Automated Machine Learning
(AutoML)

M. Lindauer F. Hutter

University of Freiburg

AutoML.org

Lectures 11:
Beyond AutoML: Algorithm Configuration and Control

Where are we? The big picture

- Introduction
- Background
  - Design spaces in ML
  - Evaluation and visualization
- Hyperparameter optimization (HPO)
  - Bayesian optimization
  - Other black-box techniques
  - More details on Gaussian processes
- Pentecost (Holiday) – no lecture
- Architecture search I + II
- Meta-Learning I + II

$\rightarrow$ Beyond AutoML: algorithm configuration and control

- Project announcement and closing

Learning Goals

After this lecture, you will be able to . . .

- define the algorithm configuration problem
- discuss differences between HPO and algorithm configuration
- explain the components of SMAC to combine Bayesian Optimization across instances
- define and give examples for the algorithm control problem
- list some further topics related AutoML and algorithm configuration

Further Material

There is one recent tutorials on algorithm configuration:

- ICML'19: Frank Hutter and Kevin Leyton-Brown on "Algorithm configuration: learning in the space of algorithm designs" `https://www.facebook.com/icml.imls/videos/vb.118896271958230/2044426569187107/`

Lecture Overview

1. Algorithm Configuration
2. SMAC: BO for Algorithm Configuration
3. Algorithm Control
4. Other Related Topics

Generalization of HPO

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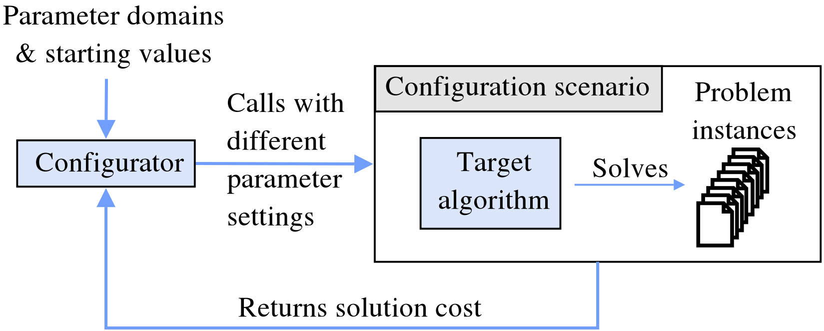
- in fact, you can optimize the performance of any algorithm by means of HPO if
  1. the algorithm at hand has parameters that influence its performance
  2. you care about the empirical performance of an algorithm
- a limitation of HPO is that we assume that we care only about a single task (i.e., dataset or input to the algorithm)

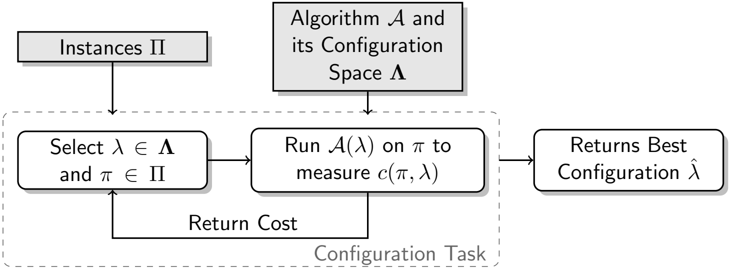
⇝ Can we find an algorithm's configuration that performs well and robustly across a set of tasks?
  - An hyperparameter configuration for a set of datasets
  - A parameter configuration of a SAT solver for a set of SAT instances
  - A parameter configuration of a AI planning solver for a set of planning problems
  - ...

