Algorithm Configuration
Challenges, Methods and Perspectives

Marius Lindauer       André Biedenkapp
What can you expect?

**Content**  Overview over well-established and new research directions

**Structure**  Combination of research insights and practical recommendations

**Hands-On**  Some simple coding examples for algorithm configuration s.t. you can directly start to play with it

**Outlook**  to new research directions and open challenges
Algorithms have Parameters!

**Evolutionary Algorithms** population size, selection strategies, mutation operators, recombination operators, step size, probabilities, ...

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But wait! (I)

🤔 But *my* algorithm has no parameters!
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- Correct: There are some algorithms that do not have parameters
- However: Algorithm parameters are simply not exposed to the user in some cases.
- Programming by Optimization could be a paradigm to address these hidden parameters [Hoos 2012]
But wait! (II)

🤔 Can’t I simply use its default settings?
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⇝ Sure! Let’s use automatic algorithm configuration!
Outline

1. What is Algorithm Configuration?
2. How can we solve AC?
3. What to watch out for?
4. Is Solving AC hard?
5. Can we learn how to solve AC?
6. Top-Down or Bottom-Up Censoring?
7. Evolving from Static to Dynamic
8. What’s next?
Algorithm Configuration Visualized

Offline tuning phase: Tune parameters on some training instances

Online application phase: Apply the found configuration to new instances

User Input

Configurator

Call with different configurations

Returns solution cost

Optimized Configuration

Algorithm

“Solves”

Training Instances

Evaluation

New Instances
Algorithm Configuration Visualized

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Algorithm Configuration – in More Detail

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Algorithm Configuration – in More Detail

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

Return Cost

Returns Best Configuration $\hat{\lambda}$

Select $\lambda \in \Lambda$ and $i \in \mathcal{I}$

Run $\mathcal{A}(\lambda)$ on $i$ to measure $c(\lambda, i)$

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

Instances $\mathcal{I}$

Configuration Task
Challenges of Algorithm Configuration

- Structured high-dimensional parameter space
  - categorical vs. continuous parameters
  - conditionals between parameters
  - between 5 and $>300$ parameters
  - low effective dimensionality

Stochastic optimization

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

Generalization across instances

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

$\Rightarrow$ combination of algorithm configuration and selection

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

[Eggensperger et al. 2019]
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Let’s configure some algorithms! (I)

Use this [Google CoLab link](https://colab.research.google.com) to configure some example algorithms.
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The AC Problem Again

Algorithm \( \mathcal{A} \) and its Configuration Space \( \Lambda \)

Select \( \lambda \in \Lambda \) and \( i \in \mathcal{I} \)

Run \( \mathcal{A}(\lambda) \) on \( i \) to measure \( c(\lambda, i) \)

Returns Best Configuration \( \hat{\lambda} \)

Instances \( \mathcal{I} \)

Return Cost

Configuration Task
The Two Main Components

Instances $\mathcal{I}$

Select $\lambda_{\text{chall}} \in \Lambda$

Return Incumbent $\lambda_{\text{inc}}$

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

Race $\lambda_{\text{chall}}$ against $\lambda_{\text{inc}}$ on $\mathcal{I}$

Returns Best Configuration $\hat{\lambda}$
Sampling of Challengers: Iterated Local Search

[Hutter et al. 2007]
Sampling of Challengers: Bayesian Optimization

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---

**Require:** Search space $\Lambda$, cost function $c$, acquisition function $u$, maximal number of function evaluations $T$

**Result:** Best configuration $\hat{\lambda}$ (according to $D$ or $\hat{c}$)

1. Initialize data $D^{(0)}$ with initial observations
2. **for** $t = 1$ **to** $T$ **do**
   3. Fit predictive model $\hat{c}^{(t)}$ on $D^{(t-1)}$
   4. Select next query point: $\lambda_t \in \arg\max_{\lambda \in \Lambda} u(\lambda; D^{(t-1)}, \hat{c}^{(t)})$
   5. Query $c(\lambda)$;
   6. Update data: $D^{(t)} \leftarrow D^{(t-1)} \cup \{(\lambda, c(\lambda))\}$

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Sampling of Challengers: Est. of Distributions

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Sampling of Challengers: Golden Search

[Pushak and Hoos. 2020]

Assumes:
- uni-modal & convex search space
- independent parameters

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Lindauer & Biedenkapp

AC: Challenges, Methods and Perspectives

Tutorial 2020 20
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Racing of Challengers: Main Idea

