Algorithm Configuration:

Learning in the Space of Algorithm Designs

Kevin Leyton-Brown

University of British Columbia
Canada CIFAR AI Chair, Amii

Frank Hutter

University of Freiburg and
Bosch Center for Artificial Intelligence

This Tutorial

High-Level Outline

Introduction, Technical Preliminaries, and a Case Study (Kevin)

Practical Methods for Algorithm Configuration (Frank)

Algorithm Configuration Methods with Theoretical Guarantees (Kevin)

Beyond Static Configuration: Related Problems and Emerging Directions (Frank)

Follow along: http://bit.ly/ACTutorial

This Tutorial

Section Outline

Introduction, Technical Preliminaries, and a Case Study (Kevin)

- **Learning in the Space of Algorithm Designs**
- Defining the Algorithm Configuration Problem
- Algorithm Runtime Prediction
- Applications and a Case Study

Follow along: http://bit.ly/ACTutorial

Algorithm Configuration

- **Algorithm configuration** is a powerful technique at the interface of ML and optimization
- It makes it possible to approach algorithm design as a **machine learning problem**
  - stop imagining that we have **good intuitions** about how to approach combinatorial optimization in practice!
  - instead, expose heuristic design choices as parameters, use **automatic methods** to search for good configurations
- Many **research challenges** in the development of methods
- Enormous scope for **applications** to practical problems

We should think about algorithm designs as a hypothesis space

Machine learning

Classical approach

- Features based on **expert insight**
- Model family selected by **hand**
- **Manual** tuning of hyperparameters

We should think about algorithm designs as a hypothesis space

Machine learning

Classical approach

- Features based on expert insight
- Model family selected by hand
- Manual tuning of hyperparameters

Deep learning

- Very **highly parameterized** models, using expert knowledge to identify appropriate invariances and model biases (e.g., convolutional structure)
- "deep": **many layers** of nodes, each depending on the last
- Use **lots of data** (plus e.g. dropout regularization) to avoid overfitting
- **Computationally intensive search** replaces human design

We should think about algorithm designs as a hypothesis space

Machine learning

Classical approach

- Features based on expert insight
- Model family selected by hand
- Manual tuning of hyperparameters

Deep learning

- Very highly parameterized models, using expert knowledge to identify appropriate invariances and model biases (e.g., convolutional structure)
- "deep": many layers of nodes, each depending on the last
- Use lots of data (plus e.g. dropout regularization) to avoid overfitting
- Computationally intensive search replaces human design

Discrete Optimization

Classical approach

- **Expert designs** a heuristic algorithm
- Iteratively conducts **small experiments** to improve the design

We should think about algorithm designs as a hypothesis space

Machine learning

Classical approach

- Features based on expert insight
- Model family selected by hand
- Manual tuning of hyperparameters

Deep learning

- Very highly parameterized models, using expert knowledge to identify appropriate invariances and model biases (e.g., convolutional structure)
- "deep": many layers of nodes, each depending on the last
- Use lots of data (plus e.g. dropout regularization) to avoid overfitting
- Computationally intensive search replaces human design

Discrete Optimization

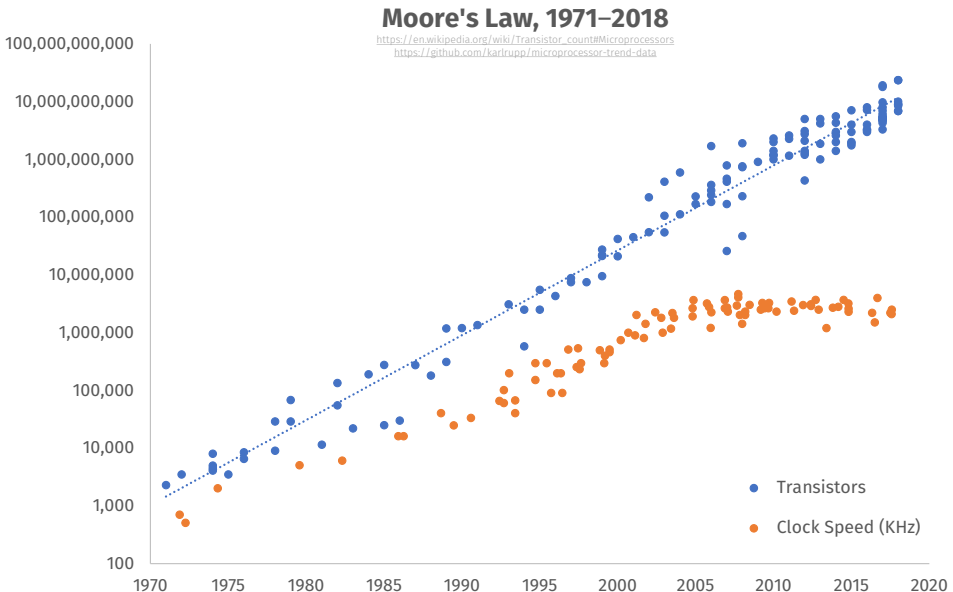
Classical approach

- Expert designs a heuristic algorithm
- Iteratively conducts small experiments to improve the design

Learning in the space of algorithm designs

- Very **highly parameterized** algorithms express a combinatorial space of heuristic design choices that make sense to an expert
- "deep": **many layers** of parameters, each depending on the last
- Use **lots of data** to characterize the distribution of interest
- **Computationally intensive search** replaces human design

Approaches that seemed crazy in 2000 make a lot of sense today...



Algorithm design in a world of learnable algorithms

Designers should:

- Shift from choosing heuristics they think will work to **exposing a wide variety of design elements** that might be sensible
  - This can be integrated into software engineering workflows; see Hoos [2012].
- get out of the business of **manual experimentation**, leaving this to automated procedures
  - this tutorial focuses mainly on **how these automated procedures work**
- **Reoptimize their designs** for new use cases rather than trying to identify a single algorithm to rule them all

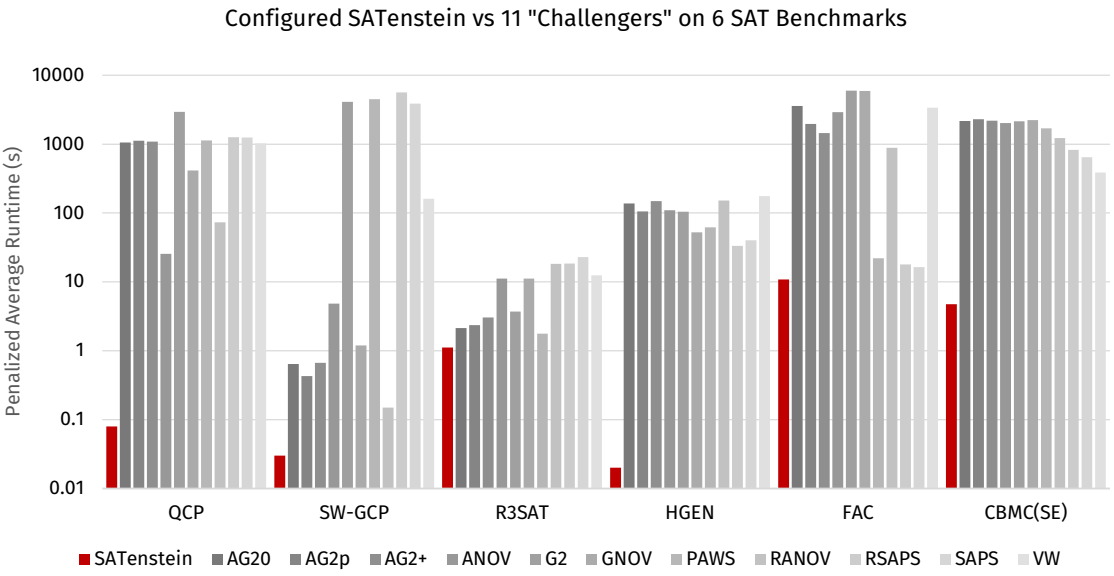
An example of how this can look: SATenstein

[Khudabukhsh, Xu, Hoos, L-B, 2009; 2016]

- **Frankenstein**'s goal:
  - Create "perfect" human being from scavenged body parts
- **SATenstein**'s goal: Create high-performance SAT solvers using components scavenged from existing solvers
  - Components drawn from or inspired by existing local search algorithms for SAT parameters determine which components are selected and how they behave (41 parameters total)
  - designed for use with algorithm configuration (3 levels of conditional params)
- SATenstein can instantiate:
  - at least **29 distinct, high-performance local-search solvers** from the literature
  - trillions of **novel solver strategies**

SATenstein outperformed the existing state of the art on each of six benchmarks

[Khudabukhsh, Xu, Hoos, L-B, 2016]



This Tutorial

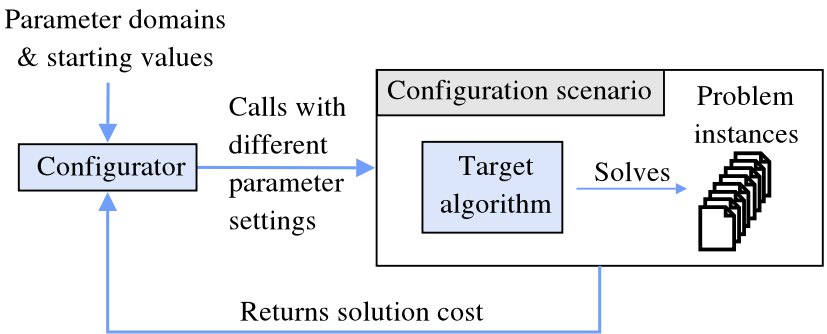
Section Outline

Introduction, Technical Preliminaries, and a Case Study (Kevin)

- Learning in the Space of Algorithm Designs
- **Defining the Algorithm Configuration Problem**
- Algorithm Runtime Prediction
- Applications and a Case Study

Follow along: http://bit.ly/ACTutorial

Algorithm Configuration Visualized



Algorithm Parameters

Parameter Types

- Continuous, integer, ordinal
- **Categorical**: finite domain, unordered, e.g., {apple, tomato, pepper}
- **Conditional**
  - allowed values of some child parameter depend on the values taken by parent parameter(s)

Parameters give rise to a structured space of configurations

- These spaces are often **huge**
  - e.g., SAT solver lingeling has 10^{947} configurations
- Changing one parameter can yield **qualitatively different behaviour**
- Overall, that's why we call it **algorithm configuration** (vs "parameter tuning")

Algorithm Configuration: General Definition

Definition (algorithm configuration)

An algorithm configuration problem is a 5-tuple $(\mathcal{A}, \mathbf{\Theta}, \mathcal{D}, \bar{\kappa}, m)$ 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 Π;
- $\bar{\kappa} < \infty$ is a **cutoff time**, after which each run of $\mathcal{A}$ will be terminated
- $m : \mathbf{\Theta} \times \Pi \to \mathbb{R}$ is a function that measures the cost incurred by $\mathcal{A}(\boldsymbol{\theta})$ on an instance $\pi \in \Pi$

Optimal configuration $\boldsymbol{\theta}^* \in \arg\min_{\boldsymbol{\theta} \in \mathbf{\Theta}} \mathbb{E}_{\pi \sim \mathcal{D}}(m(\boldsymbol{\theta}, \pi))$ minimizes expected cost

Algorithm Configuration: Definition with Runtime Objective

Definition (algorithm configuration)

An algorithm configuration problem is a 5-tuple $(\mathcal{A}, \mathbf{\Theta}, \mathcal{D}, \bar{\kappa}, R_{\bar{\kappa}})$ 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 Π;
- $\bar{\kappa} < \infty$ is a **cutoff time**, after which each run of $\mathcal{A}$ will be terminated
- $R_{\bar{\kappa}} : \mathbf{\Theta} \times \Pi \to \mathbb{R}$ is a function that measures the **time it takes to run $\mathcal{A}(\boldsymbol{\theta})$ with cutoff time $\bar{\kappa}$** on instance $\pi \in \Pi$

Optimal configuration $\boldsymbol{\theta}^* \in \arg\min_{\boldsymbol{\theta} \in \mathbf{\Theta}} \mathbb{E}_{\pi \sim \mathcal{D}}(R_{\bar{\kappa}}(\boldsymbol{\theta}, \pi))$ minimizes expected **runtime**

Beyond Runtime Optimization

Algorithm configuration methods can also be applied to objectives other than runtime optimization (though not the focus of this tutorial).

Black-Box Optimization

Optimize a function to which the algorithm **only has query access**.

Hyperparameter Optimization

Find **hyperparameters of a model** that minimize validation set loss.

This Tutorial

Section Outline

Introduction, Technical Preliminaries, and a Case Study (Kevin)

- Learning in the Space of Algorithm Designs
- Defining the Algorithm Configuration Problem
- **Algorithm Runtime Prediction**
- Applications and a Case Study

Follow along: http://bit.ly/ACTutorial

Algorithm Runtime Prediction

A key enabling technology will be the ability to solve the following problem.

A pretty vanilla application of regression?

Predict **how long an algorithm will take to run**, given:

- A set of instances D
- For each instance $i \in D$, a vector x_i of feature values
- For each instance $i \in D$ a runtime observation y_i We want a mapping $f(x) \rightarrow y$ that accurately predicts y_i given x_i

In other words, find a mapping $f(x) \rightarrow y$ that accurately predicts y_i given x_i.

Algorithm Runtime Prediction

A key enabling technology will be the ability to solve the following problem.

A pretty vanilla application of regression?

Predict **how long an algorithm will take to run**, given:

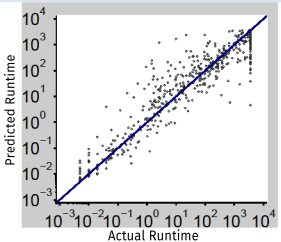
- A set of instances D
- For each instance $i \in D$, a vector x_i of feature values
- For each instance $i \in D$ a runtime observation y_i We want a mapping $f(x) \rightarrow y$ that accurately predicts y_i given x_i

In other words, find a mapping $f(x) \rightarrow y$ that accurately predicts y_i given x_i.

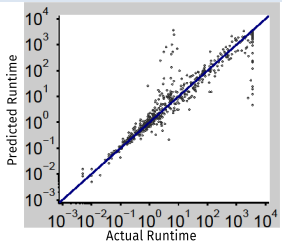
But, **is it really possible** to use supervised learning to predict the empirical behavior of an exponential-time algorithm on held-out problem inputs?

Algorithm Runtime is Surprisingly Predictable

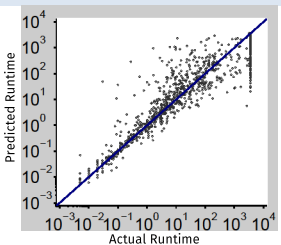
SAT Competition (Random + Handmade + Industrial) data, MINISAT solver
Random Forest (RMSE=0.47)



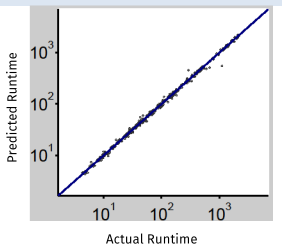
SAT: IBM hardware verification data, SPEAR solver
Random Forest (RMSE=0.38)



MIPLIB data, CPLEX 12.1 solver
Random Forest (RMSE=0.63)



Red Crested Woodpecker habitat data, CPLEX 12.1 solver
Random Forest (RMSE=0.02)



[H, Xu, L-B, Hoos, 2014]

That's Not All, Folks

[H, Xu, L-B, Hoos, 2014]

We've found that that **algorithm runtime is consistently predictable**, across:

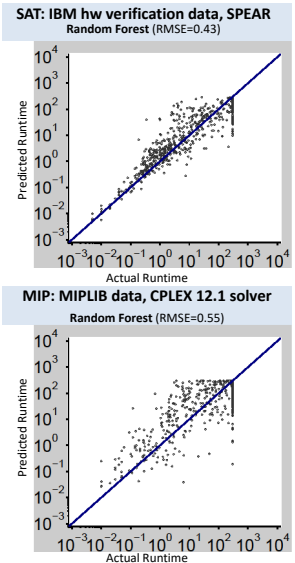
- Four **problem domains**:
  - Satisfiability (SAT)
  - Mixed Integer Programming (MIP)
  - Travelling Salesman Problem (TSP)
  - Combinatorial Auctions
- Dozens of **solvers**, including:
  - state of the art solvers in each domain
  - black-box, commercial solvers
- Dozens of **instance distributions**, including:
  - major benchmarks (SAT competitions; MIPLIB; ...)
  - real-world data (hardware verification, computational sustainability, ...)

