AutoML: Beyond AutoML

Structured Procastination

Bernd Bischl Frank Hutter Lars Kotthoff
Marius Lindauer Joaquin Vanschoren

Structured Procrastination [Kleinberg et al. 2017]

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- incumbent driven methods (such as aggressive racing with adaptive capping) provide no theoretical guarantees about runtime
- task: for a fix set of configuration, identify the one with the best average runtime
- instead of top-down capping, use bottom up capping
- start with a minimal cap-time and increase it step by step
- unsuccessful runs (with too small cap-time) are procrastinated to later

$\rightsquigarrow$ worst-case runtime guarantees

Structured Procrastination: Outline [Kleinberg et al. 2017]

Algorithm 1 Structured Procrastination

Input : finite (small) set of configurations $\mathbf{\Lambda}$, minimal cap-time κ_0, sequence of instances $i^{(1)}, \dots, i^{(N)}$
Output : best incumbent configuration $\hat{\boldsymbol{\lambda}}$

for each $\boldsymbol{\lambda} \in \mathbf{\Lambda}$ initialize a queue $Q_{\boldsymbol{\lambda}}$ with entries $(i^{(k)}, \kappa_0)$; `// small queue in the beginning`
initialize a look-up table $R(\boldsymbol{\lambda}, i) = 0$; `// optimistic runtime estimate`

Structured Procrastination: Outline [Kleinberg et al. 2017]

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while b *remains* **do**

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initialize a look-up table $R(\boldsymbol{\lambda}, i) = 0$; `// optimistic runtime estimate`
while b *remains* **do**
    determine the best $\hat{\boldsymbol{\lambda}}$ according to $R(\boldsymbol{\lambda}, \cdot)$;

Structured Procrastination: Outline [Kleinberg et al. 2017]

Algorithm 4 Structured Procrastination

Input : finite (small) set of configurations $\mathbf{\Lambda}$, minimal cap-time κ_0, sequence of instances $i^{(1)}, \dots, i^{(N)}$
Output : best incumbent configuration $\hat{\boldsymbol{\lambda}}$

```
for each λ ∈ Λ initialize a queue Q_λ with entries (i^(k), κ_0);      // small queue in the beginning
initialize a look-up table R(λ, i) = 0;                                  // optimistic runtime estimate
while b remains do
    determine the best λ̂ according to R(λ, ·);
    get first element (i^(k), κ) from Q_λ̂;
```

Structured Procrastination: Outline [Kleinberg et al. 2017]

Algorithm 5 Structured Procrastination

Input : finite (small) set of configurations $\mathbf{\Lambda}$, minimal cap-time κ_0, sequence of instances $i^{(1)}, \dots, i^{(N)}$

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

for each $\boldsymbol{\lambda} \in \mathbf{\Lambda}$ initialize a queue $Q_{\boldsymbol{\lambda}}$ with entries $(i^{(k)}, \kappa_0)$; `// small queue in the beginning`

initialize a look-up table $R(\boldsymbol{\lambda}, i) = 0$; `// optimistic runtime estimate`

while b *remains* **do**

  determine the best $\hat{\boldsymbol{\lambda}}$ according to $R(\boldsymbol{\lambda}, \cdot)$;

  get first element $(i^{(k)}, \kappa)$ from $Q_{\hat{\boldsymbol{\lambda}}}$;

  Run $\hat{\boldsymbol{\lambda}}$ on $i^{(k)}$ capped at κ;

  if *terminates* **then**

    $R(\hat{\boldsymbol{\lambda}}, i^{(k)})$:= t;

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  else
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     Insert $(i^{(k)}, 2 \cdot \kappa)$ at the end of $Q_{\hat{\boldsymbol{\lambda}}}$;

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    Insert $(i^{(k)}, 2 \cdot \kappa)$ at the end of $Q_{\hat{\boldsymbol{\lambda}}}$;
  Replenish queue $Q_{\hat{\boldsymbol{\lambda}}}$ if too small;

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Input : finite (small) set of configurations $\mathbf{\Lambda}$, minimal cap-time κ_0, sequence of instances $i^{(1)}, \ldots, i^{(N)}$
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    $R(\hat{\boldsymbol{\lambda}}, i^{(k)})$:= t;
  else
    $R(\hat{\boldsymbol{\lambda}}, i^{(k)}) := \kappa$;
    Insert $(i^{(k)}, 2 \cdot \kappa)$ at the end of $Q_{\hat{\boldsymbol{\lambda}}}$;
  Replenish queue $Q_{\hat{\boldsymbol{\lambda}}}$ if too small;
return $\hat{\boldsymbol{\lambda}} := \arg\min_{\boldsymbol{\lambda} \in \mathbf{\Lambda}} \sum_{k=1}^{N} R(\boldsymbol{\lambda}, i^{(k)})$