Observations

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Idea I: Discard poorly performing \( \lambda \)s early on
Idea II: Run promising \( \lambda \)s on many instances
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## Racing of Challengers: Main Idea

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Selection of Challengers: Aggressive Racing

[Hutter et al. 2009]

Race a challenger configuration $\lambda$ against incumbent configuration $\hat{\lambda}$:

$$\sum_{i \in I'} c(\lambda, i) > \sum_{i \in I'} c(\hat{\lambda}, i)$$

where $I'$ are the instances $\lambda$ was evaluated on

Update Incumbent $\hat{\lambda} \rightarrow \lambda$ if

(i) $\lambda$ was evaluated on the same instances as $\hat{\lambda}$ (i.e. same evidence level)

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Selection of Challengers: Statistical testing

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Objective: Decide from a set of configurations $\hat{\Lambda}$ which one(s) is the best

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3. Continue with 1. if budget remains and $|\hat{\Lambda}| > 1$
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Pitfalls & Best Practices

The goals of automated algorithm configuration include:

1. reducing the expertise required to use an algorithm
2. less human-time
3. tuning algorithms to the task at hand
4. faster development of algorithms
5. facilitating systematic and reproducible research

BUT:
1. algorithm configuration can lead to over-tuning
2. using algorithm configuration requires (at least some) expertise in algorithm configuration
3. if done wrong, waste of time and compute resources
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9 Steps to your well-performing algorithm:

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9. Validate the eventually returned configuration on your test instances
Pitfall 1: Trust your algorithm

We have encountered algorithms that

- ignored resource limitations
- returned wrong solutions
- even returned negative runtimes

Best Practice 1: Never trust your algorithm

Explicitly check and use external software to:

1. ensure resource limitations
2. terminate your algorithm
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\[ \Rightarrow \] It’s surprisingly easy to substantially slow down a shared file system

Best Practice 2: Don’t use the Shared File System

To lower the burden the file system on a HPC cluster:
- design well which files are required and which are not
- use a local (SSD) disc
Pitfall 3: Over-tuning

It’s easy to over-tune to different aspects, including:

- training instances
- random seeds
- machine type

Best Practice 3: Check for Over-Tuning

Check for over-tuning by validating your final configuration on:

- many random seeds
- a large set of unused test instances
- different hardware
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More Pitfalls and Best Practices

... can be found in [Eggensperger et al. 2019]
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Worst Case

In the worst case, AC problems are very hard:

1. very hard instances with long evaluation time
2. interactions between all parameters
3. multi-modal with many local optima
4. heterogeneous instance sets
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⇝ However, does this actually apply in practice?
Low Effective Dimensionality

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Low Effective Dimensionality

- Algorithms have often between tenths and hundreds of parameters.
- Often only less than 10 matter (⇒ low effective dimensionality)
- Importance of parameter changes depending on instance set
  [Bergstra and Bengio. 2012, Biedenkapp et al. 2018]
Intuition: parameters are either set to too high or too low

We can analyse it for example by using fANOVA

[Hutter at el. 2014, Biedenkapp et al. 2018]
Observations:

- On a single instances, the landscape might not be uni-modal, convex or smooth.
- On average across many instances, the landscapes are often uni-modal, convex and smooth (at least on solvers for discrete combinatorial problems).
Algorithm configurators...

- use racing to not evaluate each configuration on all instances
Homogeneity vs. Heterogeneity (I) [Schneider and Hoos. 2012]

Algorithm configurators...

- use racing to not evaluate each configuration on all instances
- misleading on subsets of instances if they are heterogeneous overall
Algorithm configurators...  
- use racing to not evaluate each configuration on all instances  
- misleading on subsets of instances if they are heterogeneous overall  
→ returned configurations often perform worse than default configurations in the validation phase
Homogeneity vs. Heterogeneity (II)

[Schneider and Hoos. 2012]

**Rule of Thumb**

- An instance set is homogeneous if all instances encode the same task (or problem)
- An homogeneous instance can have instances of different hardness
Homogeneity vs. Heterogeneity (II)

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- An instance set is homogeneous if all instances encode the same task (or problem)
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← smooth transition $\sim$ homogeneous
← check board pattern $\sim$ heterogeneous
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Rule of Thumb

- An instance set is homogeneous if all instances encode the same task (or problem)
- An homogeneous instance can have instances of different hardness

smooth transition \(\leadsto\) homogeneous

check board pattern \(\leadsto\) heterogeneous

\(\leadsto\) Rule of thumb does not always apply!
Per-Instance Algorithm Configuration: Hydra

[Xu et al. 2010; Xu et al. 2011]