⇝ Algorithm configuration

Algorithm Configuration Visualized



Algorithm Configuration – in More Detail



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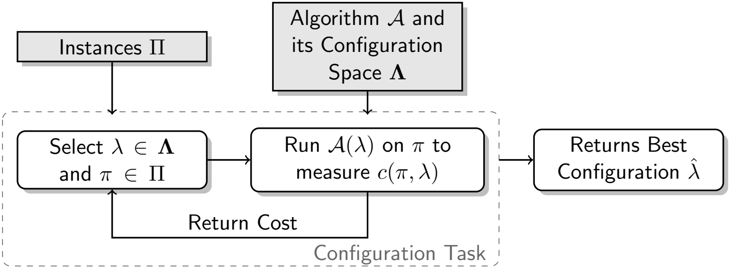

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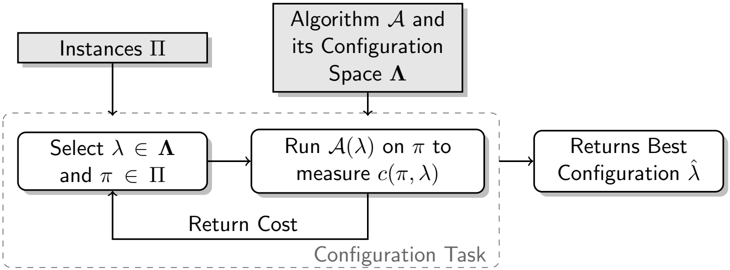

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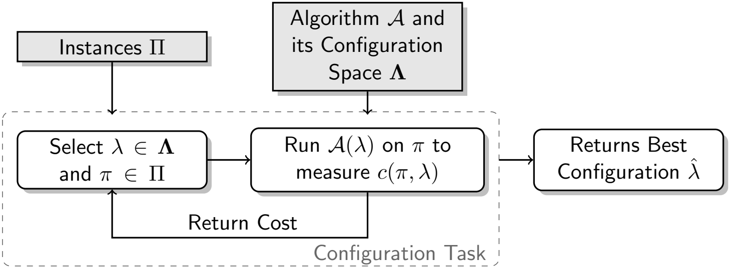

Definition

Given a parameterized algorithm $\mathcal{A}$ with possible parameter settings $\mathbf{\Lambda}$, a set of training problem instances Π, and a cost metric $c : \mathbf{\Lambda} \times \Pi \to \mathbb{R}$, the algorithm configuration problem is to find a parameter configuration $\lambda^* \in \mathbf{\Lambda}$ that minimizes c across the instances in Π.

Algorithm Configuration – Full Formal Definition

Definition

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

- $\mathcal{A}$ is a parameterized algorithm;
- $\mathbf{\Lambda}$ is the parameter configuration space of $\mathcal{A}$;
- $\mathcal{D}$ is a distribution over problem instances with domain Π;

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

Distribution of Instances

We usually have a finite number of instances from a given application

- We want to do well on that type of instances
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Like in machine learning

- We split the instances into a training set and a test set
- We configure algorithms on the training instances
- We only use the test instances afterwards
  - $\rightarrow$ unbiased estimate of generalization performance for unseen instances

Challenges of Algorithm Configuration

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  - Subsumes so-called *multi-armed bandit problem*

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  - apply algorithm configuration to homogeneous instance sets
  - Instance sets can also be heterogeneous,
    i.e., no single configuration performs well on all instances

  $\rightsquigarrow$ combination of algorithm configuration and selection

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$\rightsquigarrow$ Hyperparameter optimization is a subproblem of algorithm configuration

Lecture Overview

State-of-the-art Algorithm Configuration

SMAC: Sequential Model-based Algorithm Configuration =

- + Bayesian Optimization (instead of local search)
- + aggressive racing
- + adaptive capping (for optimizing runtime)

SMAC: Overview

Algorithm 1: SMAC

Input : instance set Π, Algorithm $\mathcal{A}$ with configuration space $\mathbf{\Lambda}$, Initial configuration λ_0, performance metric c, Configuration budget b

Output: best incumbent configuration $\hat{\lambda}$

run history H $\leftarrow$ initial design based on λ_0; // `H =` $(\lambda, \pi, c(\pi, \lambda))_i$

while b *remains* **do**

SMAC: Overview

Algorithm 2: SMAC

Input : instance set Π, Algorithm $\mathcal{A}$ with configuration space $\mathbf{\Lambda}$, Initial configuration λ_0, performance metric c, Configuration budget b