Extensions

- We can derive theoretical optimality guarantees with structured procrastination (SP)

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- In practice, plain SP is rather slow and requires the setting of some hyperparameters
- Several extensions and similar ideas:
  - [Kleinberg et al. 2019]
  - [Weisz et al. 2018]
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AutoML: Beyond AutoML

Per-Instance Algorithm Configuration

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Homogeneous vs. Heterogeneous Instances

Assumption of AC: Homogeneous Instance Distribution

- Algorithm configuration tools assume that the instance distribution is homogeneous (see video on "Best Practices for AC")
- Important because
  - there is a well-performing configuration for all (or most) instances
  - the racing algorithm can make educated decisions on subsets

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Violated assumption of AC: Hetergeneous Instance Distribution

- The racing algorithm will make inconsistent (or even wrong) decisions
- There is no single well-performing configuration for all instances

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$\leadsto$ What should we do with heterogeneous instance distributions?

Why are systems for heterogeneous instance distributions important?

1. We cannot guarantee homogeneity in practice
    1. Instances might get larger and harder
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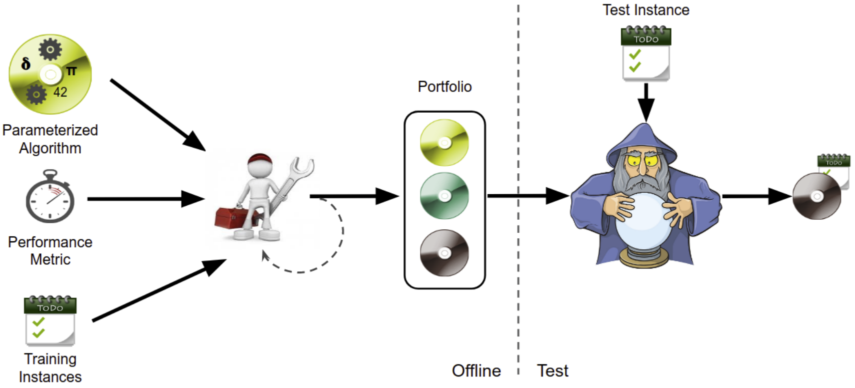
1. We cannot guarantee homogeneity in practice
   1. Instances might get larger and harder
   2. The underlying task or business case might change
2. We don't want to do algorithm configuration always from scratch
3. An adaptive configuration system would be the holy grail
   - $\rightsquigarrow$ hard to achieve

PIAC: Per-Instance Algorithm Configuration



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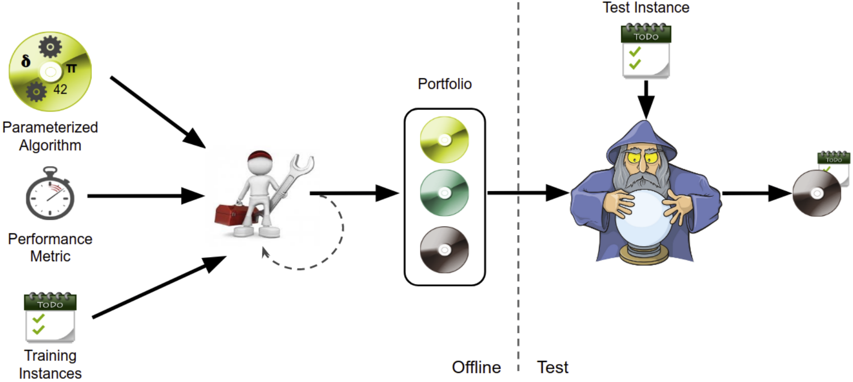

- You can use whichever kind of algorithm selection (wizard) you want
- Challenge: Building a portfolio
- Use case: Instances are heterogeneous

PIAC: Manual Expert Approach

Basic Assumption

Heterogeneous instance set can be divided into homogeneous subsets

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Heterogeneous instance set can be divided into homogeneous subsets

Manual Expert

- An expert knows the homogeneous subsets (e.g., origin of instances)
- Determine a well-performing configuration on each subset
  $\rightarrow$ portfolio of configurations
- Use Algorithm Selection to select a well-performing configuration on each instance