Idea: Find a configuration for each homogeneous subset of instances
Per-Instance Algorithm Configuration: Hydra

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**Idea:** Find a configuration for each homogeneous subset of instances
Per-Instance Algorithm Configuration: Hydra

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Idea: Find a configuration for each homogeneous subset of instances

```
Instances \( \mathcal{I} \)

Select \( \lambda \in \Lambda \) and \( i \in \mathcal{I} \)

Algorithm \( \mathcal{A} \) and its Configuration Space \( \Lambda \)

Assess \( \mathcal{A}(\lambda) \) on \( i \)

Return \( \min \{ c(\lambda), c(\mathcal{P}) \} \)

\( \mathcal{P} = \{ \lambda_1 \} \)
```
Per-Instance Algorithm Configuration: Hydra

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**Idea:** Find a configuration for each homogeneous subset of instances

\[
\begin{array}{c}
\text{Instances } \mathcal{I} \\
\downarrow \\
\text{Select } \lambda \in \Lambda \text{ and } i \in \mathcal{I} \\
\downarrow \\
\text{Assess } \mathcal{A}(\lambda||\lambda_1) \text{ on } i \\
\downarrow \\
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\end{array}
\]

\[\mathcal{P} = \{\lambda_1\}\]
Per-Instance Algorithm Configuration: Hydra

[Xu et al. 2010; Xu et al. 2011]

**Idea:** Find a configuration for each homogeneous subset of instances

- Select $\lambda \in \Lambda$ and $i \in \mathcal{I}$
- Assess $A(\lambda||\lambda_1)$ on $i$
- Return $\min\{c(\lambda), c(P)\}$
- $P = \{\lambda_1, \lambda_2\}$

Algorithm $A$ and its Configuration Space $\Lambda$
Per-Instance Algorithm Configuration: Hydra

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- **Instances** $\mathcal{I}$
- **Algorithm** $\mathcal{A}$ and its **Configuration Space** $\Lambda$
- **Select** $\lambda \in \Lambda$ and $i \in \mathcal{I}$
- **Assess** $\mathcal{A}(\lambda||\lambda_1||\lambda_2)$ on $i$
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**Similar ideas:**
- **ISAC:** 1. Cluster instances; 2. configure on each instance cluster
  [Kadioglu et al. 2010, Ansótegui et al. 2016]
- **Combination of iterative configuration and clustering** [Liu et al. 2019]
Outline

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Solving AC more than once?

Assumption: We tune the parameters of the same algorithms again and again on different instance sets.
Solving AC more than once?

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Solving AC more than once?

**Assumption:** We tune the parameters of the same algorithms again and again on different instance sets.

\[ \Rightarrow \] Learn on the first \( k \) instance sets, how to optimize on the \( k + 1 \) instance set. (Common idea in the optimization community.)
Idea 1: Try the best ones [Lindauer and Hutter. 2018]

Idea: Take the best configurations of previous runs and try them as initial design on new instances.
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**Problem:** If we have too many previous AC runs, the initial design will be too expensive.
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Problem: If we have too many previous AC runs, the initial design will be too expensive.

Idea: Select complementary configurations (Λ') across all previous instance sets (∪_j I_j):

\[
\sum_{i \in \bigcup_j I_j} \min_{\lambda \in \Lambda'} c(\lambda, i)
\]
Idea 2: Combine Surrogate Models

[Lindauer and Hutter. 2018]

Idea: Weighted combination of already trained surrogate models.
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[Lindauer and Hutter. 2018]

**Idea:** Weighted combination of already trained surrogate models.

\[
\hat{c}(\lambda,i) = w_0 + w_c \cdot \hat{c}_c(\lambda,i) + \sum_{j} w_j \cdot \hat{c}_j(\lambda,i)
\]

**Fit linear combination wrt \(w\) on hold-out set of the current obs.**
Idea 2: Combine Surrogate Models

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\leadsto \text{Fit linear combination wrt } \mathbf{w} \text{ on hold-out set of the current obs.}
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Insights from Warmstarting [Lindauer and Hutter. 2018]

1. If landscape changed too much, AC should be able to recover.
   ▶ both methods can do that
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2. Weights of combined surrogate models, prefer previous surrogates first, and later on the surrogate fitted on the current data.
If landscape changed too much, AC should be able to recover.

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Combining both ideas lead to the best speedups.
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2. Weights of combined surrogate models, prefer previous surrogates first, and later on the surrogate fitted on the current data.

