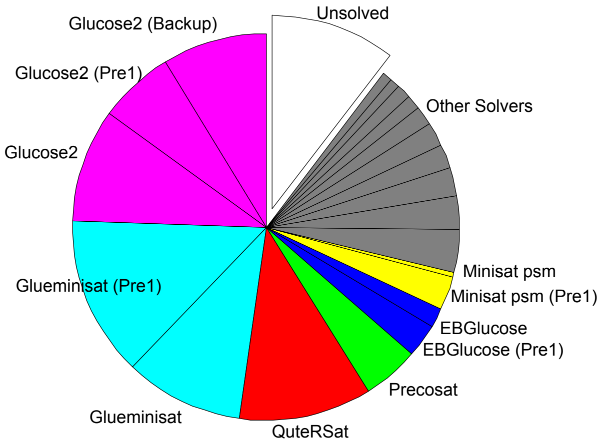


darker = higher Spearman correlation coefficient

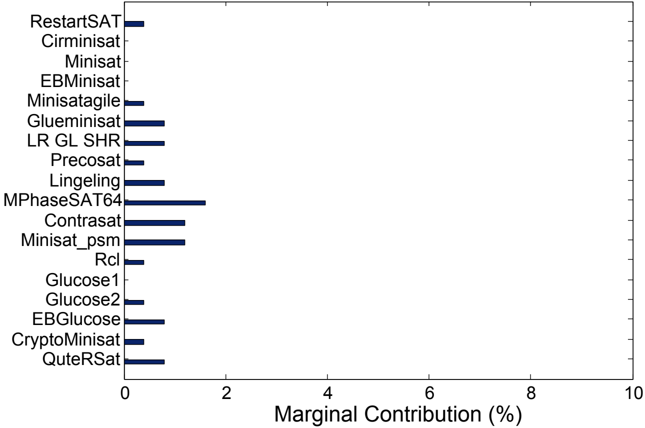
Solver Selection Frequency in SATzilla 2011 Application



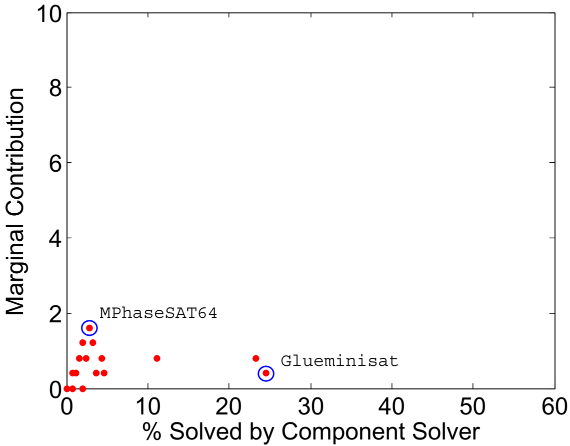
Instances Solved by SATzilla 2011 Components
Application



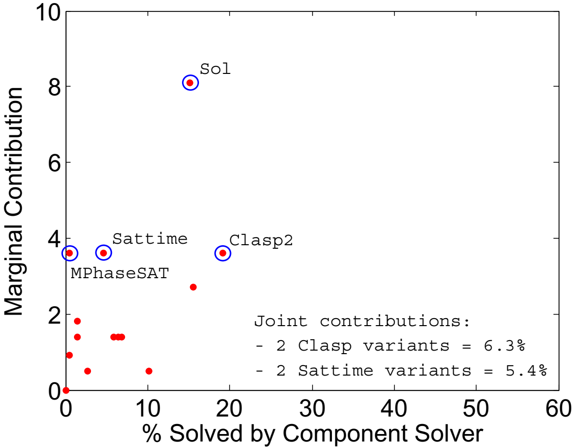
Marginal Contribution of Components
Application



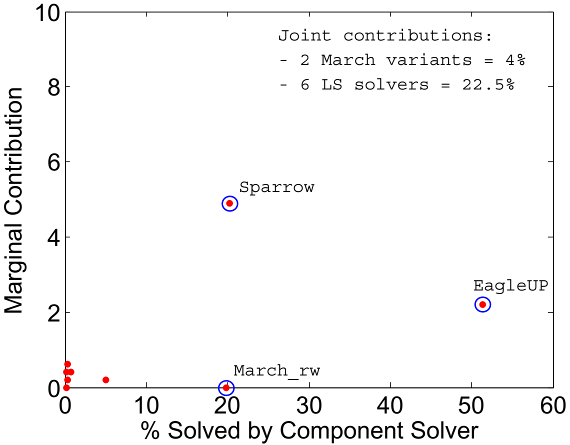
Instances Solved *vs* Marginal Contribution of Components
Application



Instances Solved *vs* Marginal Contribution of Components
Crafted



Instances Solved *vs* Marginal Contribution of Components Random



More nuanced analysis based on Shapley value:

$\rightsquigarrow$ AAAI-16 paper by Fréchette *et al.*

Bias + correction in portfolio performance evaluation:

$\rightsquigarrow$ IJCAI-16 paper by Cameron *et al.*

Leveraging parallelism

- design choices in parallel programs
  (Hamadi, Jabhour, Sais 2009)

- deriving parallel programs from sequential sources
  $\rightsquigarrow$ concurrent execution of optimised designs
  (parallel portfolios)
  (Hoos, Leyton-Brown, Schaub, Schneider 2012)

- parallel design optimisers
  (*e.g.*, Hutter, Hoos, Leyton-Brown 2012)

- use of cloud resources (parallel runs of design optimisers, ...)
  (Geschwender, Hutter, Kotthoff, Malitsky, Hoos, Leyton-Brown 2014)

Take-home Message

Programming by Optimisation ...

- leverages computational power to construct better software
- enables creative thinking about design alternatives
- produces better performing, more flexible software
- facilitates scientific insights into
  - efficacy of algorithms and their components
  - empirical complexity of computational problems

... changes how we build and use high-performance software

More Information:

- www.prog-by-opt.net/Tutorials/IJCAI-17
- www.prog-by-opt.net
- PbO article in Communications of the ACM (Hoos 2012)
- Talk by Kleinberg *et al.*: Tue, 15:15, Room 216
  Talk by Lindauer *et al.*: Fri, 10:50, Room 203
  Invited talk by HH at CP/ICLP/SAT: Tue, 08/29, 9:00
- Forthcoming book (Morgan & Claypool)

If PbO works for you:

- Make our day – let us know!
- Share the joy – tell everyone else!