Instance-Specific Algorithm Configuration: ISAC [Kadioglu et al. 2010]

Idea

Training:

1. Cluster instances into homogeneous subsets
   (using g-means in the instance feature space)
2. Apply algorithm configuration (here GGA) on each instance set

Instance-Specific Algorithm Configuration: ISAC [Kadioglu et al. 2010]

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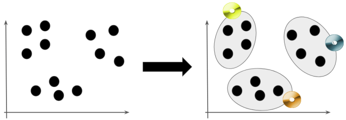
Test:

1. Determine the nearest cluster (k-NN with $k = 1$) in feature space
2. Apply optimized configuration of this cluster



Hydra [Xu et al. 2010]

Idea

- Iteratively add configurations to a portfolio $\mathbf{P}$, start with $\mathbf{P} = \emptyset$
- In each iteration, determine configuration that is complementary to $\mathbf{P}$

  $\rightsquigarrow$ Maximize marginal contribution to $\mathbf{P}$

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Marginal contribution of a configuration $\boldsymbol{\lambda}$ to a portfolio $\mathbf{P}$:

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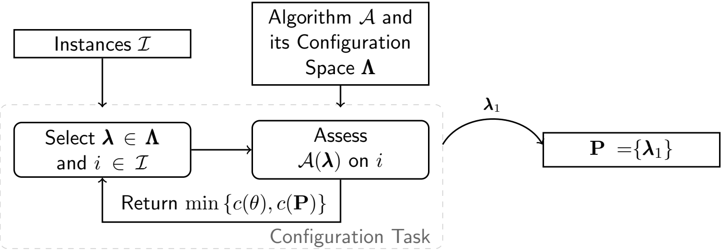

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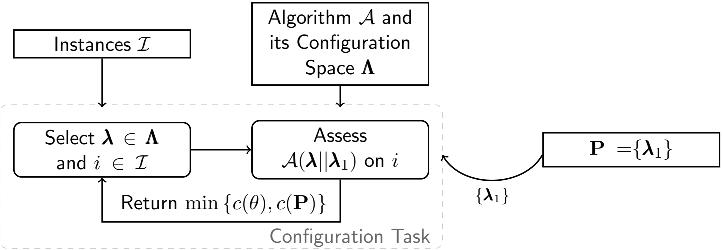

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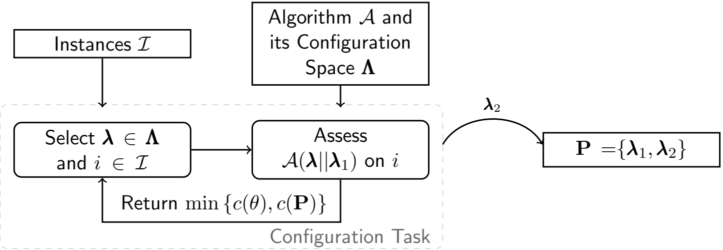

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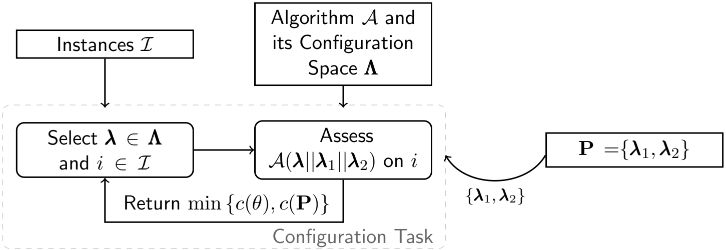
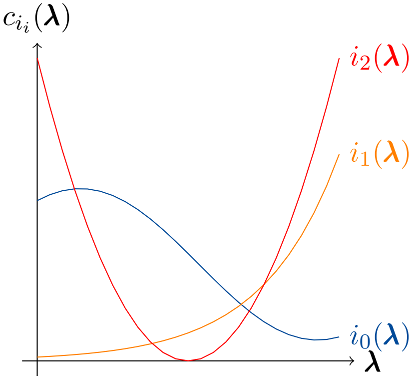


Heterogeneous example



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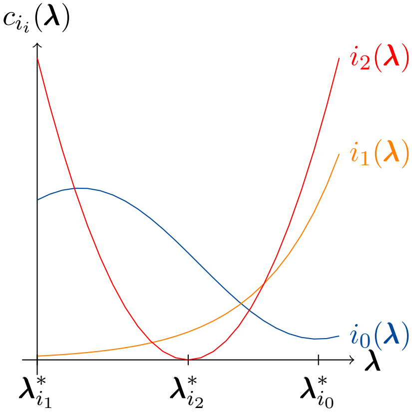