Output: best incumbent configuration $\hat{\lambda}$

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while b *remains* **do**

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Algorithm 3: SMAC

Input : instance set Π, Algorithm $\mathcal{A}$ with configuration space $\mathbf{\Lambda}$, Initial configuration λ_0, performance metric c, Configuration budget b

Output: best incumbent configuration $\hat{\lambda}$

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while b *remains* **do**

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Algorithm 4: SMAC

Input : instance set Π, Algorithm $\mathcal{A}$ with configuration space $\mathbf{\Lambda}$, Initial configuration λ_0, performance metric c, Configuration budget b

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while b *remains* **do**

  $\hat{f} \leftarrow$ train empirical performance model based on run history H;

  $\mathbf{\Lambda}_{challengers} \leftarrow$ select configurations based on $\hat{f}$;

  $\hat{\lambda}$, H $\leftarrow$ intensify($\mathbf{\Lambda}_{challengers}$, $\hat{\lambda}$); `// racing and capping`

Algorithm 5: SMAC

Input : instance set Π, Algorithm $\mathcal{A}$ with configuration space $\mathbf{\Lambda}$, Initial configuration λ_0, performance metric c, Configuration budget b

Output: best incumbent configuration $\hat{\lambda}$

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return $\hat{\lambda}$

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  - How does this relate to cross-validation?
- Problem: How to set N? Problems of large N? Small N?
  - Problem of large N: evaluations are slow
  - Problem of small N: overfitting to a small set of instances
  - $\leadsto$ Tradeoff: Choose N of moderate size

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Question: Which N instances should we use?

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Answer: the same N instances, so that we compare apples with apples

(but: using the same instances can also yield overtuning)

If we sampled different instances for each configuration:

- Some configurations would randomly get easier instances
- Those configurations would look better than they really are

Comparisons on N instances

Question: For randomized algorithms, how should we set the seeds?

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In summary, for each run of Basic(N):
pick N (instance, seed) pairs and use them for evaluating each λ.
(Different Basic(N) runs can use different instances and seeds.)

The concept of overtuning

Very related to overfitting in machine learning

- Performance improves on the training set
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More pronounced for more heterogeneous benchmark sets

- But it even happens for very homogeneous sets
- Indeed, one can even overfit on a single instance, to the seeds used for training

Overtuning Visualized

- Example: minimizing SLS solver runlengths for a single SAT instance
- Training cost, e.g., with N=100:
  average runlengths across 100 runs with different seeds
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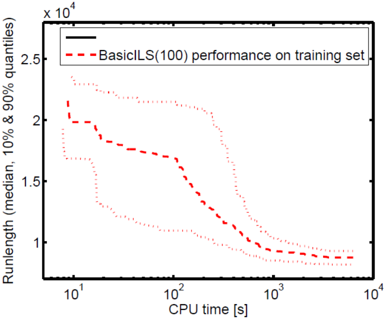

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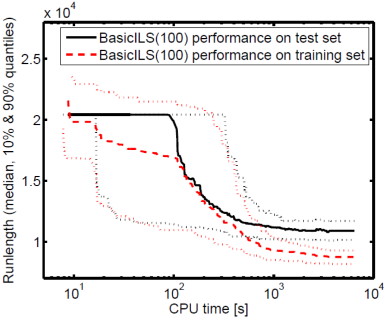

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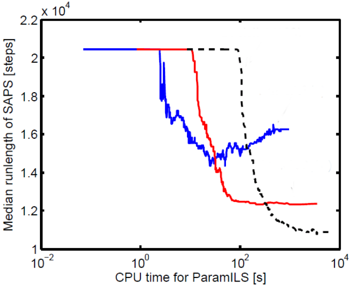

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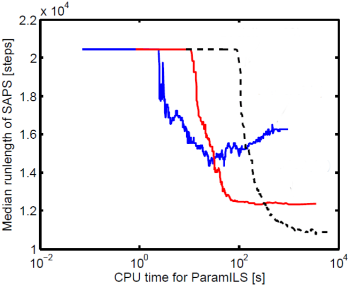