What About Modeling Algorithm Parameters, Too?

- So far we've considered the runtime of **single, black box algorithms**
- Our goal in this tutorial is understanding algorithm performance as a function of an **algorithm's parameters**
  - with the ultimate aim of optimizing this function
- Can we predict the performance of **parameterized algorithm families**?

What About Modeling Algorithm Parameters, Too?

- So far we've considered the runtime of **single, black box algorithms**
- Our goal in this tutorial is understanding algorithm performance as a function of an **algorithm's parameters**
  - with the ultimate aim of optimizing this function
- Can we predict the performance of **parameterized algorithm families**?
  - Performance is worse than before, but we're generalizing simultaneously to **unseen problem instances** and **unseen parameter configurations**
    - On average, correct within roughly **half an order of magnitude**
  - Despite discontinuities, an algorithm's performance is well approximated by a **relatively simple function** of its parameters



So, how does it work?

In fact, it's a somewhat trickier regression problem than initially suggested

- mixed continuous/**discrete**
- **high-dimensional**, though often with low effective dimensionality
- **very noisy** response variable (e.g., exponential runtime distribution)

Plus there are some extra features that will be nice to have

- compatibility with **censored observations**
- ability to offer **uncertainty estimates** at test time

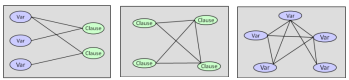
We've tried a lot of different approaches

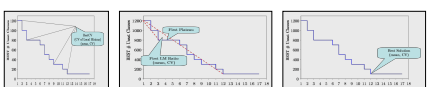
- linear/ridge/lasso/polynomial; SVM; MARS; Gaussian processes; deep nets; ...

...to date, we've had the most success with **random forests of regression trees**

It's most important to get features right. For example, in SAT:

- Problem **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
- Cumulative # of **unit propagations** at different depths
- **Local search probing**
- **Linear programming** relaxation





$$\begin{aligned} \text{maximize:} \quad & \sum_{k \in C} \left(\sum_{i \in L, i \in k} v_i + \sum_{j \in L, i \notin k} (1 - v_j) \right) \\ \text{subject to:} \quad & \sum_{i \in k, i \in L} v_i + \sum_{j \in k, j \in L} (1 - v_j) \geq 1 \qquad \forall k \in C \\ & v_i \in \{0, 1\} \qquad \forall i \end{aligned}$$

This Tutorial

Section Outline

Introduction, Technical Preliminaries, and a Case Study (Kevin)

- Learning in the Space of Algorithm Designs
- Defining the Algorithm Configuration Problem
- Algorithm Runtime Prediction
- **Applications and a Case Study**

Follow along: http://bit.ly/ACTutorial

Algorithm Configuration: Many Applications

FCC spectrum auction

[Auction]omics

IBM ILOG **Mixed integer programming**

Analytics & Optimization

ORTEC OPTIMIZE YOUR WORLD

Social gaming

zynga

Scheduling and Resource Allocation

actenum

Applications by Colleagues

- Exam timetabling
- Motion, person tracking
- RNA sequence-structure alignment
- Protein Folding

Algorithm Competitions

- SAT, MIP, TSP, AI planning, ASP, SMT, timetabling, protein folding, ...

Applications by Others

- Kidney exchange
- Linear algebra subroutines
- Java garbage collection
- Computer GO
- Linear algebra subroutines
- Evolutionary Algorithms
- ML: Classification

A Case Study

[L-B, Milgrom & Segal, 2017; Newman, Fréchette & L-B, 2017]

Over 13 months in 2016–17 the FCC held an "incentive auction" to **repurpose radio spectrum** from broadcast television to wireless internet

In total, the auction yielded **$19.8 billion**

- over $10 billion was paid to 175 broadcasters for **voluntarily relinquishing their licenses** across 14 UHF channels (84 MHz)
- Stations that continued broadcasting were assigned **potentially new channels** to fit as densely as possible into the channels that remained
- The government **netted over $7 billion** (used to pay down the national debt) after covering costs

Feasibility Testing

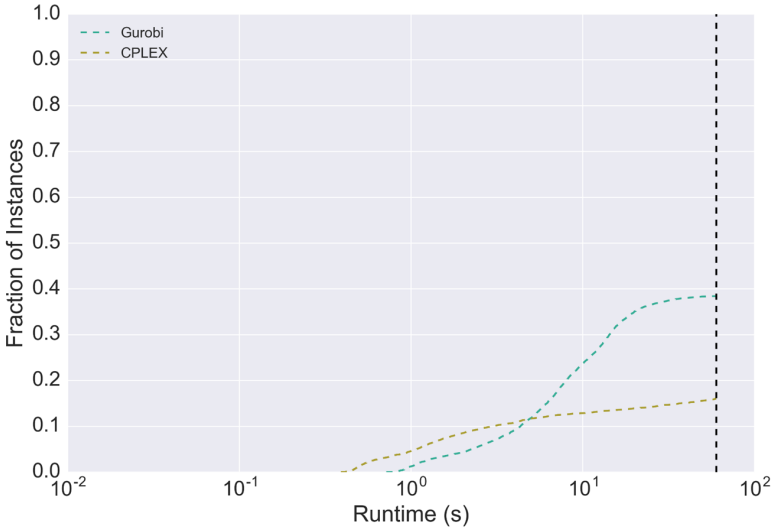
- A key subproblem in the auction:
  - asking "could station x **leave the auction** and go back on-air into the reduced band of spectrum, alongside all other stations X who have already done the same?
  - about 100K such problems arise per auction
  - about 20K are nontrivial

- A hard **graph-colouring problem**
  - 2990 stations (nodes)
  - 2.7 million interference constraints (channel-specific interference)
  - Initial skepticism about whether this problem could be solved exactly at a national scale
- What happens when we can't solve an instance:
  - Needed a minimum of two price decrements per 8h business day
  - each feasibility check was allowed a maximum of one minute
  - Treat **unsolved problems as infeasible**, raising the amount they're paid

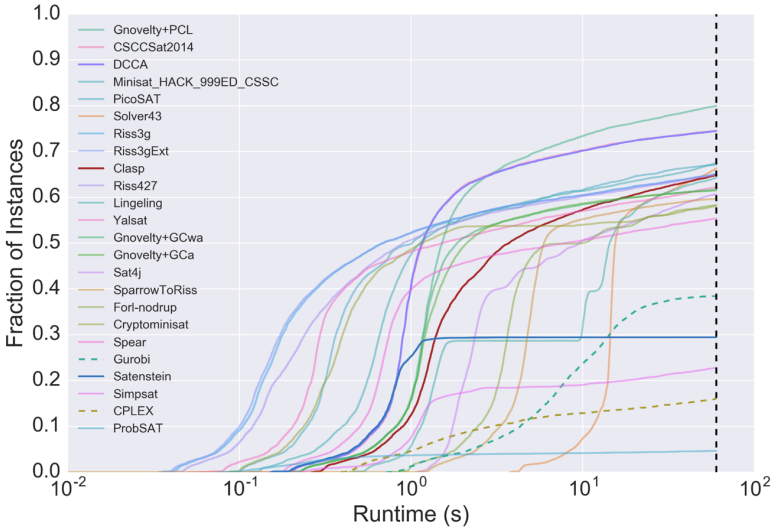
First, We Need Some Data

- We wrote a full **reverse auction simulator** (open source)
- **Generated valuations** by sampling from a model due to Doraszelski et al. [2016]
- Assumptions:
  - 84 MHz clearing target
  - stations participated when their private value for continuing to broadcast was smaller than their opening offer for going off-air
  - 1 min timeout given to SATFC
- 20 simulated auctions $\Rightarrow$ **60,057 instances**
  - 2,711–3,285 instances per auction
  - all not solvable by directly augmenting the previous solution
  - about 3% of the problems encountered in full simulations
- Our goal: solve problems within a **one-minute cutoff**

The Incumbent Solution: MIP Encoding



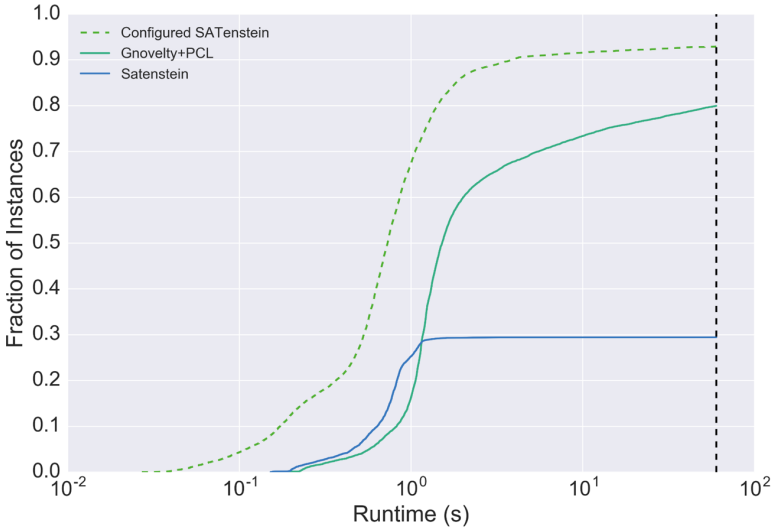
What about trying SAT solvers?



Setting Up an Algorithm Design Hypothesis Space

- Choice of complete or local-search **solver**
  - with which solver parameters
    - and, depending on solver, conditional subparameters?
- Various **problem-specific speedups**
  (each of which furthermore had parameters of its own)
  - reusing previous solutions
  - problem decomposition
  - caching similar solutions
  - removing underconstrained stations
- And further **problem-independent heuristics**
  - constraint propagation preprocessor
  - different SAT encodings

Algorithm Configuration to the Rescue



Algorithm Portfolios

[L-B, Nudelman, Shoham, 2002-2009; Xu, Hutter, Hoos, L-B, 2007-12]

Often **different solvers perform well on different instances**

- Idea: build an **algorithm portfolio**, consisting of different algorithms that can work together to solve a problem
- **SATzilla**: state-of-the-art portfolio developed by my group
  - machine learning to choose algorithm on a per-instance basis
- Or, just run all the algorithms together in parallel

Algorithm Portfolios

[L-B, Nudelman, Shoham, 2002-2009; Xu, Hutter, Hoos, L-B, 2007-12]

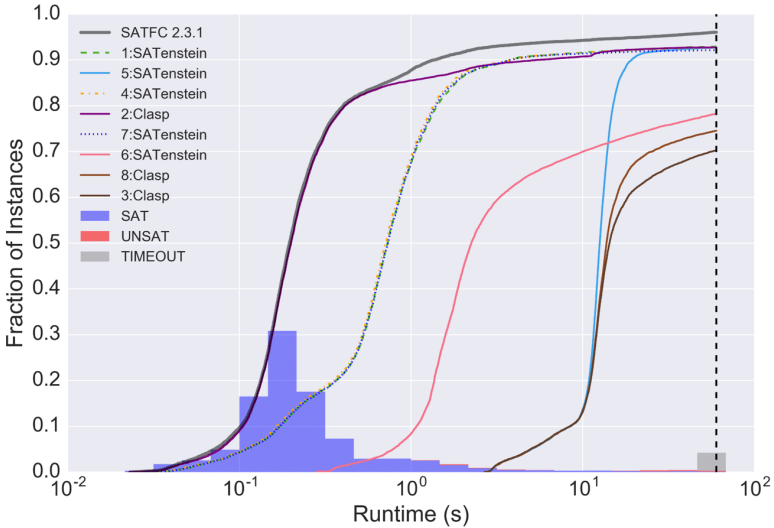
Often **different solvers perform well on different instances**

- Idea: build an **algorithm portfolio**, consisting of different algorithms that can work together to solve a problem
- **SATzilla**: state-of-the-art portfolio developed by my group
  - machine learning to choose algorithm on a per-instance basis
- Or, just run all the algorithms together in parallel

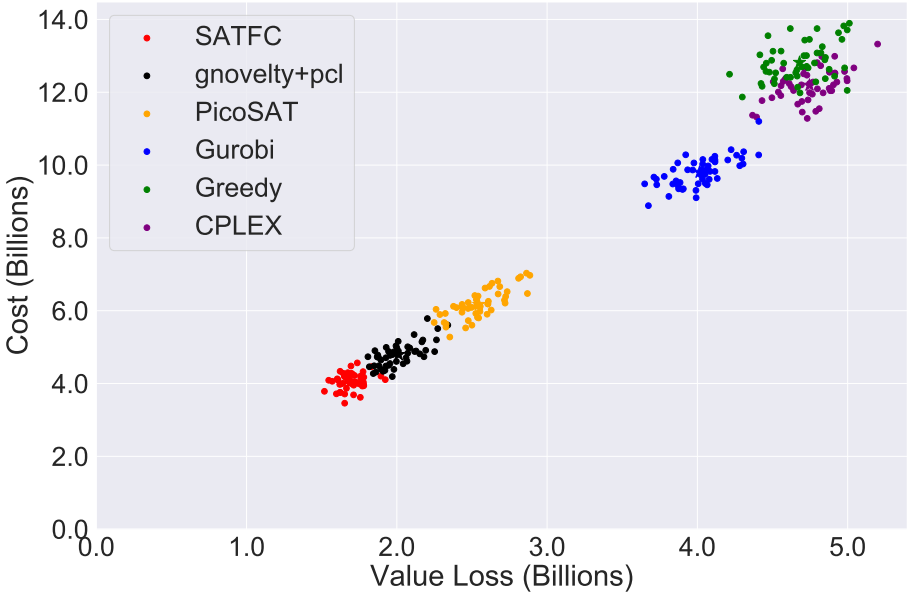
Hydra: use algorithm configuration to **learn a portfolio** of complementary algorithms

- augment an additional portfolio P by targeting instances on which P performs poorly
- Give the algorithm configuration method a dynamic performance metric:
  - performance of alg s when s outperforms P; performance of P

Performance of the Algorithm Portfolio



Economic Impact of a Stronger Solver



This Tutorial

High-Level Outline

Introduction, Technical Preliminaries, and a Case Study (Kevin)

Practical Methods for Algorithm Configuration (Frank)

Algorithm Configuration Methods with Theoretical Guarantees (Kevin)

Beyond Static Configuration: Related Problems and Emerging Directions (Frank)

Follow along: http://bit.ly/ACTutorial

This Tutorial

Section Outline

Practical Methods for Algorithm Configuration (Frank)

- **Sequential Model-Based Algorithm Configuration (SMAC)**
- Details on the Bayesian Optimization in SMAC
- Other Algorithm Configuration Methods
- Case Studies and Evaluation

Follow along: http://bit.ly/ACTutorial

The basic components of algorithm configuration methods

Recall the core of the algorithm configuration definition

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

The two components of algorithm configuration methods

- How to select a new configuration to evaluate?
- How to compare this configuration to the best so far?