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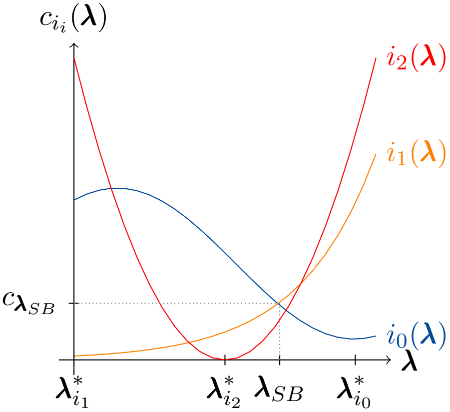

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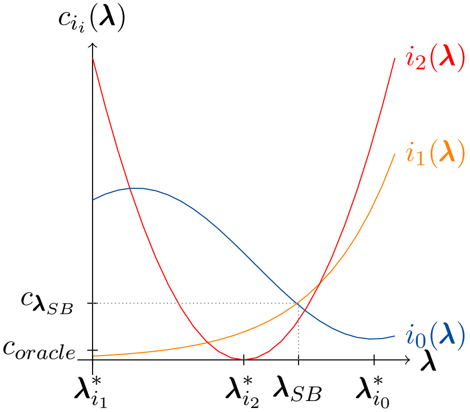
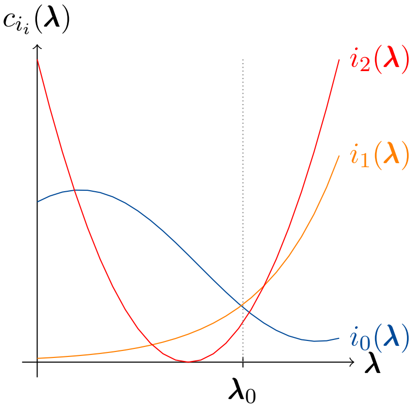


Hydra: Iteration 1



Search initial well performing configuration. Add $\boldsymbol{\lambda}_0$ to $\mathbf{P}$

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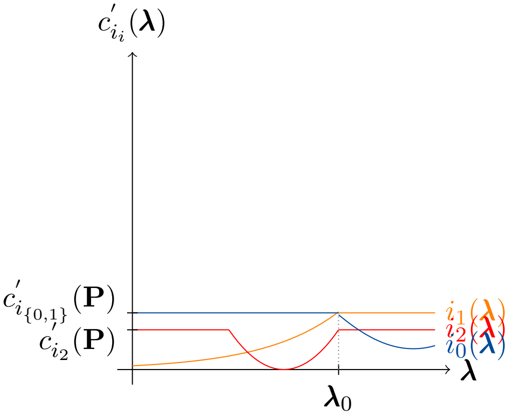
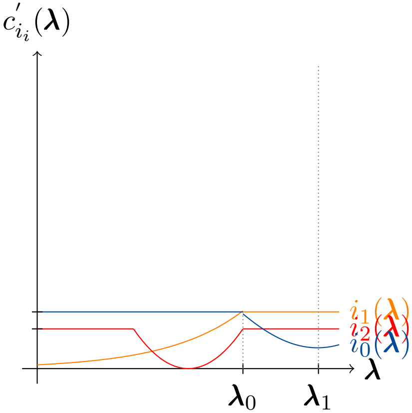


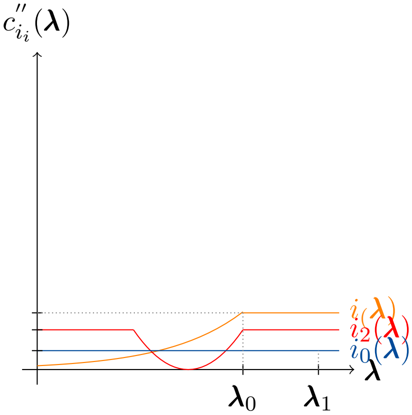
Update metric

Hydra: Iteration 2



Search well performing configuration complementary to $\mathbf{P}$.
Add $\boldsymbol{\lambda}_1$ to $\mathbf{P}$.