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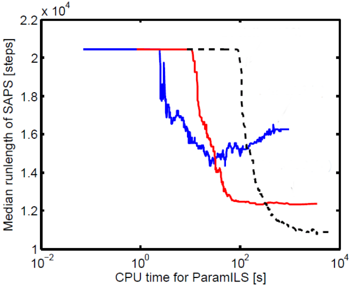

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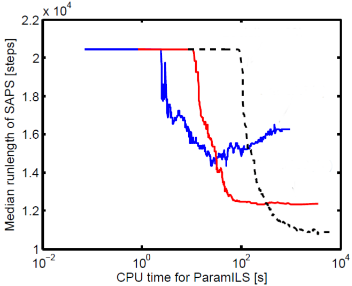

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Correct Answer: 1

Aggressive Racing (inspired by FocusedILS)

Intuition: get the best of both worlds

- Perform more runs for good configurations
  - to avoid overtuning
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In the beginning: $N(\lambda) = 0$ for every configuration λ

Aggressive Racing

Definition: domination

λ_1 dominates λ_2 if

- $N(\lambda_1) \geq N(\lambda_2)$ and
- $\hat{c}_{N(\lambda_2)}(\lambda_1) \leq \hat{c}_{N(\lambda_2)}(\lambda_2)$.

I.e.: we have at least as many runs for λ_1 and its cost is at least as low.

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- Over time: perform extra runs of λ^* to gain more confidence in it

Toy Example

- Let λ^* be the incumbent (evaluated on π_1, π_2, π_3)
- We'll look at challengers λ' and λ''

	π_1	π_2	π_3
λ^*	3	2	10

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λ''	3		

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λ''	3	1	

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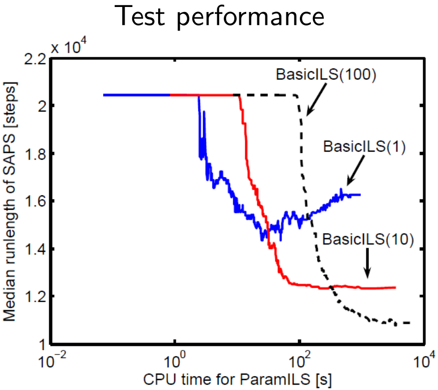
λ''	3	1	5

- new incumbent: $\lambda^* \leftarrow \lambda''$
- Perform an additional run for new λ^* to increase confidence over time

Racing achieves the best of both worlds

Aggressive racing (aka FocusedILS): Fast progress and no overtuning



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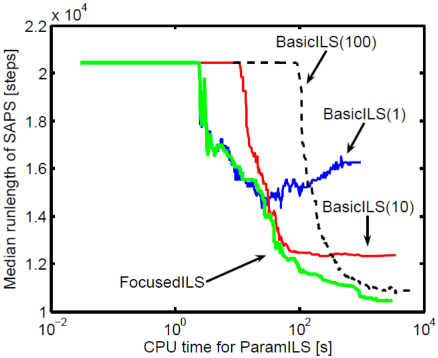
Test performance



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  - Terminate evaluation of λ' once guaranteed to be worse than λ^*

$\leadsto$ To compare against λ^* based on N runs,
we can terminate evaluation of λ' after time $\sum_{i=1}^{N} c(\lambda^*, \pi_i)$

Toy-Example: Adaptive capping

runtime cutoff $\kappa = 300$, comparison based on 2 instances (using $\hat{c}_3$)

	π_1	π_2
λ^*	4	2

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Without adaptive capping		
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Toy-Example: Adaptive capping

runtime cutoff $\kappa = 300$, comparison based on 2 instances (using $\hat{c}_3$)

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Note: To combine adaptive capping with BO, we need to impute the censored observations caused by adaptive capping.