Sequential Model-based AC (SMAC): high-level overview

Algorithm 1: SMAC (high-level overview)

Learn a model $\hat{m}$ from performance data so far: $\hat{m} : \mathbf{\Theta} \times \Pi \rightarrow \mathbb{R}$
Use model $\hat{m}$ to select promising configurations $\mathbf{\Theta}_{new}$

Sequential Model-based AC (SMAC): high-level overview

Algorithm 1: SMAC (high-level overview)

Learn a model $\hat{m}$ from performance data so far: $\hat{m} : \mathbf{\Theta} \times \Pi \to \mathbb{R}$
Use model $\hat{m}$ to select promising configurations $\mathbf{\Theta}_{new}$
Compare $\mathbf{\Theta}_{new}$ against best configuration so far by executing new algorithm runs

Sequential Model-based AC (SMAC): high-level overview

Algorithm 1: SMAC (high-level overview)

Initialize by executing some runs and collecting their performance data

repeat

- Learn a model $\hat{m}$ from performance data so far: $\hat{m} : \mathbf{\Theta} \times \Pi \rightarrow \mathbb{R}$
- Use model $\hat{m}$ to select promising configurations $\mathbf{\Theta}_{new}$
- Compare $\mathbf{\Theta}_{new}$ against best configuration so far by executing new algorithm runs

until *time budget exhausted*

Sequential Model-based AC (SMAC): high-level overview

Algorithm 1: SMAC (high-level overview)

Initialize by executing some runs and collecting their performance data

repeat

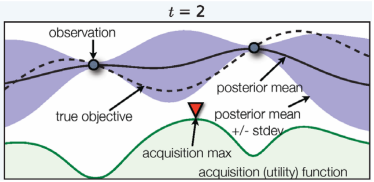
- Learn a model $\hat{m}$ from performance data so far: $\hat{m} : \mathbf{\Theta} \times \Pi \to \mathbb{R}$
- Use model $\hat{m}$ to select promising configurations $\mathbf{\Theta}_{new}$ $\rightsquigarrow$ **Bayesian optimization**
- Compare $\mathbf{\Theta}_{new}$ against best configuration so far by executing new algorithm runs

until *time budget exhausted*

Bayesian Optimization

General approach

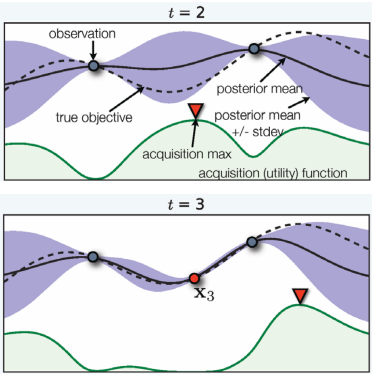
- Fit a probabilistic model to the collected function samples $\langle \boldsymbol{\theta}, f(\boldsymbol{\theta}) \rangle$
- Use the model to guide optimization, trading off exploration *vs* exploitation



Bayesian Optimization

General approach

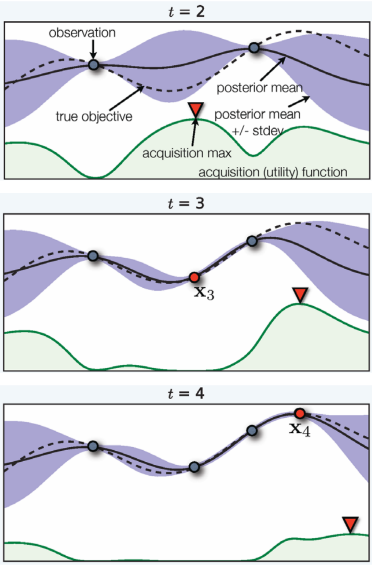
- Fit a probabilistic model to the collected function samples $\langle \boldsymbol{\theta}, f(\boldsymbol{\theta}) \rangle$
- Use the model to guide optimization, trading off exploration *vs* exploitation



Bayesian Optimization

General approach

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



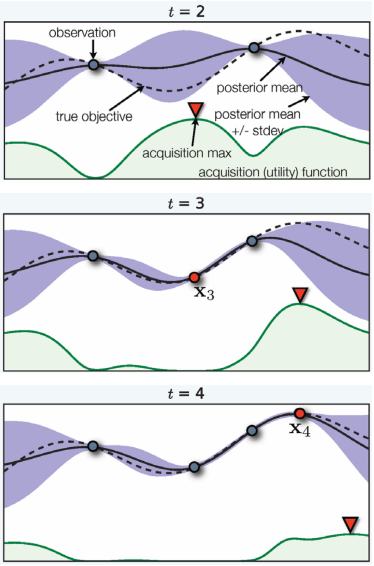
Bayesian Optimization

General approach

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

Popular 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]



Sequential Model-based AC (SMAC): high-level overview

Algorithm 1: SMAC (high-level overview)

Initialize by executing some runs and collecting their performance data

repeat

Learn a model $\hat{m}$ from performance data so far: $\hat{m} : \Theta \times \Pi \to \mathbb{R}$

Use model $\hat{m}$ to select promising configurations Θ_{new}

$\rightsquigarrow$ **Bayesian optimization with random forests**

Compare Θ_{new} against best configuration so far by executing new algorithm runs

$\rightsquigarrow$ **How many instances to evaluate for $\theta \in \Theta_{new}$?**

until *time budget exhausted*

How many instances to evaluate per configuration?

Performance on individual instances often does not generalize

- Instance hardness varies (from milliseconds to hours)
- Aim to minimize cost in expectation over instances: $c(\boldsymbol{\theta}) = \mathbb{E}_{\pi \sim \mathcal{D}}(m(\boldsymbol{\theta}, \pi))$

How many instances to evaluate per configuration?

Performance on individual instances often does not generalize

- Instance hardness varies (from milliseconds to hours)
- Aim to minimize cost in expectation over instances: $c(\boldsymbol{\theta}) = \mathbb{E}_{\pi \sim \mathcal{D}}(m(\boldsymbol{\theta}, \pi))$

Simplest, suboptimal solution: use N instances for each evaluation

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

SMAC's racing approach: focus on configurations that might beat the incumbent

- Race new configurations against the best known **incumbent configuration** $\hat{\theta}$
  - Use same instances (and seeds) as previously used for $\hat{\boldsymbol{\theta}}$
  - Aggressively discard new configuration $\boldsymbol{\theta}$ if it performs worse than $\hat{\boldsymbol{\theta}}$ on shared runs

SMAC's racing approach: focus on configurations that might beat the incumbent

- Race new configurations against the best known **incumbent configuration** $\hat{\theta}$
  - Use same instances (and seeds) as previously used for $\hat{\boldsymbol{\theta}}$
  - Aggressively discard new configuration $\boldsymbol{\theta}$ if it performs worse than $\hat{\boldsymbol{\theta}}$ on shared runs
    - No requirement for statistical domination
      (this would be inefficient since there are exponentially many bad configurations)
    - Search component allows to return to $\boldsymbol{\theta}$ even if it is discarded based on current runs

SMAC's racing approach: focus on configurations that might beat the incumbent

- Race new configurations against the best known **incumbent configuration** $\hat{\theta}$
  - Use same instances (and seeds) as previously used for $\hat{\boldsymbol{\theta}}$
  - Aggressively discard new configuration $\boldsymbol{\theta}$ if it performs worse than $\hat{\boldsymbol{\theta}}$ on shared runs
    - No requirement for statistical domination
      (this would be inefficient since there are exponentially many bad configurations)
    - Search component allows to return to $\boldsymbol{\theta}$ even if it is discarded based on current runs
  - Add more runs for $\hat{\boldsymbol{\theta}}$ over time $\rightsquigarrow$ build up confidence in $\hat{\boldsymbol{\theta}}$

SMAC's racing approach: focus on configurations that might beat the incumbent

- Race new configurations against the best known **incumbent configuration $\hat{\theta}$**
  - Use same instances (and seeds) as previously used for $\hat{\boldsymbol{\theta}}$
  - Aggressively discard new configuration $\boldsymbol{\theta}$ if it performs worse than $\hat{\boldsymbol{\theta}}$ on shared runs
    - No requirement for statistical domination
      (this would be inefficient since there are exponentially many bad configurations)
    - Search component allows to return to $\boldsymbol{\theta}$ even if it is discarded based on current runs
  - Add more runs for $\hat{\boldsymbol{\theta}}$ over time $\rightsquigarrow$ build up confidence in $\hat{\boldsymbol{\theta}}$

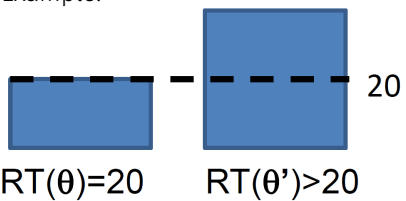
Observation

Let $\boldsymbol{\Theta}$ be finite. Then, the **probability that SMAC finds the true optimal parameter configuration $\theta^* \in \boldsymbol{\Theta}$ approaches 1** as the number of executed runs goes to infinity.

Saving More Time: Adaptive Capping

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

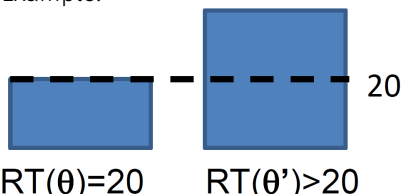
- Is $\boldsymbol{\theta}'$ better than $\boldsymbol{\theta}$?
  - Example:



Saving More Time: Adaptive Capping

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

- Is $\boldsymbol{\theta}'$ better than $\boldsymbol{\theta}$?
  - Example:

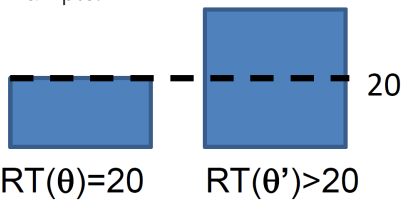


- Can terminate evaluation of $\boldsymbol{\theta}'$ once it is guaranteed to be worse than $\boldsymbol{\theta}$

Saving More Time: Adaptive Capping

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

- Is $\boldsymbol{\theta}'$ better than $\boldsymbol{\theta}$?
  - Example:



- Can terminate evaluation of $\boldsymbol{\theta}'$ once it is guaranteed to be worse than $\boldsymbol{\theta}$

Observation

Let Θ be finite. Then, the **probability that SMAC with adaptive capping finds the true optimal parameter configuration $\theta^* \in \Theta$ approaches 1** the number of executed runs goes to infinity.

Sequential Model-based AC (SMAC): summary

Algorithm 1: SMAC

Initialize by executing some runs and collecting their performance data

repeat

Learn a model $\hat{m}$ from performance data so far: $\hat{m} : \mathbf{\Theta} \times \Pi \to \mathbb{R}$

Use model $\hat{m}$ to select promising configurations $\mathbf{\Theta}_{new}$

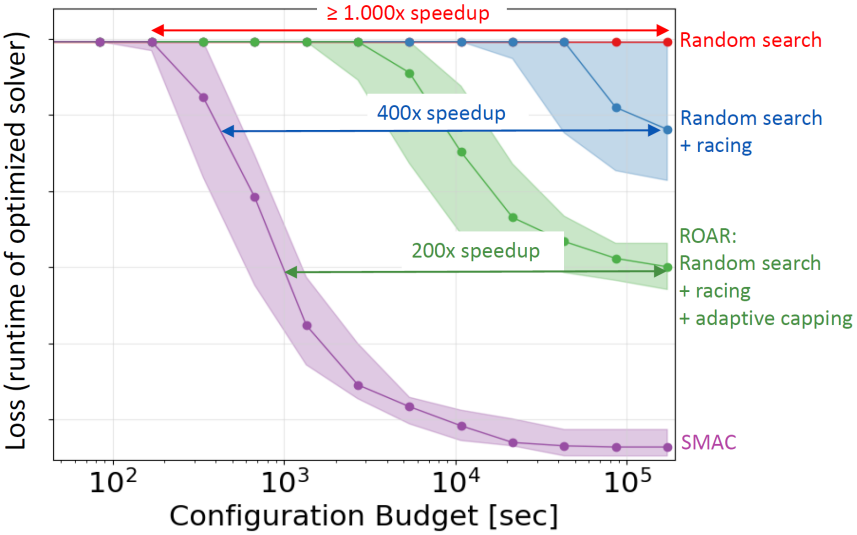
$\rightsquigarrow$ **Bayesian optimization with random forests**

Compare $\mathbf{\Theta}_{new}$ against best configuration so far by executing new algorithm runs

$\rightsquigarrow$ **Aggressive racing and adaptive capping**

until *time budget exhausted*

All of SMAC's components matter for performance



Example: Optimizing CPLEX on combinatorial auctions (Regions 100)

This Tutorial

Section Outline

Practical Methods for Algorithm Configuration (Frank)

- Sequential Model-Based Algorithm Configuration (SMAC)
- **Details on the Bayesian Optimization in SMAC**
- Other Algorithm Configuration Methods
- Case Studies and Evaluation

Follow along: http://bit.ly/ACTutorial

AC poses many non-standard challenges to Bayesian optimization

Complex parameter space

- High dimensionality (low effective dimensionality) [Wang et al, 2013; Garnett et al., 2013]
- Mixed continuous/discrete parameters [H., 2009; H. et al, 2014]
- Conditional parameters [Swersky et al, 2013; H. & Osborne, 2013; Levesque et al., 2017]

AC poses many non-standard challenges to Bayesian optimization

Complex parameter space

- High dimensionality (low effective dimensionality) [Wang et al, 2013; Garnett et al., 2013]
- Mixed continuous/discrete parameters [H., 2009; H. et al, 2014]
- Conditional parameters [Swersky et al, 2013; H. & Osborne, 2013; Levesque et al., 2017]

Non-standard noise

- Non-Gaussian noise [Williams et al, 2000; Shah et al, 2018; Martinez-Cantinet al, 2018]
- Heteroscedastic noise [Le et al, Wang & Neal, 2012]

AC poses many non-standard challenges to Bayesian optimization

Complex parameter space

- High dimensionality (low effective dimensionality) [Wang et al, 2013; Garnett et al., 2013]
- Mixed continuous/discrete parameters [H., 2009; H. et al, 2014]
- Conditional parameters [Swersky et al, 2013; H. & Osborne, 2013; Levesque et al., 2017]

Non-standard noise

- Non-Gaussian noise [Williams et al, 2000; Shah et al, 2018; Martinez-Cantinet al, 2018]
- Heteroscedastic noise [Le et al, Wang & Neal, 2012]

Efficient use in off-the-shelf Bayesian optimization

- Robustness of the model [Malkomes and Garnett, 2018]
- Model overhead [Quiñonero-Candela & Rasmussen, 2005; Bui et al, 2018; H. et al, 2010; Snoek et al, 2015]

AC poses many non-standard challenges to Bayesian optimization

Complex parameter space

- High dimensionality (low effective dimensionality) [Wang et al, 2013; Garnett et al., 2013]
- Mixed continuous/discrete parameters [H., 2009; H. et al, 2014]
- Conditional parameters [Swersky et al, 2013; H. & Osborne, 2013; Levesque et al., 2017]

Non-standard noise

- Non-Gaussian noise [Williams et al, 2000; Shah et al, 2018; Martinez-Cantinet al, 2018]
- Heteroscedastic noise [Le et al, Wang & Neal, 2012]

Efficient use in off-the-shelf Bayesian optimization

- Robustness of the model [Malkomes and Garnett, 2018]
- Model overhead [Quiñonero-Candela & Rasmussen, 2005; Bui et al, 2018; H. et al, 2010; Snoek et al, 2015]

We'll use random forests to address all these; but we need **uncertainty estimates**

Adaptation of regression trees: storing empirical variance in every leaf

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

$\text{param}_3 \in \{\text{red}\}$ | $\text{param}_3 \in \{\text{blue, green}\}$

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

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

$\text{feature}_2 \leq 3.5$ | $\text{feature}_2 > 3.5$

param 1	feature 2	param 3	runtime
false	2	red	3.7

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

$\mu = 18.6$
$\sigma^2 = 4.72$

$\mu = 3.7$
$\sigma^2 = 0$

$\mu = 1.65$
$\sigma^2 \approx 0.20$

Random Forests with Uncertainty Predictions

- Random forest as a **mixture model** of T trees [H. et al., 2014]
- Predict with each of the forest's trees: μ_t and σ_t^2 for tree t
- Predictive distribution: $\mathcal{N}(\mu, \sigma^2)$ with

$$\mu = \frac{1}{T} \sum_{t=1}^{T} \mu_t$$

$$\sigma^2 = \left(\frac{1}{T} \sum_{t=1}^{T} \sigma_t^2 \right) + \frac{1}{T} \left(\sum_{t=1}^{T} \mu_t^2 \right) - \mu^2$$

mean of the variances

variance of the means

Another recent variant for uncertainty in random forests: Mondrian forests

[Lakshminarayanan, Roy & Teh, 2015; Lakshminarayanan, Roy & Teh, 2016]

A key modification of random forests: sampling split points

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

$\text{param}_2 \leq 3.5$ $\text{param}_2 > 3.5$

param 1	param 2	param 3	runtime
false	2	red	3.7

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

- To obtain this split, the split point should be somewhere between **L=2**, **U=5**
- Standard: split at mid-point $\frac{1}{2}(L+U) = 3.5$
- Now instead: **sample split point from Uniform [L,U]**

A key modification of random forests: sampling split points

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

$\text{param}_2 \leq 3.5$ $\quad$ $\text{param}_2 > 3.5$

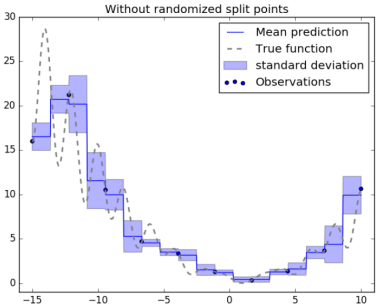
param 1	param 2	param 3	runtime
false	2	red	3.7