Hydra: Iteration 2



Update metric

Cedalion [Seipp et al. 2015]

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- Optimize a schedule of configurations with algorithm configuration

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- Iteratively add a configuration with a time slot t to a schedule $\mathcal{S} \oplus \langle \boldsymbol{\lambda}, t \rangle$

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- Iteratively add a configuration with a time slot t to a schedule $\mathcal{S} \oplus \langle \boldsymbol{\lambda}, t \rangle$
- In each iteration, only optimize on instances not solved so far
- The time slot is a further parameter in the configuration space

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- Iteratively add a configuration with a time slot t to a schedule $\mathcal{S} \oplus \langle \boldsymbol{\lambda}, t \rangle$
- In each iteration, only optimize on instances not solved so far
- The time slot is a further parameter in the configuration space
- Optimize marginal contribution per time spent:

$$\frac{c(\mathcal{S}) - c(\mathcal{S} \oplus \langle \boldsymbol{\lambda}, t \rangle)}{t}$$

Submodularity

Observation

- Performance metrics of Hydra and Cedalion are submodular
  - Family of functions
  - Adding an element to a set reduces the function value
  - Diminishing returns: decrease of the value reduction over time

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Definition (Submodularity of f)

For every $X, Y \subseteq Z$ with $X \subseteq Y$ and every $x \in Z - Y$ we have that
$f(X \cup \{x\}) - f(X) \geq f(Y \cup \{x\}) - f(Y)$

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Advantage

We can bound the error of the portfolio/schedule:
At most away from optimum by factor of 0.63 (see [Streeter and Golovin. 2008])

Dynamic Instance Grouping [Liu et al. 2018]

Idea

- Similar to ISAC: group instances into clusters
- Similar to Hydra: refine clusters and configurations over several iterations

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Main Idea

1. Group instances randomly into clusters
2. run AC on each cluster
3. Update clusters based on performance (estimates)
4. Go to 2. if budget is not empty
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1. Group instances randomly into clusters
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- increase the configuration budget in each iteration
  - first clusterings will have a poor quality $\rightarrow$ small configuration time
  - later clusterings will be better $\rightarrow$ more configuration time

AutoML: Beyond AutoML

Racing for Algorithm Configuration

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State-of-the-art Algorithm Configuration

SMAC: Sequential Model-based Algorithm Configuration [Hutter et al. 2011]

- Bayesian Optimization +
- aggressive racing +
- adaptive capping (for optimizing runtime)

SMAC: Overview [Hutter et al. 2011]

Algorithm 1 SMAC

Input : instance set $\mathcal{I}$, Algorithm $\mathcal{A}$ with configuration space $\mathbf{\Lambda}$, Initial configuration $\boldsymbol{\lambda}_0$, performance metric c, Configuration budget b

run history $\mathcal{D}_{\text{Hist}} \leftarrow$ initial design based on $\boldsymbol{\lambda}_0$; // $\mathcal{D}_{\texttt{Hist}} = (\boldsymbol{\lambda}, i, c(i, \boldsymbol{\lambda}))_i$

while b *remains* **do**

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Algorithm 2 SMAC

Input : instance set $\mathcal{I}$, Algorithm $\mathcal{A}$ with configuration space $\mathbf{\Lambda}$, Initial configuration $\boldsymbol{\lambda}_0$, performance metric c, Configuration budget b

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  $\hat{c} \leftarrow$ train empirical performance model based on run history $\mathcal{D}_{\text{Hist}}$;

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return $\hat{\boldsymbol{\lambda}}$

Comparisons on N instances [Hutter et al. 2009]

- Basic(N) uses a pretty basic comparison: $\mathit{better}_N(\boldsymbol{\lambda}', \boldsymbol{\lambda})$:
  - Compare $\boldsymbol{\lambda}'$ and $\boldsymbol{\lambda}$ based on N instances

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- Problem: How to set N? Problems of large N? Small N?

Comparisons on N instances [Hutter et al. 2009]

- Basic(N) uses a pretty basic comparison: *better*$_N(\boldsymbol{\lambda}', \boldsymbol{\lambda})$:
  - Compare $\boldsymbol{\lambda}'$ and $\boldsymbol{\lambda}$ based on N instances
  - 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

  $\rightsquigarrow$ Tradeoff: Choose N of moderate size

Comparisons on N instances [Hutter et al. 2009]

Question: Which N instances should we use?