3. Combining both ideas lead to the best speedups.

4. We sped up SMAC by a factor of 4.3 on average and up to a factor of 165.
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Assumption: we would like to minimize runtime of algorithms

\[ \sim \text{overall invested time: 450 sec} \]
Top-Down Capping [Hutter et al. 2009]

- Assumption: we would like to minimize runtime of algorithms

\[ \approx \text{overall invested time: 275 sec (instead of 450 sec)} \]
Bottom-Up Procrastination

[Kleinberg et al. 2017, Kleinberg et al. 2019]

- Assumption: we would like to minimize runtime of algorithms

⇝ overall invested time: 225 sec (instead of 450 and 275 sec)
- Generalize this idea to evaluate configurations on pairs of random seeds and instances
- performance guarantees of AC methods
Bottom-Up Procrastination

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Algorithm Configuration Recap

Selection and Configuration:

Instances $\mathcal{I}$

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

Select $\lambda \in \Lambda$ and $i \in \mathcal{I}$

Run $\mathcal{A}(\lambda)$ on $i$ to measure $c(\lambda, i)$

Returns Best Configuration $\hat{\lambda}$

Important observation: Many algorithms are iterative by design $\Rightarrow$ fixed configurations are not optimal for each iteration
Algorithm Configuration Recap

- Important observation: Many algorithms are iterative by design
  - fixed configurations are not optimal for each iteration

- Configuration Task
  - Instances $\mathcal{I}$
  - Algorithm $\mathcal{A}$ and its Configuration Space $\Lambda$
  - Select $\lambda \in \Lambda$ and $i \in \mathcal{I}$
  - Run $\mathcal{A}(\lambda)$ on $i$ to measure $c(\lambda, i)$
  - Returns Best Configuration $\hat{\lambda}$
  - Return Cost

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Algorithms have Dynamic Parameters!

Evolutionary Algorithms population size, selection strategies, mutation operators, recombination operators, step size, probabilities, ...

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**Evolutionary Algorithms** population size, selection strategies, mutation operators, recombination operators, step size, probabilities, ...

**Satisfiability Solving** Search strategies (local vs. tree-based), variable selection heuristic, restart probability, deletion heuristic, ...

**Machine Learning** model class (linear, non-linear, tree, ...), model complexity, regularization, preprocessing, data augmentation, ...

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\(^1\)Gregor Papa: "Dynamic Parameter Changing During the Run to Speed Up Evolutionary Algorithms"
What Can We Do? (I)

🤔 Manually design heuristics to adapt the parameter online.
  ▶ Requires substantial expert knowledge
  ⇝ specialized heuristics for specific domains
  ▶ Very time-consuming
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🤔 Manually design heuristics to adapt the parameter online.
  ► Requires substantial expert knowledge
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🤔 Use Algorithm Configuration/Selection to choose a heuristic.
  ► Limited approach
  ⇻ does not make use of information during the algorithms execution
What Can We Do? (II)

🤔 Learn to configure from scratch

- Requires access to the algorithms internal statistics
- Data-driven approach
What Can We Do? (II)

🤔 Learn to configure from scratch
  - Requires access to the algorithms internal statistics
  - Data-driven approach

🤔 Warmstart from expert knowledge
  - Potentially more sample efficient
  - Which expert should we learn from?

Lindauer & Biedenkapp
AC: Challenges, Methods and Perspectives
Tutorial 2020
Dynamic Algorithm Configuration

[Biedenkapp et al. 2020]
Dynamic Algorithm Configuration

[Biedenkapp et al. 2020]

Dynamic Config. $\pi$

apply action $a_2$

(set parameter $h$)

Algorithm $A$

state $s_3$

reward $r_3$

instance 0

$h = a_2$
Dynamic Algorithm Configuration

[Biedenkapp et al. 2020]

apply action $a_4$

(set parameter $h$)

Dynamic Config. $\pi$

state $s_3$

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Algorithm $A$

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Dynamic Algorithm Configuration

[Dynamic Configuration \( \pi \)]

(set parameter \( h \))

apply action \( a_2 \)

Dynamic Config. \( \pi \)

Algorithm \( A \)

state \( s_3 \)

reward \( r_3 \)

instance 1

\( h = a_2 \)
Dynamic Algorithm Configuration

[Biedenkapp et al. 2020]
Dynamic Algorithm Configuration

[Biedenkapp et al. 2020]
Dynamic Algorithm Configuration

[Diedenkapp et al. 2020]

Dynamic Config. $\pi$

apply action $a_2$

(set parameter $h$)

Algorithm $A$

state $s_3$

reward $r_3$

instance 2

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Dynamic Algorithm Configuration

[Biedenkapp et al. 2020]

How can DAC look inside the algorithm? I.e. what is a state?
Looking Inside Algorithms: Desiderata

1. Cheap to compute
2. Quantify the progress of the algorithm
3. Available at each decision point
Looking Inside Algorithms: Desiderata

1. Cheap to compute
2. Quantify the progress of the algorithm
3. Available at each decision point

⇝ Make use of internal statistics
Looking Inside Algorithms

- **EAs**
  - population fitness [Sharma et al. 2019, Shala et al. 2020]
  - stdev population fitness [Sharma et al. 2019]
  - cumulative evolution path length [Shala et al. 2020]
  - ...