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

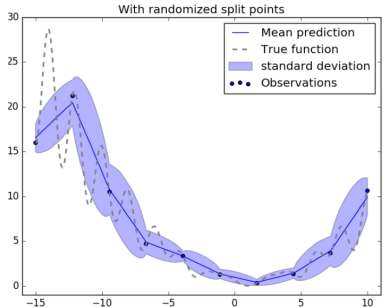
- To obtain this split, the split point should be somewhere between **L=2**, **U=5**
- Standard: split at mid-point $\frac{1}{2}(L+U) = 3.5$
- Now instead: **sample split point from Uniform [L,U]**

Random forests with better uncertainty estimates

- Sampling split points is crucial to obtain smooth uncertainty estimates



Split at mid point 0.5 (L+U)

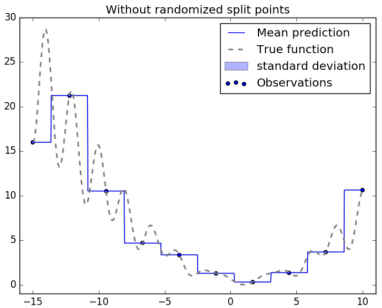


Split at sample from Uniform[L, U]

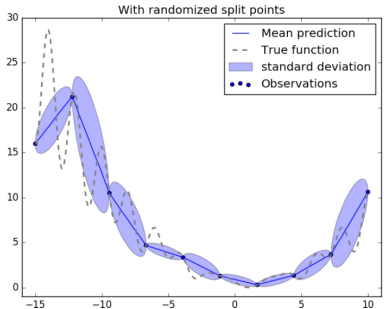
1000 trees, min. number of points per leaf = 1; with bootstrapping

Random forests with better uncertainty estimates

- Sampling split points is crucial to obtain smooth uncertainty estimates



Split at mid point 0.5 (L+U)



Split at sample from Uniform[L, U]

1000 trees, min. number of points per leaf = 1; without bootstrapping

Aggregating Model Predictions Across Multiple Instances

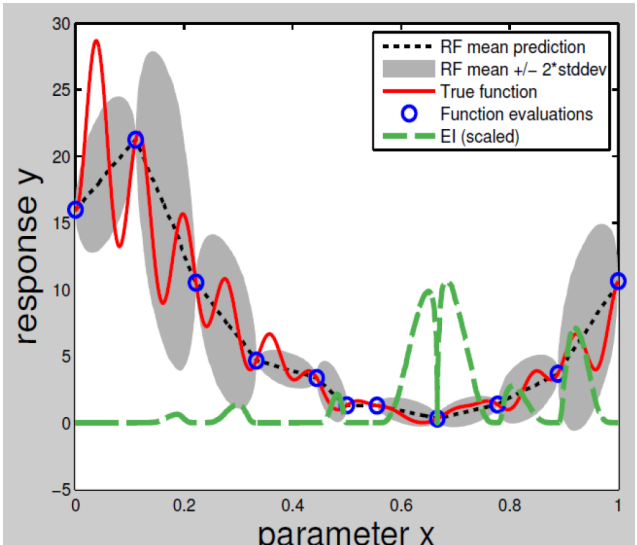
Problem

- Model $\hat{m} : \boldsymbol{\Theta} \times \Pi \rightarrow \mathbb{R}$ predicts for one instance at a time
- We want a model that marginalizes over instances: $\hat{f}(\boldsymbol{\theta}) = \mathbb{E}_{\pi \sim \mathcal{D}}(\hat{m}(\boldsymbol{\theta}, \pi))$

Solution

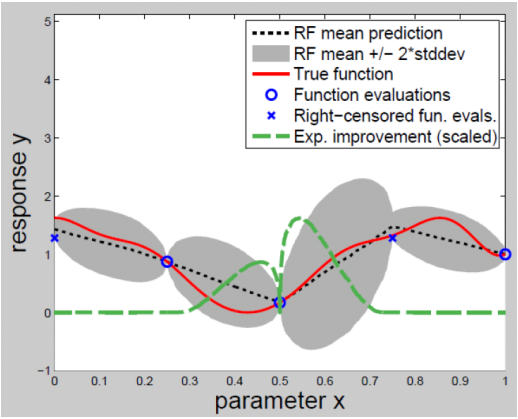
- Intuition: predict for each instance and then average
- More efficient implementation in random forests
  - Keep track of fraction of instances compatible with each leaf
  - Weight the predictions of the leaves accordingly

Bayesian optimization with random forests



Bayesian optimization with censored data

- Terminating poor runs early yields **censored** data points
  - ⇝ we only know a **lower bound** for some data points
- Use an EM-style approach to fill in censored values [Schmee & Hahn, 1979; H. et al, 2013]



Handling of conditional parameters in random forests

- Only split on a parameter if it's guaranteed to be active in the current node
  - Splits higher up in the tree must guarantee parent parameters to have right values

Handling of conditional parameters in random forests

- Only split on a parameter if it's guaranteed to be active in the current node
  - Splits higher up in the tree must guarantee parent parameters to have right values
- Empirically, both GPs and RFs have their advantages [Eggensperger et al, 2013]

Low-dimensional, continuous

Experiment	#evals	SMAC Valid. loss	Spearmint Valid. loss	TPE Valid. loss
branin (0.398)	200	0.655±0.27	**0.398**±0.00	0.526± 0.13
har6 (-3.322)	200	-2.977±0.11	**-3.133**±0.41	-2.823±0.18
Log.Regression	100	8.6±0.9	**7.3**±0.2	8.2±0.6
LDA ongrid	50	**1269.6**±2.9	1272.6±10.3	1271.5±3.5
SVM ongrid	100	**24.1**±0.1	24.6±0.9	24.2±0.0

Handling of conditional parameters in random forests

- Only split on a parameter if it's guaranteed to be active in the current node
  - Splits higher up in the tree must guarantee parent parameters to have right values
- Empirically, both GPs and RFs have their advantages [Eggensperger et al, 2013]

Low-dimensional, continuous

Experiment	#evals	SMAC Valid. loss	Spearmint Valid. loss	TPE Valid. loss
branin (0.398)	200	0.655±0.27	**0.398**±0.00	0.526± 0.13
har6 (-3.322)	200	-2.977±0.11	**-3.133**±0.41	-2.823±0.18
Log.Regression	100	8.6±0.9	**7.3**±0.2	8.2±0.6
LDA ongrid	50	**1269.6**±2.9	1272.6±10.3	1271.5±3.5
SVM ongrid	100	**24.1**±0.1	24.6±0.9	24.2±0.0
HP-NNET convex	200	**18.3**±1.9	20.0±0.9	18.5±1.4
HP-NNET MRBI	200	**48.3**±1.80	51.4±3.2	48.9±1.4
HP-DBNET convex	200	**15.4**±0.8	17.45±5.6	16.1±0.5
Auto-WEKA	30h	**27.5**±4.9	40.64±7.2	35.5±2.9

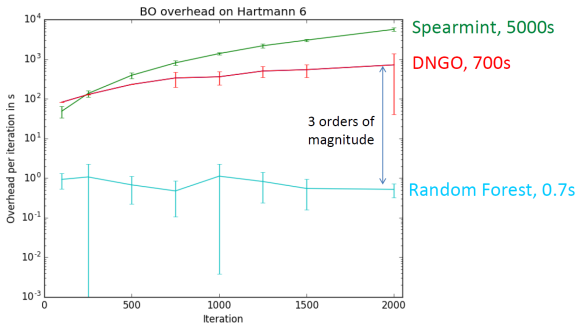
High-dimensional, conditional

Computational efficiency of random forests and standard Gaussian processes

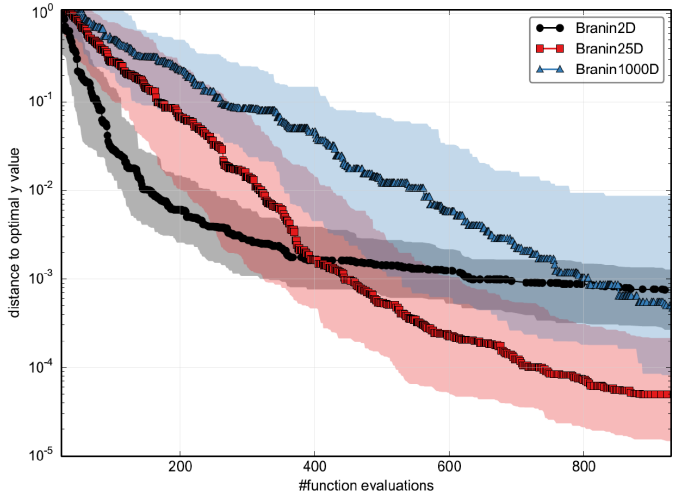
Computational complexity for N data points (and T trees in a forest)

	Random forests	Standard GPs
Training	$O(TN \log^2 N)$	$O(N^3)$
Prediction	$O(T \log N)$	$O(N^2)$

Empirical scaling of runtime with the number of data points:



Scaling with high dimensions (low effective dimensionality)



2 important dimensions (Branin test function)

+ additional unimportant dimensions, following Wang et al [2013]

This Tutorial

Section Outline

Practical Methods for Algorithm Configuration (Frank)

- Sequential Model-Based Algorithm Configuration (SMAC)
- Details on the Bayesian Optimization in SMAC
- **Other Algorithm Configuration Methods**
- Case Studies and Evaluation

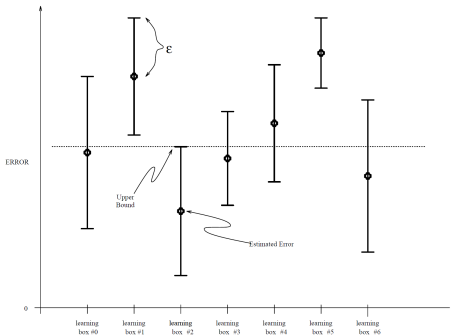
Follow along: http://bit.ly/ACTutorial

There are many continuous blackbox optimization methods

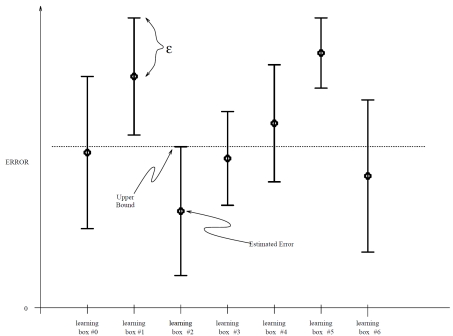
- Evolutionary strategies, e.g., CMA-ES [Hansen & Ostermeier, 2001; Hansen, 2016]
  - Strong results for **continuous hyperparameter optimization** [Friedrichs & Igel, 2004], especially with parallel resources [Loshchilov & H., 2016]
  - Also strong results for **optimizing NN parameters**, especially when only approximate gradients are available (RL) [Salimans et al, 2017; Conti et al, 2018, Chrabaszcz et al, 2018]
- Differential evolution [Storn and Price, 1997]
- Particle swarm optimization [Kennedy & Eberhart, 1995]

$\rightsquigarrow$ For continuous parameter spaces, these could be used instead of Bayesian optimization

There are many approaches for model selection



There are many approaches for model selection



- E.g., Hoeffding races [Maron & Moore, 1993]
- To compare a set of configurations (or algorithms):
  - Use Hoeffding's bound to compute a confidence band for each configuration
  - Stop evaluating configuration when its lower bound is above another's upper bound

F-race and Iterated F-race

F-race [Birattari et al, 2002]

- Similar idea as Hoeffding races
- But uses a statistical test instead to check whether $\boldsymbol{\theta}$ is inferior
  - Namely, the F-test, followed by pairwise t-tests

Iterated F-Race [López-Ibáñez et al, 2016]

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

$\rightsquigarrow$ Focus on solution quality optimization

The ParamILS Framework

Iterated local search in parameter configuration space [H. et al, 2007; H. et al, 2009]

Animation credit: Holger Hoos

The ParamILS Framework

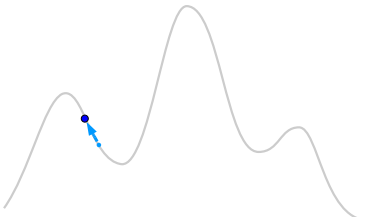
Iterated local search in parameter configuration space [H. et al, 2007; H. et al, 2009]

Initialisation

Animation credit: Holger Hoos

The ParamILS Framework

Iterated local search in parameter configuration space [H. et al, 2007; H. et al, 2009]

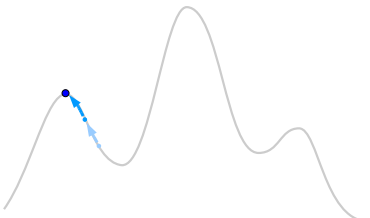


Local Search

Animation credit: Holger Hoos

The ParamILS Framework

Iterated local search in parameter configuration space [H. et al, 2007; H. et al, 2009]

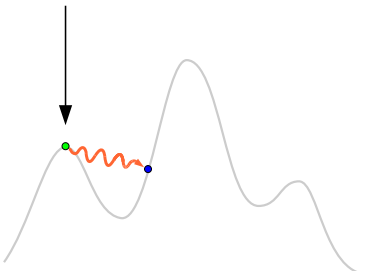


Local Search

Animation credit: Holger Hoos

The ParamILS Framework

Iterated local search in parameter configuration space [H. et al, 2007; H. et al, 2009]

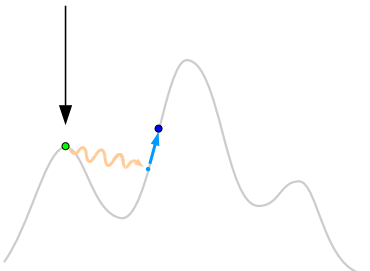


Perturbation

Animation credit: Holger Hoos

The ParamILS Framework

Iterated local search in parameter configuration space [H. et al, 2007; H. et al, 2009]

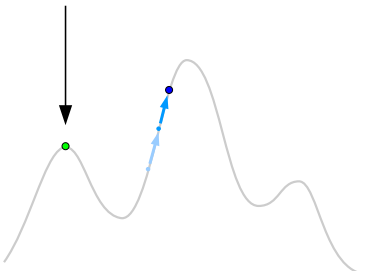


Local Search

Animation credit: Holger Hoos

The ParamILS Framework

Iterated local search in parameter configuration space [H. et al, 2007; H. et al, 2009]

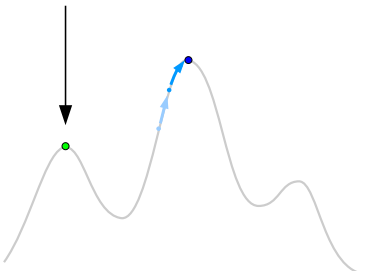


Local Search

Animation credit: Holger Hoos

The ParamILS Framework

Iterated local search in parameter configuration space [H. et al, 2007; H. et al, 2009]

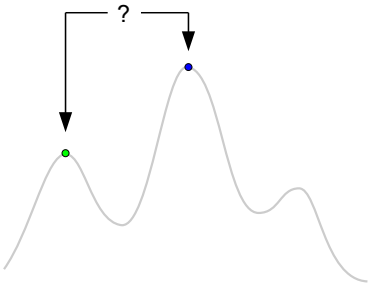


Local Search

Animation credit: Holger Hoos

The ParamILS Framework

Iterated local search in parameter configuration space [H. et al, 2007; H. et al, 2009]

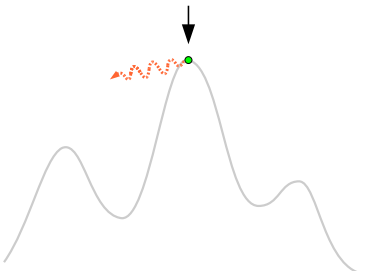


Selection (using Acceptance Criterion)

Animation credit: Holger Hoos

The ParamILS Framework

Iterated local search in parameter configuration space [H. et al, 2007; H. et al, 2009]