SMAC: Overview

Algorithm 6: SMAC

Input : instance set Π, Algorithm $\mathcal{A}$ with configuration space $\mathbf{\Lambda}$, Initial configuration λ_0, performance metric c, Configuration budget b

Output: best incumbent configuration $\hat{\lambda}$

run history H $\leftarrow$ initial design based on λ_0; `// H =` $(\lambda, \pi, c(\pi, \lambda))_i$

while b *remains* **do**

- $\hat{f} \leftarrow$ train empirical performance model based on run history H;
- $\mathbf{\Lambda}_{challengers} \leftarrow$ select configurations based on $\hat{f}$; `// BO with EI`
- $\hat{\lambda}$, H $\leftarrow$ intensify($\mathbf{\Lambda}_{challengers}$, $\hat{\lambda}$); `// racing and capping`

return $\hat{\lambda}$

Lecture Overview

Dynamic Heuristics

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- What examples for dynamic heuristics can you think of?
- other examples: restart probability of search, mutation rate of evolutionary algorithms, . . .

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- Still not guaranteed that optimal setting of learning rate schedules will lead to optimal learning rate behavior
  - Learning rate schedules are only heuristics

Algorithm Control [Biedenkapp et al. 2019]

- Goal: control a (set of) hyperparameter(s) during the run
- Problem can be defined as an MDP $\mathcal{M} := (\mathcal{S}, \mathcal{A}, \mathcal{T}, \mathcal{R})$

State Space $\mathcal{S}$ At each time step t, internal state s_t of the target algorihtm being controlled.

Action space $\mathcal{A}$ Given a state s_t, the controller has to decide how to change the value $v \in \mathcal{A}_h$ of a hyperparameter h.

Transition Function $\mathcal{T}$ dynamics of the algorithm at hand transitioning from s_t to s_{t+1} by applying action a_t with probability $t(s_t, a_t, s_{t+1})$

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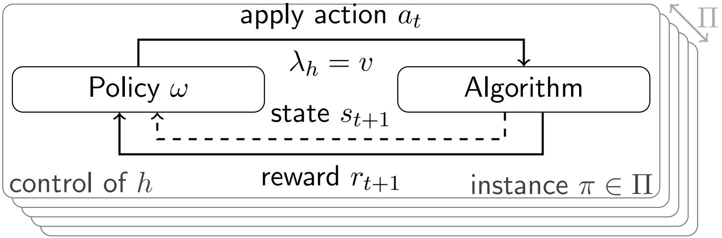
$$\omega^*(s) \in \arg\max_{a \in \mathcal{A}} \mathcal{R}(s, a) + \mathcal{Q}_{\omega^*}(s, a)$$

$$\mathcal{Q}_\omega(s, a) = \mathbb{E}_\omega \left[\sum_{k=0}^{\infty} \gamma^k r_{t+k+1} | s_t = s, a_t = a \right]$$

Algorithm Control across Instances [Biedenkapp et al. 2019]



Following the same arguments as for algorithm configuration, we want to learn a robust policy across instances $\pi \in \Pi$

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  $\rightsquigarrow$ more robust policies which generalize better to new instances
- heterogeneous instances
  - instances have different characteristics s.t. the policy has to be adapted to the instance at hand

  $\rightsquigarrow$ we might have to characterize the instances by using instance features (aka meta features)

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- Idea II (DNN): If we have randomized algorithms and we are interested in the algorithm's performance distribution, DNNs perform better [Eggensperger et al. '18]

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$\rightsquigarrow$ CAVE for analyzing AutoML experiments:
`https://github.com/automl/CAVE`

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- Benchmark III (AClib) Benchmarks and cheap-to-run surrogate benchmarks for algorithm configuration

Learning Goals

After this lecture, you are able to . . .

- define the algorithm configuration problem
- discuss differences between HPO and algorithm configuration
- explain the components of SMAC to combine Bayesian Optimization across instances
- define and give examples for the algorithm control problem
- list some further topics related AutoML and algorithm configuration

Literature [These are links]

- SMAC [Sequential Model-Based Optimization for General Algorithm Configuration]
- [Pitfalls and Best Practices in Algorithm Configuration]
- [Towards White-box Benchmarks for Algorithm Control]
- [CAVE: Configuration Assessment, Visualization and Evaluation]