- **AI Planning** [Speck et al. 2020]
  - average heuristic value
  - minimal heuristic value
  - #possible next planning states
  - ...

- **NN Optimization** [Daniel et al. 2016]
  - predictive change in function value
  - disagreement of function values
  - uncertainty
  - ...

Looking Inside Algorithms

- EAs $\leadsto$ better generalization
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Looking Inside Algorithms

- **EAs** $\leadsto$ better generalization
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\[^2\) presented at PPSN in poster session 2\]
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Next I: Neural Networks?

🤔 "everyone" uses neural networks these days.
Models in algorithm configuration are still random forests?
"everyone" uses neural networks these days. Models in algorithm configuration are still random forests?

**Towards DNNs for AC (I): Prediction of Runtime Distributions**

[Eggersperger et al. 2018]

- **Algorithm** $\mathcal{A}$
- **Training instances** $i \in \mathcal{I}_{\text{train}}$
- **Run** $\mathcal{A}$ $k$ times on each $i \in \mathcal{I}_{\text{train}}$
- **Compute instance features** $\mathbf{x}_{\text{meta}}(i)$ for each $i \in \mathcal{I}_{\text{train}}$
- **Data:** $\left\langle \mathbf{x}_{\text{meta}}(i), t(i) \right\rangle_{1 \ldots k}$
- **Estimate RTD family** $\mathcal{D}$
- **Fit RTD model** $\hat{m} : \mathbf{x}_{\text{meta}}(i) \mapsto \theta$
- **New instance** $i_{n+1}$
- **Compute features** $\mathbf{x}_{\text{meta}}(i_{n+1})$
- **Use** $\hat{m}$ **to predict** $\mathcal{D}$'s parameters $\theta$ **for** $i_{n+1}$
Next II: Neural Networks?

🤔 How to handle censored data (from capping of runs) in DNNs?
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🤔 How to handle censored data (from capping of runs) in DNNs?

Towards DNNs for AC (II): Handling of Censored Data

[Eggensperger et al. 2020]

\[- \log \mathcal{L} \left( (\hat{\mu}_i, \hat{\sigma}_i^2)_{i=1}^n \mid D \right) = - \sum_{i=1}^n \log \left( \phi(Z_i)^{1-I_i}(1 - \Phi(Z_i))^{I_i} \right)\]
Next II: Multi-Objective Optimization?

Can we consider more than one objective?

![Diagram showing memory consumption vs. runtime with dominated and non-dominated configurations marked.]
Next II: Multi-Objective Optimization?

Can we consider more than one objective?

Challenges:

1. How to sample promising (non-dominated) configurations?

2. How to efficiently determine that a configuration is really on the Pareto front across all instances?

[Blot et al. 2016]
Next III: What are interesting AC benchmarks?

🤔 I developed a new configurator, but on which benchmarks should I benchmark it?

AClib

[Hutter et al. 2014]

- 84 AC scenarios
- 18 target algorithms and their configuration spaces
- 45 instance sets
- 6 AI domains
- 6 configurators

⇝ To make development cheaper, you can benchmark on surrogate benchmarks

[Eggensperger et al. 2018]

⇝ Open which of these are interesting?

▶ not too easy, not too hard, diverse set, different characteristics, representative, . . .

https://bitbucket.org/mlindauer/aclib2/
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Take Home Message

1. Algorithm Configuration improves the performance of your algorithms
Take Home Message

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2. There are different state-of-the-art AC approaches
Take Home Message

1. **Algorithm Configuration improves the performance of your algorithms**
2. **There are different state-of-the-art AC approaches**
3. **Using algorithm configuration is nevertheless fairly easy these days**
Take Home Message

1. Algorithm Configuration improves the performance of your algorithms
2. There are different state-of-the-art AC approaches
3. Using algorithm configuration is nevertheless fairly easy these days
4. Many open questions for the research community to be answered
Thank you!