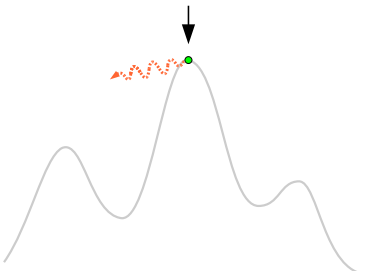


Perturbation

Animation credit: Holger Hoos

The ParamILS Framework

Iterated local search in parameter configuration space [H. et al, 2007; H. et al, 2009]



Perturbation

Animation credit: Holger Hoos

ParamILS predates SMAC; **aggressive racing & adaptive capping originate here**

Gender-based Genetic Algorithm (GGA) [Ansotegui et al, 2009]

Genetic algorithm:

- Population of individuals as genomes (i.e., solution candidates)
- Modify population by
  - Mutations (i.e., random changes)
  - Crossover (i.e., combination of 2 parents to form an offspring)

Gender-based Genetic Algorithm (GGA) [Ansotegui et al, 2009]

Genetic algorithm:

- Population of individuals as genomes (i.e., solution candidates)
- Modify population by
  - Mutations (i.e., random changes)
  - Crossover (i.e., combination of 2 parents to form an offspring)

Genetic algorithm for algorithm configuration

- **Genome = parameter configuration**
- Crossover: Combine 2 configurations to form a new configuration

Gender-based Genetic Algorithm (GGA) [Ansotegui et al, 2009]

Genetic algorithm:

- Population of individuals as genomes (i.e., solution candidates)
- Modify population by
  - Mutations (i.e., random changes)
  - Crossover (i.e., combination of 2 parents to form an offspring)

Genetic algorithm for algorithm configuration

- **Genome = parameter configuration**
- Crossover: Combine 2 configurations to form a new configuration

Two genders in the population (competitive and non-competitive)

- Selection pressure only on one gender
- Preserves diversity of the population

GGA: Racing and Capping

Can exploit parallel resources

- **Evaluate population members in parallel**
- Adaptive capping: can stop when the first k succeed

GGA: Racing and Capping

Can exploit parallel resources

- **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}

This Tutorial

Section Outline

Practical Methods for Algorithm Configuration (Frank)

- Sequential Model-Based Algorithm Configuration (SMAC)
- Details on the Bayesian Optimization in SMAC
- Other Algorithm Configuration Methods
- **Case Studies and Evaluation**

Follow along: http://bit.ly/ACTutorial

Configuration of a SAT Solver for Verification [H. et al, FMCAD 2007]

SAT-encoded instances from formal verification

- Software verification [Babić & Hu; CAV '07]
- IBM bounded model checking [Zarpas; SAT '05]

State-of-the-art tree search solver for SAT-based verification

- Spear, developed by Domagoj Babić at UBC
- 26 parameters, 8.34×10^{17} configurations

Configuration of a SAT Solver for Verification [H. et al, FMCAD 2007]

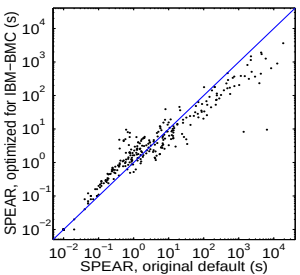
- Ran ParamILS, 2 days $\times$ 10 machines
  - On a training set from each of hardware and software verification

Configuration of a SAT Solver for Verification [H. et al, FMCAD 2007]

- Ran ParamILS, 2 days $\times$ 10 machines
  - On a training set from each of hardware and software verification
- Compared to manually-engineered default
  - 1 week of performance tuning
  - Competitive with the state of the art
  - Comparison on unseen test instances

Configuration of a SAT Solver for Verification [H. et al, FMCAD 2007]

- Ran ParamILS, 2 days $\times$ 10 machines
  - On a training set from each of hardware and software verification
- Compared to manually-engineered default
  - 1 week of performance tuning
  - Competitive with the state of the art
  - Comparison on unseen test instances

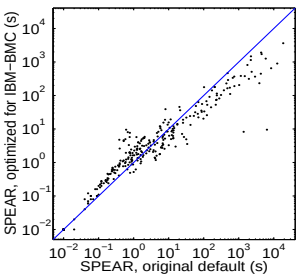


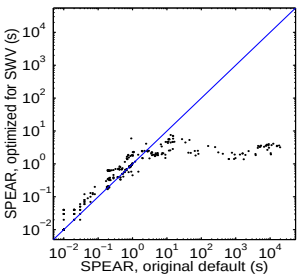
IBM Hardware verification:

4.5-fold speedup on average

Configuration of a SAT Solver for Verification [H. et al, FMCAD 2007]

- Ran ParamILS, 2 days $\times$ 10 machines
  - On a training set from each of hardware and software verification
- Compared to manually-engineered default
  - 1 week of performance tuning
  - Competitive with the state of the art
  - Comparison on unseen test instances





IBM Hardware verification:

4.5-fold speedup on average

Software verification: **500-fold speedup**

$\rightsquigarrow$ won QF_BV category in **2007 SMT competition**

Configuration of a Commercial MIP Solver [H. et al, CPAIOR 2010]

Mixed integer programming (MIP)

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

Combines efficiency of solving linear programs with representational power of integer variables

Configuration of a Commercial MIP Solver [H. et al, CPAIOR 2010]

Mixed integer programming (MIP)

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

Combines efficiency of solving linear programs with representational power of integer variables

Commercial MIP Solver CPLEX

- Leading solver for 15 years (at the time)
- Licensed by over 1000 universities and 1300 corporations
- 76 parameters, 10^{47} configurations

Configuration of a Commercial MIP Solver [H. et al, CPAIOR 2010]

Mixed integer programming (MIP)

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

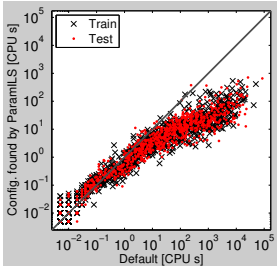
Combines efficiency of solving linear programs with representational power of integer variables

Commercial MIP Solver CPLEX

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

Improvements by configuration with ParamILS

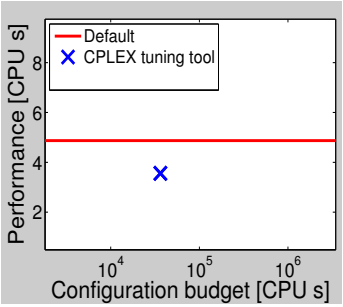
- Between 2× and 50× speedups to solve optimally
- Later work with CPLEX team: up to **10 000× speedups**
- Reduction of optimality gap: 1.3× to 8.6 ×



Wildlife corridor instances

Comparison to CPLEX Tuning Tool [H. et al, CPAIOR 2010]

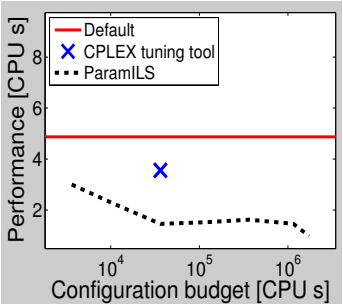
- CPLEX tuning tool
  - Introduced in version 11 (late 2007, after *ParamILS*)
  - Evaluates predefined good configurations, returns best one
  - Required runtime varies (from $< 1h$ to weeks)



CPLEX on MIK instances

Comparison to CPLEX Tuning Tool [H. et al, CPAIOR 2010]

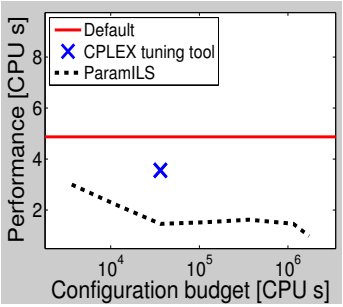
- CPLEX tuning tool
  - Introduced in version 11 (late 2007, after *ParamILS*)
  - Evaluates predefined good configurations, returns best one
  - Required runtime varies (from $< 1h$ to weeks)
- *ParamILS*: anytime algorithm
  - At each time step, keeps track of its incumbent



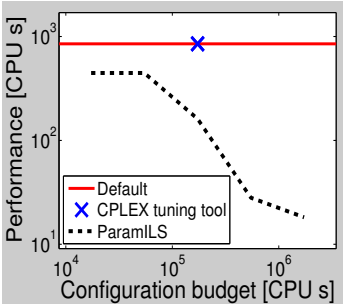
CPLEX on MIK instances

Comparison to CPLEX Tuning Tool [H. et al, 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



CPLEX on MIK instances



CPLEX on SUST instances

Note: lower is better

SMAC further improved performance for both of these case studies

AC scenario	GGA	ParamILS	SMAC
CPLEX on CLS	5.36	2.12	**1.77**
CPLEX on CORLAT	20.47	9.57	**5.38**
CPLEX on RCW2	63.65	54.09	**49.69**
CPLEX on Regions200	7.09	**3.04**	**3.09**
SPEAR on IBM	– –	801.32	**775.15**
SPEAR on SWV	– –	1.26	**0.87**

Configurable SAT Solver Competition (CSSC) [H. et al, AIJ 2015]

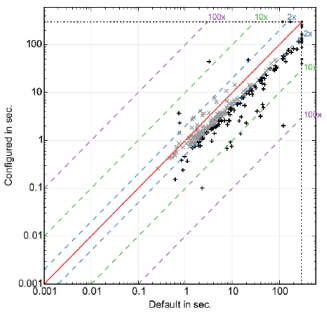
Annual SAT competition

- Scores SAT solvers by their performance across instances
- Medals for best average performance with solver defaults
- Implicitly highlights solvers with good defaults

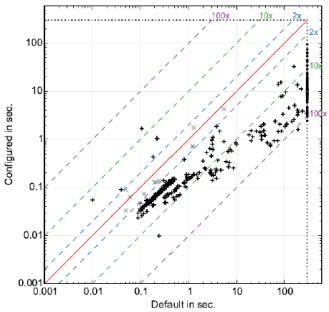
Configurable SAT Solver Challenge (CSSC)

- Better reflects an application setting: homogeneous instances
- Can automatically optimize parameters
- Medals for best **performance after configuration**
  - Based on configuration by all of SMAC, ParamILS and GGA

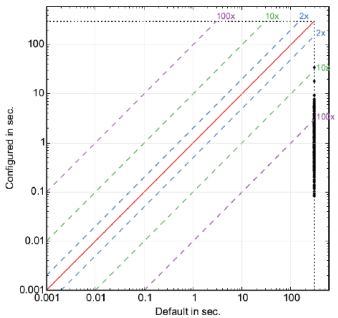
CSSC result #1: Solver performance often improved a lot



Lingeling on CircuitFuzz:
Timeouts: 119 → 107



Clasp on n-queens:
Timeouts: 211 → 102



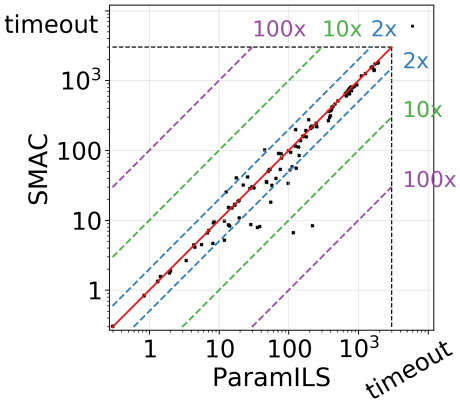
probSAT on unif rnd 5-SAT:
Timeouts: 250 → 0

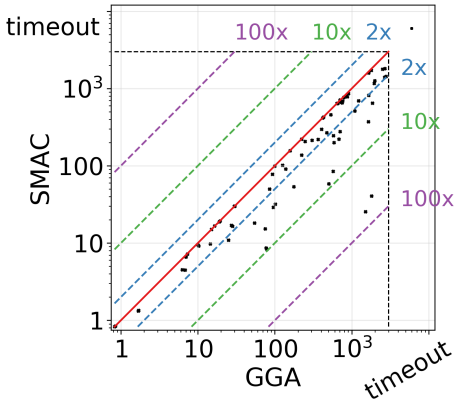
CSSC result #2: Automated configuration changed algorithm rankings

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

CSSC result #3: SMAC yielded larger speedups than ParamILS and GGA





Each dot: performance achieved by the two configurators being compared for one solver on one benchmark distribution

This Tutorial

High-Level Outline

Introduction, Technical Preliminaries, and a Case Study (Kevin)

Practical Methods for Algorithm Configuration (Frank)

Algorithm Configuration Methods with Theoretical Guarantees (Kevin)

Beyond Static Configuration: Related Problems and Emerging Directions (Frank)

Follow along: http://bit.ly/ACTutorial

Algorithm Configuration

- It's trivial to achieve **optimality in the limit**
  - what makes an algorithm configurator good is finding good configurations quickly
- So far our focus, like most of the literature, has been on empirical performance
- Let's now consider obtaining **meaningful theoretical guarantees about worst-case running time**
  - This section follows Kleinberg, L-B & Lucier [2017]
    - but uses notation consistent with the rest of this tutorial

This Tutorial

Section Outline

Algorithm Configuration Methods with Theoretical Guarantees (Kevin)

Technical Setup

Structured Procrastination (the case of few configurations)

Extensions to Structured Procrastination (many configurations and more)

LeapsAndBounds

CapsAndRuns

Structured Procrastination with Confidence

Related Work and Further Reading

Follow along: http://bit.ly/ACTutorial

Problem Definition Redux

(Notation you'll need for this section, slide 1/2)

An **algorithm configuration problem** is defined by $(\mathcal{A}, \mathbf{\Theta}, \mathcal{D}, \bar{\kappa}, R)$:

- $\mathcal{A}$ is a parameterized **algorithm**
- $\mathbf{\Theta}$ is the parameter **configuration space** of $\mathcal{A}$
  - We use θ to identify particular configurations
- $\mathcal{D}$ is a **probability distribution over input instances** with domain Π; typically the uniform distribution over a benchmark set
  - We use π to identify (input instance, random seed) pairs, which we call *instances*
- $\bar{\kappa} < \infty$ is a **max cutoff time**, after which each run of $\mathcal{A}$ will be terminated
- $R_\kappa(\theta, \pi)$ is the **runtime** of configuration $\theta \in \mathbf{\Theta}$ on instance π, with cutoff time κ
  - $R_\kappa(\theta) = \mathbb{E}_{\pi \sim \mathcal{D}}[R_\kappa(\theta, \pi)]$ denotes **expected κ-capped running time** of θ
  - $R(\theta) = R_{\bar{\kappa}}(\theta)$ denotes **expected running time** of θ
- $\kappa_0 > 0$ is the **minimum runtime**: $R(\theta, \pi) \geq \kappa_0$ for all θ and π

Approximately Optimal Configurations

(Notation you'll need for this section, slide 2/2)

Let **OPT** $= \min_\theta\{R(\theta)\}$.

Definition (ϵ-Optimality)

Given $\epsilon > 0$, find $\theta^* \in \mathbf{\Theta}$ such that $R(\theta^*) \leq (1+\epsilon)\text{OPT}$.

- If θ's average running time is driven by **a small set of exceedingly bad inputs that occur very rarely**, then we'd need to run θ on *many* inputs
- Implies worst-case bounds scaling **linearly with** $\bar{\kappa}$ even when OPT $\ll \bar{\kappa}$

Approximately Optimal Configurations

(Notation you'll need for this section, slide 2/2)

Let **OPT** $= \min_\theta\{R(\theta)\}$.

Definition (ϵ-Optimality)

Given $\epsilon > 0$, find $\theta^* \in \mathbf{\Theta}$ such that $R(\theta^*) \leq (1+\epsilon)$OPT.

- If θ's average running time is driven by **a small set of exceedingly bad inputs that occur very rarely**, then we'd need to run θ on *many* inputs
- Implies worst-case bounds scaling **linearly with** $\bar{\kappa}$ even when OPT $\ll \bar{\kappa}$

We **relax our objective** by allowing the running time of θ^* to be *capped* at some threshold value κ for a δ fraction of (instance, seed) pairs

Definition ((ϵ, δ)-Optimality)

A configuration θ^* is (ϵ, δ)-*optimal* if there exists some threshold κ for which $R_\kappa(\theta^*) \leq (1+\epsilon)$**OPT** and $\Pr_{\pi\sim\mathcal{D}}\left(R(\theta^*, \pi) > \kappa\right) \leq \delta$.

Existing Approaches

Definition (incumbent-driven)

An algorithm configuration procedure is **incumbent-driven** if, whenever an algorithm run is performed, the captime is either $\bar{\kappa}$ or (an amount proportional to) the runtime of a previously performed algorithm run.

Existing algorithm configuration procedures are incumbent driven:

F-race [Birattari *et al.*, 2002], ParamILS [Hutter *et al.*, 2007; 2009], GGA [Ansótegui *et al.*, 2009; 2015], irace [López-Ibáñez *et al.*, 2016], ROAR and SMAC [Hutter *et al.*, 2011]

Theorem (running time lower bound)

*Any (ϵ, δ)-optimal incumbent-driven search procedure has worst-case expected runtime that scales at least **linearly with** $\bar{\kappa}$.*

This Tutorial

Section Outline

Algorithm Configuration Methods with Theoretical Guarantees (Kevin)

- Technical Setup
- **Structured Procrastination** (the case of few configurations)
- Extensions to Structured Procrastination (many configurations and more)
- LeapsAndBounds
- CapsAndRuns
- Structured Procrastination with Confidence
- Related Work and Further Reading

Follow along: http://bit.ly/ACTutorial

Structured Procrastination

- A time management scheme due to Stanford philosopher John Perry
  [Perry, 1996; 2011 Ig Nobel Prize in Literature]
  - Keep a set of **daunting tasks that you procrastinate to avoid**, thereby accomplishing other tasks
  - Eventually, replace each daunting task with **a new task that is even more daunting**, and so complete the first task

Structured Procrastination

- A time management scheme due to Stanford philosopher John Perry
  [Perry, 1996; 2011 Ig Nobel Prize in Literature]
  - Keep a set of **daunting tasks that you procrastinate to avoid**, thereby accomplishing other tasks
  - Eventually, replace each daunting task with **a new task that is even more daunting**, and so complete the first task
- Similarly, the Structured Procrastination algorithm configuration procedure [Kleinberg, Lucier & L-B, 2017]:
  - maintains **sets of tasks** *(for each configuration θ, a queue of runs to perform)*;
  - starts with the **easiest tasks** *(shortest captimes)*;
  - **procrastinates** when these tasks prove daunting *(puts them back on the queue)*.

Structured Procrastination

- A time management scheme due to Stanford philosopher John Perry
  [Perry, 1996; 2011 Ig Nobel Prize in Literature]
  - Keep a set of **daunting tasks that you procrastinate to avoid**, thereby accomplishing other tasks
  - Eventually, replace each daunting task with **a new task that is even more daunting**, and so complete the first task
- Similarly, the Structured Procrastination algorithm configuration procedure
  [Kleinberg, Lucier & L-B, 2017]:
  - maintains **sets of tasks** *(for each configuration θ, a queue of runs to perform)*;
  - starts with the **easiest tasks** *(shortest captimes)*;
  - **procrastinates** when these tasks prove daunting *(puts them back on the queue)*.

Key insight

Only spend a long time running a given configuration on a given instance after having failed to find any other (configuration, instance) pair that could be evaluated more quickly.

Structured Procrastination

For now we consider the case of **few configurations**; let $|\mathbf{\Theta}| = n$

Structured Procrastination

For now we consider the case of **few configurations**; let $|\mathbf{\Theta}| = n$

1. Initialize a **bounded-length queue** Q_θ of (instance, captime) pairs for each configuration θ
   - instances randomly sampled from $\mathcal{D}$ with randomly sampled seeds
   - initial captimes of κ_0
2. Calculate **approximate expected runtime** for each θ
   - zero for configurations on which no runs have yet been performed
   - else average runtimes, treating capped runs as though they finished

Structured Procrastination

For now we consider the case of **few configurations**; let $|\mathbf{\Theta}| = n$

1. Initialize a **bounded-length queue** Q_θ of (instance, captime) pairs for each configuration θ
2. Calculate **approximate expected runtime** for each θ
   - zero for configurations on which no runs have yet been performed
   - else average runtimes, treating capped runs as though they finished
3. Choose the task **optimistically predicted to be easiest**: the (instance, captime) pair at the head of the queue corresponding to the θ with smallest approximate expected runtime

Structured Procrastination

For now we consider the case of **few configurations**; let $|\mathbf{\Theta}| = n$

1. Initialize a **bounded-length queue** Q_θ of (instance, captime) pairs for each configuration θ
2. Calculate **approximate expected runtime** for each θ
3. Choose the task **optimistically predicted to be easiest**: the (instance, captime) pair at the head of the queue corresponding to the θ with smallest approximate expected runtime
4. If the task does not complete within its captime, **procrastinate**: **double the captime** and put the task at the tail of Q_θ
   - We'll do many other runs before we'll forecast this to be the easiest task

Structured Procrastination

For now we consider the case of **few configurations**; let $|\mathbf{\Theta}| = n$

1. Initialize a **bounded-length queue** Q_θ of (instance, captime) pairs for each configuration θ
2. Calculate **approximate expected runtime** for each θ
3. Choose the task **optimistically predicted to be easiest**: the (instance, captime) pair at the head of the queue corresponding to the θ with smallest approximate expected runtime
4. If the task does not complete within its captime, **procrastinate**: **double the captime** and put the task at the tail of Q_θ
   - We'll do many other runs before we'll forecast this to be the easiest task
5. If execution has not yet been interrupted, goto 2

Structured Procrastination

For now we consider the case of **few configurations**; let $|\mathbf{\Theta}| = n$

1. Initialize a **bounded-length queue** Q_θ of (instance, captime) pairs for each configuration θ
2. Calculate **approximate expected runtime** for each θ
3. Choose the task **optimistically predicted to be easiest**: the (instance, captime) pair at the head of the queue corresponding to the θ with smallest approximate expected runtime
4. If the task does not complete within its captime, **procrastinate**: **double the captime** and put the task at the tail of Q_θ
5. If execution has not yet been interrupted, goto 2
6. Return the configuration that **we spent the most total time running**
   - it might seem more intuitive to return the configuration with best approximate expected runtime, but this isn't statistically stable

Running Structured Procrastination

The user must specify

- an **algorithm configuration problem** $(\mathcal{A}, \mathbf{\Theta}, \mathcal{D}, \bar{\kappa}, R, \kappa_0)$;
- a **precision** ϵ (how far solutions can be from optimal);
- a **failure probability** ζ (max probability with which guarantees can fail to hold).

The user does not need to specify δ (the fraction of **"outlying" instances** on which running times may be capped)

- this parameter is gradually reduced as the algorithm runs
- when the algorithm is stopped, it returns the δ for which it is guaranteed to have found an (ϵ, δ)-optimal configuration

Structured Procrastination: Running Time

Theorem (worst-case running time, few configurations)

For any $\delta > 0$, an execution of the Structured Procrastination algorithm ***identifies an (ϵ, δ)-optimal configuration with probability at least $1 - \zeta$*** *within worst-case expected time*

$$O\left(\frac{n}{\delta\epsilon^2}\ln\left(\frac{n\ln\bar{\kappa}}{\zeta\delta\epsilon^2}\right)OPT\right).$$

Structured Procrastination: Running Time

Theorem (worst-case running time, few configurations)

For any $\delta > 0$, an execution of the Structured Procrastination algorithm ***identifies an (ϵ, δ)-optimal configuration with probability at least $1 - \zeta$*** *within worst-case expected time*

$$O\left(\frac{n}{\delta\epsilon^2} \ln\left(\frac{n \ln \bar{\kappa}}{\zeta\delta\epsilon^2}\right) OPT\right).$$

Structured Procrastination: Running Time

Theorem (worst-case running time, few configurations)

For any $\delta > 0$, an execution of the Structured Procrastination algorithm ***identifies an (ϵ, δ)-optimal configuration with probability at least $1 - \zeta$*** *within worst-case expected time*

$$O\left(\frac{n}{\delta\epsilon^2} \ln\left(\frac{n \ln \bar{\kappa}}{\zeta\delta\epsilon^2}\right) OPT\right).$$

Theorem (running time lower bound for few configurations)

Suppose an algorithm configuration procedure is guaranteed to select an (ϵ, δ)-optimal configuration with probability at least $\frac{1}{2}$. Its worst-case expected running time ***must be at least $\Omega\left(\frac{n}{\delta\epsilon^2} OPT\right)$.***

This Tutorial

Section Outline

Algorithm Configuration Methods with Theoretical Guarantees (Kevin)

- Technical Setup
- Structured Procrastination (the case of few configurations)
- **Extensions to Structured Procrastination** (many configurations and more)
- LeapsAndBounds
- CapsAndRuns
- Structured Procrastination with Confidence
- Related Work and Further Reading

Follow along: http://bit.ly/ACTutorial

The Case of Many Configurations

- We need a **different approach** if we want to handle infinitely many configurations—our current guarantees are superlinear in n
  - Relax the requirement that we find performance close to that of OPT
  - Instead, seek a configuration with performance close to **the best that remains after we exclude the γ fraction of fastest configurations** from $\mathbf{\Theta}$ (call this $\mathbf{OPT}_\gamma$)
    - in other words, seek **a configuration within the top-performing $\lfloor 1/\gamma \rfloor$-quantile**

Definition ($(\epsilon, \delta, \gamma)$-Optimality)

A configuration θ^* is $(\epsilon, \delta, \gamma)$-*optimal* if there exists some threshold κ for which $R_\kappa(\theta^*) \leq (1+\epsilon)\,\mathbf{OPT}_\gamma$ and $\Pr_{\pi\sim\mathcal{D}}\left(R(\theta^*, \pi) > \kappa\right) \leq \delta$.

Extending Structured Procrastination to Many Configurations

We **extend the Structured Procrastination algorithm** to seek the best among a random sample of $1/\gamma$ configurations

- It **gradually reduces both δ and γ** to tighten guarantees
  - reduces γ by sampling more configurations
  - sets $\delta = \gamma^\omega$

Theorem

***For any γ, ω and with $\delta = \gamma^\omega$**, an execution of the Structured Procrastination algorithm identifies an $(\epsilon, \delta, \gamma)$-optimal configuration with probability at least $1 - \zeta$ in worst-case expected time*

$$O\left(\frac{1}{\delta\gamma\epsilon^2}\ln\left(\frac{\ln\bar{\kappa}}{\zeta\delta\gamma\epsilon^2}\right)\mathit{OPT}_\gamma\right).$$

Extending Structured Procrastination to Many Configurations

Theorem

For any γ, ω and with $\delta = \gamma^\omega$, an execution of the Structured Procrastination algorithm identifies an $(\epsilon, \delta, \gamma)$-optimal configuration with probability at least $1 - \zeta$ in worst-case expected time

$$O\left(\frac{1}{\delta\gamma\epsilon^2}\ln\left(\frac{\ln\bar{\kappa}}{\zeta\delta\gamma\epsilon^2}\right)OPT_\gamma\right).$$

Theorem (running time lower bound for many configurations)

Suppose an algorithm configuration procedure is guaranteed to select an $(\epsilon, \delta, \gamma)$-optimal configuration with probability at least $\frac{1}{2}$. Its worst-case expected running time ***must be at least*** $\Omega\left(\frac{1}{\delta\gamma\epsilon^2}OPT_\gamma\right)$.

Practical extensions

Theorem (compatibility with Bayesian optimization & local search)

Suppose that half of the configurations sampled in Structured Procrastination are ***generated in a way that depends arbitrarily on previous observations****. Then worst-case runtime is increased by at most a factor of 2.*

Theorem (linear speedups when parallelized)

Suppose that Structured Procrastination is ***executed by p processors running in parallel****. Then, provided it is run for a sufficiently long time (linear in p), worst-case runtime decreases by at least a factor of $p - 1$.*

This Tutorial

Section Outline

Algorithm Configuration Methods with Theoretical Guarantees (Kevin)

- Technical Setup
- Structured Procrastination (the case of few configurations)
- Extensions to Structured Procrastination (many configurations and more)
- **LeapsAndBounds**
- CapsAndRuns
- Structured Procrastination with Confidence
- Related Work and Further Reading

Follow along: http://bit.ly/ACTutorial

LeapsAndBounds

- A second, **approximately optimal** algorithm configuration technique due to Weisz, György & Szepesvári [2018]
- Improves on SP's worst-case performance by:
  - **removing dependence on** $\bar{\kappa}$ (replaced with OPT, usually much smaller)
  - tightening the worst-case performance bound by a log factor
- **Empirically outperforms** SP
  - based on very limited experiments, but likely true overall
- But is **not anytime**: requires both ϵ, δ as inputs

LeapsAndBounds: How it Works

The algorithm at a glance:

1. Attempt to guess an (initially) low value of OPT
2. Try to find a configuration whose mean is smaller than this guess
   - Discard configurations whose mean is large **relative to the current guess**
   - Use **fewer samples** to estimate mean runtime of configurations with **low runtime variance** across instances
3. If none, double the guess and repeat

LeapsAndBounds: Running Time

Theorem (worst-case running time)

For any $\epsilon \in (0, 1/3)$, $\delta \in (0, 1)$, an execution of LeapsAndBounds ***identifies an (ϵ, δ)-optimal configuration with probability at least $1 - \zeta$*** *within worst-case expected time*

$$O\left(\frac{n}{\delta\epsilon^2} \ln\left(\frac{n \ln \mathbf{OPT}}{\zeta}\right) OPT\right).$$

Structured Procrastination

Compare to Structured Procrastination:

$$O\left(\frac{n}{\delta\epsilon^2} \ln\left(\frac{n \ln \bar{\kappa}}{\zeta\delta\epsilon^2}\right) \mathrm{OPT}\right).$$

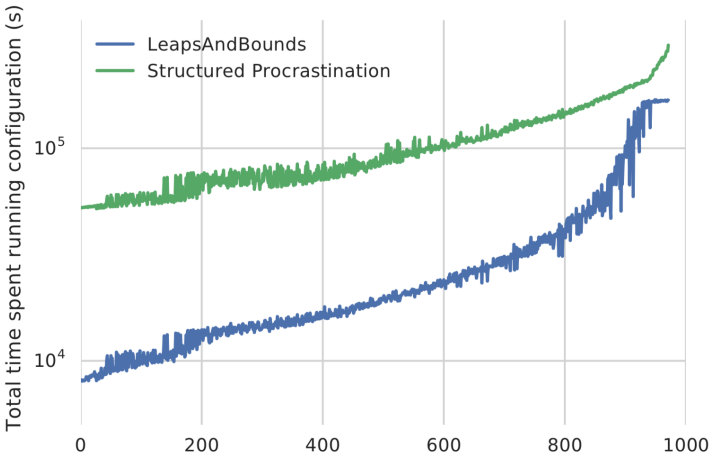
LeapsAndBounds: Empirical Performance

972 `minisat` configurations running on 20,118 nontrivial `CNFuzzDD` SAT problems

Time to prove $(\epsilon = 0.2, \delta = 0.2)$-optimality: **SP 1,169** CPU days; **L&B 369** CPU days

LeapsAndBounds: Empirical Performance

972 `minisat` configurations running on 20,118 nontrivial `CNFuzzDD` SAT problems
Time to prove $(\epsilon = 0.2, \delta = 0.2)$-optimality: **SP 1,169** CPU days; **L&B 369** CPU days



This Tutorial

Section Outline

Algorithm Configuration Methods with Theoretical Guarantees (Kevin)

- Technical Setup
- Structured Procrastination (the case of few configurations)
- Extensions to Structured Procrastination (many configurations and more)
- LeapsAndBounds
- **CapsAndRuns**
- Structured Procrastination with Confidence
- Related Work and Further Reading

Follow along: http://bit.ly/ACTutorial

CapsAndRuns

- Recent extension to LeapsAndBounds [Weisz, György & Szepesvári, ICML 2019]
  - **Tue Jun 11th 04:20–04:25 PM Room 103**

CapsAndRuns

- Recent extension to LeapsAndBounds [Weisz, György & Szepesvári, ICML 2019]
  - **Tue Jun 11th 04:20–04:25 PM Room 103**
- **Adapts to easy problem instances** by eliminating configurations that are dominated by other configurations
- Also provides an **improved bound** for non-worst-case instances
  - scales with suboptimality gap, $\frac{R(\theta)}{R(\theta)-OPT}$, instead of ϵ^{-1}
  - dependence on ϵ and δ individually, rather than product $\epsilon\delta$
- Bounds are also improved by defining (ϵ, δ)-optimality w.r.t. $OPT_{\delta/2}$, the optimal configuration when capping runs at the $\delta/2$-quantile, rather than OPT
- Still **not anytime**

CapsAndRuns: How it Works

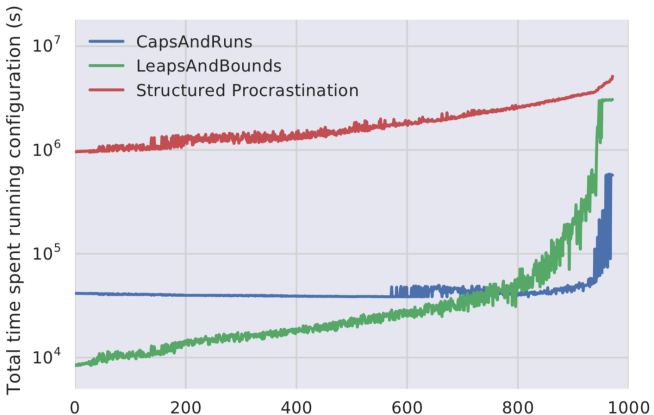
Proceeds in **two phases**:

- Phase 1: **Estimate** $(1-\delta)$**-quantile** of each configuration's runtime over $\mathcal{D}$
- Phase 2: **Estimate mean runtime** of each configuration using the **quantile** from Phase 1 as **captime**
- Return configuration with **minimum estimated mean**

CapsAndRuns: Empirical Results

972 `minisat` configurations running on 20,118 nontrivial `CNFuzzDD` SAT problems

Time to prove $(\epsilon = 0.05, \delta = 0.2)$-optimality (CPU days): **SP 20,643**; **L&B 1,451**; **C&R: 586**



$(\epsilon = 0.05, \delta = 0.2)$ [Weisz, György & Szepesvári, ICML 2019]

This Tutorial

Section Outline

Algorithm Configuration Methods with Theoretical Guarantees (Kevin)

- Technical Setup
- Structured Procrastination (the case of few configurations)
- Extensions to Structured Procrastination (many configurations and more)
- LeapsAndBounds
- CapsAndRuns
- **Structured Procrastination with Confidence**
- Related Work and Further Reading

Follow along: http://bit.ly/ACTutorial

Structured Procrastination with Confidence

- Recent extension to Structured Procrastination [Kleinberg, L-B, Lucier & Graham, arXiv 2019]
- **Adapts to easy problem instances** by maintaining confidence bounds on each configuration's runtime
- Anytime algorithm: δ is **gradually refined** during the search process
  - helpful when user can't predict the relationship between these parameters and runtime
  - also improves performance: by starting with large values of δ, SPC **eliminates bad configurations early on**
- SPC's running time matches (up to log factors) the running time of a hypothetical "optimality verification procedure" that knows the identity of the optimal configuration
  - i.e., SPC takes about as long to prove (ϵ, δ)-optimality as our hypothetical verification procedure would need to demonstrate that fact to a skeptic
  - **When verification is easy, SPC is fast**

Recall: Structured Procrastination

1. Initialize a **bounded-length queue** Q_θ of (instance, captime) pairs for each configuration θ
2. Calculate **approximate expected runtime** for each θ
3. Choose the task **optimistically predicted to be easiest**: the (instance, captime) pair at the head of the queue corresponding to the i with smallest approximate expected runtime
4. If the task does not complete within its captime, **procrastinate**: **double the captime** and put the task at the tail of Q_θ
5. If execution has not yet been interrupted, goto 2
6. Return the configuration that **we spent the most total time running**

Structured Procrastination with Confidence

1. Initialize a **bounded-length queue** Q_θ of (instance, captime) pairs for each configuration θ
2. Calculate ~~**approximate expected runtime**~~ **lower confidence bound on expected runtime** for each θ
3. Choose the task **optimistically predicted to be easiest**: the (instance, captime) pair at the head of the queue corresponding to the i with smallest approximate expected runtime
4. If the task does not complete within its captime, **procrastinate**: **double the captime** and put the task at the tail of Q_θ
5. If execution has not yet been interrupted, goto 2
6. Return the configuration that **we spent the most total time running**

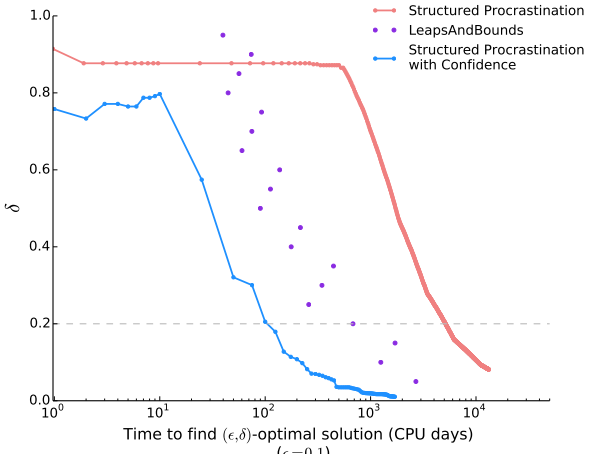
Structured Procrastination with Confidence

1. Initialize a **bounded-length queue** Q_θ of (instance, captime) pairs for each configuration θ
2. Calculate ~~**approximate expected runtime**~~ **lower confidence bound on expected runtime** for each θ
3. Choose the task **optimistically predicted to be easiest**: the (instance, captime) pair at the head of the queue corresponding to the i with smallest approximate expected runtime
4. If the task does not complete within its captime, **procrastinate**: **double the captime** and put the task at the tail of Q_θ
5. If execution has not yet been interrupted, goto 2
6. ~~Return the configuration that **we spent the most total time running**~~ **Return the configuration that either solved or attempted the greatest number of instances**

Structured Procrastination with Confidence: Empirical Performance

972 `minisat` configurations running on 20,118 nontrivial `CNFuzzDD` SAT problems

Time to prove $(\epsilon = 0.1, \delta = 0.2)$-optimality: **SP 5,150**; **L&B 680**; **SPC 150** (CPU days)



[Kleinberg, L-B, Lucier & Graham, 2019]

This Tutorial

Section Outline

Algorithm Configuration Methods with Theoretical Guarantees (Kevin)

- Technical Setup
- Structured Procrastination (the case of few configurations)
- Extensions to Structured Procrastination (many configurations and more)
- LeapsAndBounds
- CapsAndRuns
- Structured Procrastination with Confidence
- **Related Work and Further Reading**

Follow along: http://bit.ly/ACTutorial

Related Work: Bandits

- Bandits:
  - Optimism in the face of uncertainty [Auer, Cesa-Bianchi & Fischer 2002, Bubeck & Cesa-Bianchi 2012]
  - bandits with **correlated arms** that scale to large experimental design settings [Kleinberg 2006; Kleinberg, Slivkins & Upfal 2008; Chaudhuri, Freund & Hsu 2009, Bubeck, Munos, Stoltz & Szepesvári 2011, Srinivas, Krause, Kakade & Seeger 2012, Cesa-Bianchi & Lugosi 2012, Munos 2014]
- However, our runtime minimization objective is **crucially different** from more general objective functions targeted in most bandits literature:
  - cost of pulling an arm **measured in the same units** as the minimization objective function
  - freedom to **set a maximum amount** κ we are willing to pay in pulling an arm; if true cost exceeds κ, we pay only κ but learn only that true cost was higher
- Beyond the assumption that **all arms involve the same, fixed cost**:
  - **Variable costs** and a fixed overall budget, but no capping [Guha & Munagala 2007, Tran-Thanh, Chapman, Rogers & Jennings 2012, Badanidiyuru, Kleinberg, & Slivkins 2013]
  - The algorithm can *specify* a **maximum cost to be paid** when pulling an arm, but never pays less than that amount [Kandasamy, Dasarathy, Poczos & Schneider 2016]
  - Observations are **censored if they exceed a given budget** [Ganchev, Nevmyvaka, Kearns & Vaughan 2010]

Other Important Related Work

- **Hyperparameter optimization**
  - Key initial work [Bergstra, Bardenet, Bengio & Kégl 2011,Thornton, H, Hoos & L-B 2013]
  - Hyperband: uses similar theoretical tools [Li, Jamieson, DeSalvo, Rostamizadeh, & Talwalkar 2016]

- **Learning-theoretic foundations**
  - Gupta & Roughgarden [2017]: framed configuration and selection in terms of learning theory
  - Sample-efficient, special-purpose algorithms for particular classes of problems
    - combinatorial partitioning problems (clustering, max-cut, etc) [Balcan, Nagarajan, Vitercik & White 2017]
    - branching strategies in tree search [Balcan, Dick, Sandholm & Vitercik 2018]
    - various algorithm selection problems [Balcan, Dick & Vitercik 2018]

This Tutorial

High-Level Outline

Introduction, Technical Preliminaries, and a Case Study (Kevin)

Practical Methods for Algorithm Configuration (Frank)

Algorithm Configuration Methods with Theoretical Guarantees (Kevin)

Beyond Static Configuration: Related Problems and Emerging Directions (Frank)

Follow along: http://bit.ly/ACTutorial

This Tutorial

Section Outline

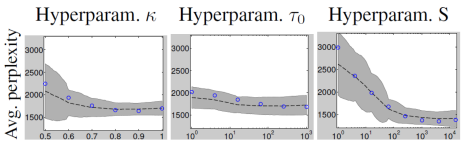
Beyond Static Configuration: Related Problems and Emerging Directions (Frank)

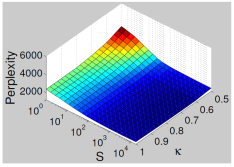
- **Parameter Importance**
- Algorithm Selection
- End-to-End Learning of Combinatorial Solvers
- Integrating ML and Combinatorial Optimization

Follow along: http://bit.ly/ACTutorial

Global effect of a parameter

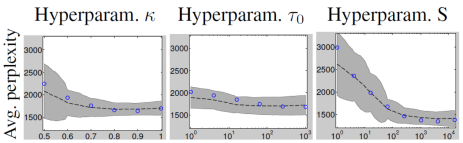
- To quantify the global effect of one or more parameters, we can **marginalize predicted performance across all settings of all other parameters** [H., Hoos & L-B, 2014]

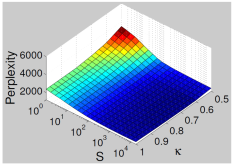




Global effect of a parameter

- To quantify the global effect of one or more parameters, we can **marginalize predicted performance across all settings of all other parameters** [H., Hoos & L-B, 2014]





In regression trees, we can do this **efficiently**:

$$\text{avg}(v) = \sum_{\theta_2 \in \Theta_2} \cdots \sum_{\theta_n \in \Theta_n} \frac{1}{|\Theta_2|} \cdots \frac{1}{|\Theta_n|} f(v, \theta_2, \ldots, \theta_n)$$

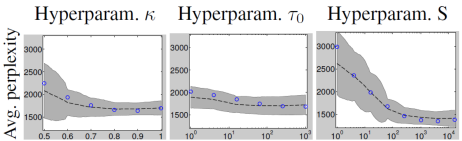
$$\approx \sum_{\theta_2 \in \Theta_2} \cdots \sum_{\theta_n \in \Theta_n} \frac{1}{|\Theta_2|} \cdots \frac{1}{|\Theta_n|} \hat{f}(v, \theta_2, \ldots, \theta_n)$$

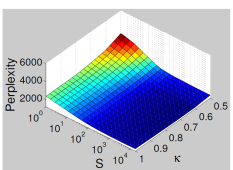
$$= \sum_{\theta_2 \in \Theta_2} \cdots \sum_{\theta_n \in \Theta_n} \frac{1}{|\Theta_2|} \cdots \frac{1}{|\Theta_n|} \sum_{P_i \in \mathcal{P}} \mathbb{I}(\langle v, \theta_2, \ldots, \theta_n \rangle \in P_i) \cdot c(P_i)$$

$$= \sum_{P_i \in \mathcal{P}} \frac{|\Theta_2{}^{(i)}| \cdots |\Theta_n{}^{(i)}|}{|\Theta_2| \cdots |\Theta_n|} \cdot \mathbb{I}(v \in \Theta_1{}^{(i)}) \cdot c(P_i)$$

Linear time computation

Functional analysis of variance (fANOVA) [H., Hoos & L-B, 2014]





- By definition, the variance of predictor $\hat{f}$ across its domain $\boldsymbol{\Theta}$ is:

$$\mathbb{V} = \frac{1}{||\boldsymbol{\Theta}||} \int (\hat{f}(\boldsymbol{\theta}) - \hat{f}_0)^2 d\boldsymbol{\theta}$$

- Functional ANOVA [Sobol, 1993] **decomposes this variance into components** due to each subset of the parameters N:

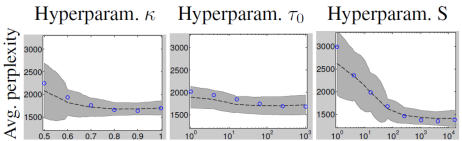
$$\mathbb{V} = \sum_{U \subset N} \mathbb{V}_U, \text{ where } \mathbb{V}_U = \frac{1}{||\boldsymbol{\Theta}_U||} \int \hat{f}_U^2(\boldsymbol{\theta}_U) d\boldsymbol{\Theta}_U$$

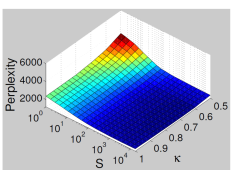
Functional analysis of variance (fANOVA) [H., Hoos & L-B, 2014]

"Main effect" S explains 65% of variance

"Interaction effect" of S&κ explains another 18%

Computing this took milliseconds





- By definition, the variance of predictor $\hat{f}$ across its domain $\boldsymbol{\Theta}$ is:

$$\mathbb{V} = \frac{1}{||\boldsymbol{\Theta}||} \int (\hat{f}(\boldsymbol{\theta}) - \hat{f}_0)^2 d\boldsymbol{\theta}$$

- Functional ANOVA [Sobol, 1993] **decomposes this variance into components** due to each subset of the parameters N:

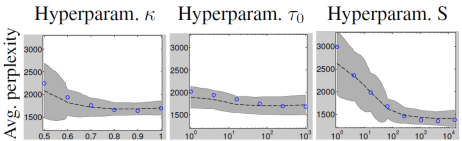
$$\mathbb{V} = \sum_{U \subset N} \mathbb{V}_U, \text{ where } \mathbb{V}_U = \frac{1}{||\boldsymbol{\Theta}_U||} \int \hat{f}_U^2(\boldsymbol{\theta}_U) d\boldsymbol{\Theta}_U$$

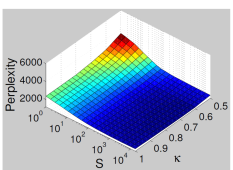
Functional analysis of variance (fANOVA) [H., Hoos & L-B, 2014]

"Main effect" S explains 65% of variance

"Interaction effect" of S&κ explains another 18%

Computing this took milliseconds





- By definition, the variance of predictor $\hat{f}$ across its domain $\boldsymbol{\Theta}$ is:

$$\mathbb{V} = \frac{1}{||\boldsymbol{\Theta}||} \int (\hat{f}(\boldsymbol{\theta}) - \hat{f}_0)^2 d\boldsymbol{\theta}$$

- Functional ANOVA [Sobol, 1993] **decomposes this variance into components** due to each subset of the parameters N:

$$\mathbb{V} = \sum_{U \subset N} \mathbb{V}_U, \text{ where } \mathbb{V}_U = \frac{1}{||\boldsymbol{\Theta}_U||} \int \hat{f}_U^2(\boldsymbol{\theta}_U) d\boldsymbol{\Theta}_U$$

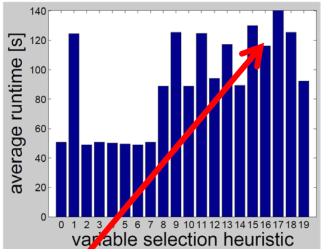
Theorem

In regression trees, main effects can be computed in linear time.

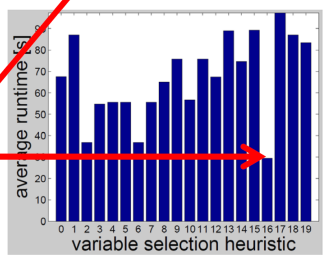
Functional ANOVA example for SAT solver Spear [H., Hoos & L-B, 2014]

- SAT solver Spear: 26 parameters
- Posthoc analysis of data gathered from optimization with SMAC

- **93% of variation in runtimes is due to a single parameter**: the **variable selection heuristic**.
- Analysis took seconds



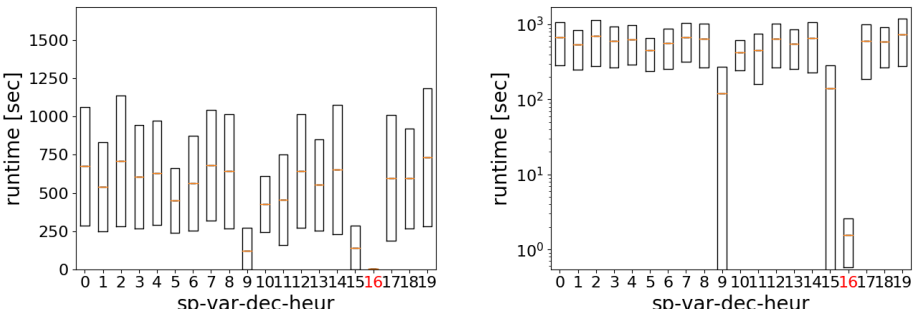
Data set: bounded model checking



Data set: software verification

Local parameter importance (LPI): changing each parameter around the incumbent

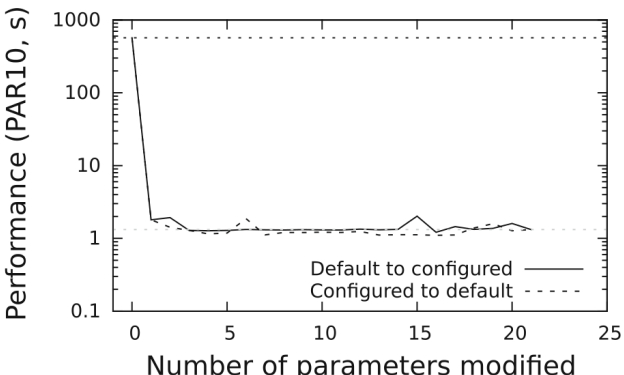
- What is the **local effect of varying one parameter of the incumbent**?
  - Use relative changes to quantify local parameter importance
  - Can also be done based on the predictive model of algorithm performance [Biedenkapp et al, 2018]



Results for Spear on SWV

Ablation between default and incumbent configuration

- Greedily change the parameter that improves performance most [Fawcett et al. 2013]
  - Can also be done based on the predictive model of algorithm performance [Biedenkapp et al, 2017]



Results for Spear on SWV

This Tutorial

Section Outline

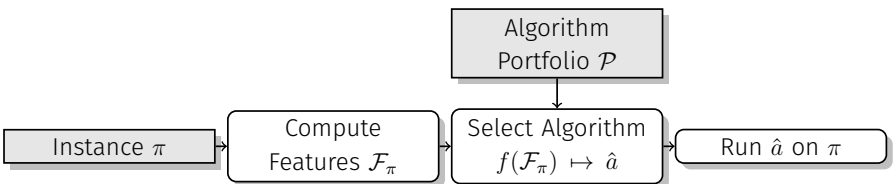
Beyond Static Configuration: Related Problems and Emerging Directions (Frank)

- Parameter Importance
- **Algorithm Selection**
- End-to-End Learning of Combinatorial Solvers
- Integrating ML and Combinatorial Optimization

Follow along: http://bit.ly/ACTutorial

Algorithm selection

- In this tutorial, we focussed on finding a single configuration that performs well on average: $\arg\min_{\boldsymbol{\theta} \in \boldsymbol{\Theta}} \mathbb{E}_{\pi \sim \mathcal{D}}(m(\boldsymbol{\theta}, \pi))$
- We can also learn a function that picks the best configuration $\boldsymbol{\theta} \in \boldsymbol{\Theta}$ or algorithm $a \in \mathcal{P}$ per instance π with features $\mathcal{F}_\pi$: $\arg\min_{f:\Pi \to \boldsymbol{\Theta}} \mathbb{E}_{\pi \sim \mathcal{D}}(m(f(\mathcal{F}_\pi), \pi))$



- There is a rich literature on this **algorithm selection** problem [L-B et al, 2003 Xu et al, 2008; Smith-Miles, 2009; Xu et al, 2012; Kotthoff, 2014; Malitsky et al, 2013; Lindauer et al, 2015; Lorregia et al, 2016]

Example SAT Challenge 2012

Rank	RiG	Solver	#solved
–	–	Virtual Best Solver (VBS)	568
1	1	SATzilla2012 APP	531
2	2	SATzilla2012 ALL	515
3	1	Industrial SAT Solver	499
–	–	lingeling (SAT Competition 2011 Bronze)	488
4	2	interactSAT	480
5	1	glucose	475
6	2	SINN	472
7	3	ZENN	468
8	4	Lingeling	467
9	5	linge_dyphase	458
10	6	simpsat	453

The VBS (virtual best solver) is an oracle algorithm selector of competition entries.
(pink: algorithm selectors, blue: portfolios, green: single-engine solvers)

Automated construction of portfolios from a single algorithm

- **Algorithm Configuration**
  - Strength: find a single configuration with strong performance for a given cost metric
  - Weakness: for heterogeneous instance sets, there is often no configuration that performs great for all instances
- **Algorithm Selection**
  - Strength: works well for heterogeneous instance sets due to per-instance selection
  - Weakness: in standard algorithm selection, the set of algorithms $\mathcal{P}$ to choose from typically only contains a few algorithms
- **Putting the two together** [Kadioglu et al, 2010; Xu et al, 2010]
  - Use algorithm configuration to determine useful configurations
  - Use algorithm selection to select from them based on instance characteristics

Warmstarting of algorithm configuration [Lindauer & H., 2018]

- Humans often **don't start from scratch** when tuning an algorithm's parameters
  - They use their previous experience
  - E.g., tuning CPLEX for a few applications tells you which parameters tend to be important

Warmstarting of algorithm configuration [Lindauer & H., 2018]

- Humans often **don't start from scratch** when tuning an algorithm's parameters
  - They use their previous experience
  - E.g., tuning CPLEX for a few applications tells you which parameters tend to be important
- We would also like to make use of previous AC runs on other distributions
  - Option 1: initialize from **strong previous configurations**
  - Option 2: **reuse the previous models** (weighted by how useful they are)
  - Combination of 1+2 often works best

Warmstarting of algorithm configuration [Lindauer & H., 2018]

- Humans often **don't start from scratch** when tuning an algorithm's parameters
  - They use their previous experience
  - E.g., tuning CPLEX for a few applications tells you which parameters tend to be important
- We would also like to make use of previous AC runs on other distributions
  - Option 1: initialize from **strong previous configurations**
  - Option 2: **reuse the previous models** (weighted by how useful they are)
  - Combination of 1+2 often works best
- Results
  - Can yield large speedups ($> 100\times$) when similar configurations work well
  - Does not substantially slow down the search if misleading
  - On average: $4\times$ speedups over running SMAC from scratch

This Tutorial

Section Outline

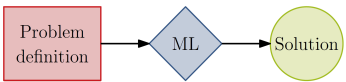
Beyond Static Configuration: Related Problems and Emerging Directions (Frank)

- Parameter Importance
- Algorithm Selection
- **End-to-End Learning of Combinatorial Solvers**
- Integrating ML and Combinatorial Optimization

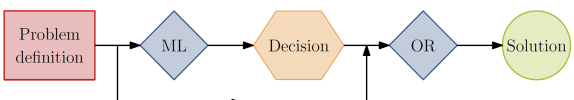
Follow along: http://bit.ly/ACTutorial

Categorization of ML for Combinatorial Optimization / Operations Research (OR)

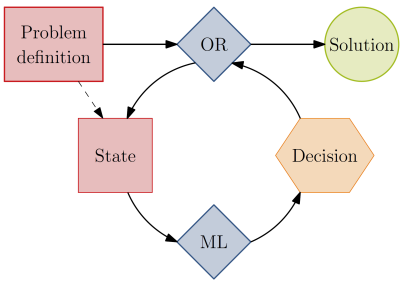
- Recent survey article [Yoshua Bengio, Andrea Lodi and Antoine Prouvost, 2018]
  - Define three categories of combinining ML and OR



ML acts alone to solve the problem



ML augments OR with valuable information



Integrating ML into OR; OR algorithm repeatedly calls the same model to make decisions

End-to-end learning of algorithms (in general)

Learn a neural network with parameters ϕ that defines an algorithm

- The network's parameters ϕ are trained to optimize the true objective (or a proxy)
- The network is queried for each action of the algorithm

End-to-end learning of algorithms (in general)

Learn a neural network with parameters ϕ that defines an algorithm

- The network's parameters ϕ are trained to optimize the true objective (or a proxy)
- The network is queried for each action of the algorithm

Examples

- Learning to learn with gradient descent [Andrychowicz et al, 2016] / learning to optimize [Li & Malik, 2017]: parameterize an update rule for base-level NN parameters $\mathbf{w}$:

$$\mathbf{w}_{t+1} = \mathbf{w}_t + g(\nabla f(\mathbf{w}_t), \phi)$$

End-to-end learning of algorithms (in general)

Learn a neural network with parameters ϕ that defines an algorithm

- The network's parameters ϕ are trained to optimize the true objective (or a proxy)
- The network is queried for each action of the algorithm

Examples

- Learning to learn with gradient descent [Andrychowicz et al, 2016] / learning to optimize [Li & Malik, 2017]: parameterize an update rule for base-level NN parameters $\mathbf{w}$:

$$\mathbf{w}_{t+1} = \mathbf{w}_t + g(\nabla f(\mathbf{w}_t), \phi)$$

- Learning a gradient-free optimizer's update rule [Chen et al, 2017]
- Learning unsupervised learning rules [Metz et al, 2019]
- AlphaZero [Silver et al, 2018], etc

End-to-end learning of combinatorial problems

Learning to solve Euclidean TSP

- Pointer networks [Vinyals et al, 2015]
  - RNN to encode TSP instance
  - Another RNN with attention-like mechanism to predict probability distribution over next node
  - Trained with supervised learning, using optimal solutions to TSP instances
- Reinforcement learning avoids need for optimal solutions
  - Train an RNN [Bello et al, 2017] or a graph neural network [Kool et al, 2019]
- Directly predict the permutation [Emami & Ranka, 2018; Nowak et al, 2017]
- Learn a greedy heuristic to choose next node [Dai et al, 2018]

End-to-end learning of combinatorial problems

Learning to solve SAT

- NeuroSAT [Selsam et al, 2019]
  - Use permutation invariant graph neural network
  - Learn a message passing algorithm for solving new instances
- SATNet [Wang et al, 2019]
  - Differentiable approximate MaxSAT solver
  - Can be integrated as a component of a deep learning system (e.g., “visual Sudoku”)
- Learning to predict satisfiability [Cameron et al, 2019]
  - Even at the phase transition, with 80% accuracy
  - Using exchangeable deep networks

This Tutorial

Section Outline

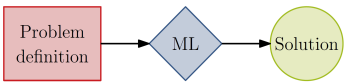
Beyond Static Configuration: Related Problems and Emerging Directions (Frank)

- Parameter Importance
- Algorithm Selection
- End-to-End Learning of Combinatorial Solvers
- **Integrating ML and Combinatorial Optimization**

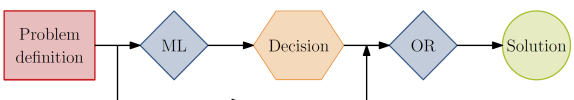
Follow along: http://bit.ly/ACTutorial

Categorization of ML for Combinatorial Optimization / Operations Research (OR)

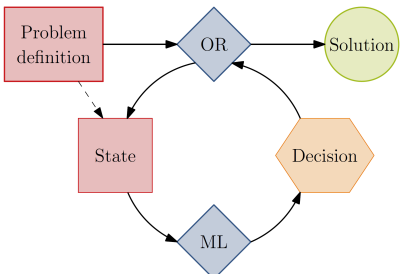
- Recent survey article [Yoshua Bengio, Andrea Lodi and Antoine Prouvost, 2018]
  - Defines three categories of combinining ML and OR



ML acts alone to solve the problem



ML augments OR with valuable information



Integrating ML into OR; OR algorithm repeatedly calls the same model to make decisions

Learning to make simple decisions online

Dynamic restart policies

- For a randomized algorithm
- Based on an initial observation window of a run, predict whether this run is good or bad (and thus whether to restart) [Kautz et al, 2002; Horvitz et al, 2001]

Learning to make simple decisions online

Dynamic restart policies

- For a randomized algorithm
- Based on an initial observation window of a run, predict whether this run is good or bad (and thus whether to restart) [Kautz et al, 2002; Horvitz et al, 2001]

Dynamic algorithm portfolios

- Run several algorithms in parallel
- Decide time shares adaptively based on algorithms' progress

  [Carchrae & Beck, 2014; Gagliolo & Schmidhuber, 2006]

Learning to make simple decisions online

Dynamic restart policies

- For a randomized algorithm
- Based on an initial observation window of a run, predict whether this run is good or bad (and thus whether to restart) [Kautz et al, 2002; Horvitz et al, 2001]

Dynamic algorithm portfolios

- Run several algorithms in parallel
- Decide time shares adaptively based on algorithms' progress

  [Carchrae & Beck, 2014; Gagliolo & Schmidhuber, 2006]

Learning in which search nodes to apply primal heuristics

- Primal heuristics can find feasible solutions in branch-and-bound
- Too expensive to apply in every node $\rightsquigarrow$ learn when to apply [Khalil et al, 2017]

Learning to select/switch between algorithms online

Learning to select a sorting algorithm at each node

- Keep track of a state (e.g., length of sequence left to be sorted recursively)
- Choose algorithm to use for subtree based on state using RL [Lagoudakis & Littmann, 2000]
  - E.g., QuickSort for long sequences, InsertionSort for short ones

Learning to select branching rules for DPLL in SAT solving

- Keep track of a backtracking state
- Choose branching rule based on state using RL [Lagoudakis & Littmann, 2001]

Parameter control

Adapting algorithm parameters online

- A strict **generalization of algorithm configuration**
  - just pick a fixed setting and never change it

Parameter control

Adapting algorithm parameters online

- A strict **generalization of algorithm configuration**
  - just pick a fixed setting and never change it
- A strict **generalization of per-instance algorithm configuration (PIAC)**
  - just select configuration once in the beginning per instance, never change

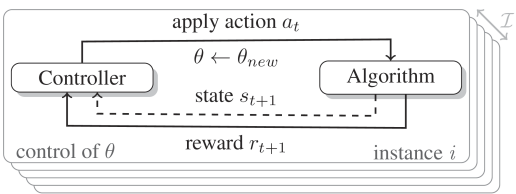
Parameter control

Adapting algorithm parameters online

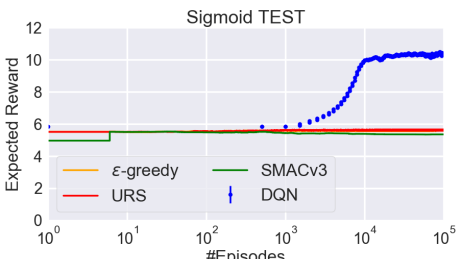
- A strict **generalization of algorithm configuration**
  - just pick a fixed setting and never change it
- A strict **generalization of per-instance algorithm configuration (PIAC)**
  - just select configuration once in the beginning per instance, never change
- A strict **generalization of algorithm selection** (finite set of algorithms $\mathcal{P}$)
  - special case of PIAC with one categorical parameter with domain $\mathcal{P}$

Parameter control: a reinforcement learning problem

- Formulation of the single-instance case as an MDP [Adriaensen & Nowe, 2016]
  - But a strong policy for a single instance may not generalize
- Formulation of the general problem as a **contextual MDP** to learn to generalize across instances [Biedenkapp et al, 2019]



Shared state & action spaces
Different transition and reward functions



First promising results on toy functions

Conclusions

Summary

- Algorithm configuration: **learning in the space of algorithm designs**
- **Practical AC methods** are very mature; often able to speed up state-of-the-art algorithms by orders of magnitude
- Much recent progress on **AC with worst-case runtime guarantees**; likely to impact practice soon
- **Related problems:** parameter importance; algorithm selection; end-to-end learning; other ways of integrating ML with combinatorial optimization

Further resources

- **Code** available for SMAC, CAVE (parameter importance), Auto-WEKA, Auto-sklearn
- See http://automl.org for **more material**; also, we're hiring: http://automl.org/jobs