1. N different instances for each configuration
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If we sampled different instances for each configuration:

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

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In summary, for each run of Basic(N):
pick N (instance, seed) pairs and use them for evaluating each $\boldsymbol{\lambda}$.
(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
- Performance does not improve on the test set, and may even degrade

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More pronounced for 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
- Test cost of $\hat{\boldsymbol{\lambda}}$ here based on 1000 new seeds

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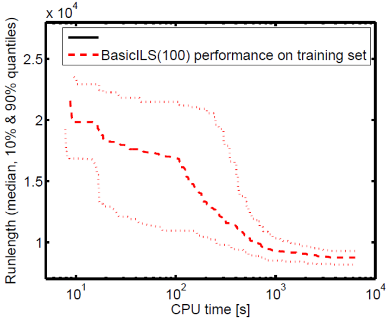

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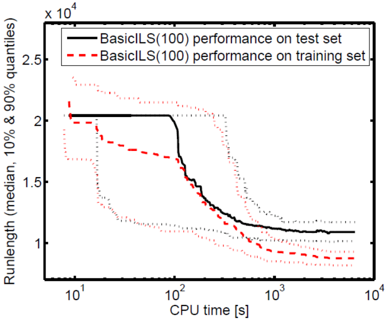

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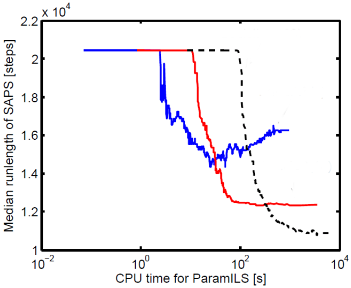

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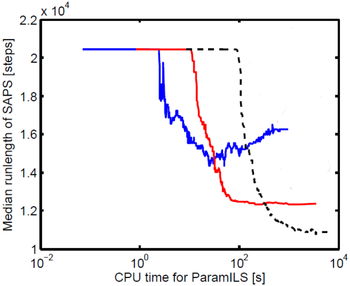

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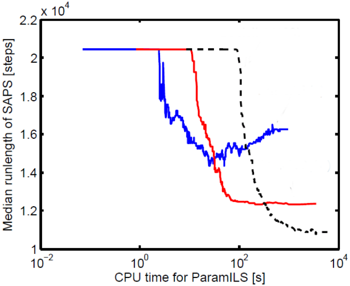

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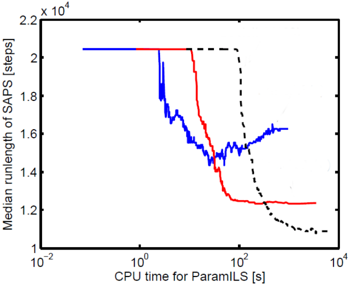

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Correct Answer: 1

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Intuition: get the best of both worlds

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  - to avoid overtuning
- Quickly reject poor configurations
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In the beginning: $N(\boldsymbol{\lambda}) = 0$ for every configuration $\boldsymbol{\lambda}$

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Definition: domination

$\boldsymbol{\lambda}^{(1)}$ dominates $\boldsymbol{\lambda}^{(2)}$ if

- $N(\boldsymbol{\lambda}^{(1)}) \geq N(\boldsymbol{\lambda}^{(2)})$ and
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I.e.: we have at least as many runs for $\boldsymbol{\lambda}^{(1)}$ and its cost is at least as low.

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- Over time: perform extra runs of $\hat{\boldsymbol{\lambda}}$ to gain more confidence in it

Toy Example

- Let $\hat{\boldsymbol{\lambda}}$ be the incumbent (evaluated on $i^{(1)}, i^{(2)}, i^{(3)}$)
- We'll look at challengers $\boldsymbol{\lambda}'$ and $\boldsymbol{\lambda}''$

	$i^{(1)}$	$i^{(2)}$	$i^{(3)}$
$\hat{\boldsymbol{\lambda}}$	3	2	10

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	$\rightarrow$ reject, since $\hat{c}_2(\boldsymbol{\lambda}') = 6 > \hat{c}_2(\hat{\boldsymbol{\lambda}}) = 2.5$		

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$\boldsymbol{\lambda}''$	3	1	

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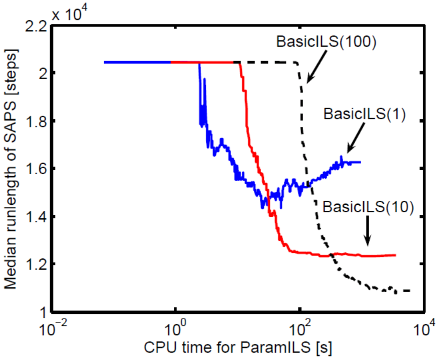
- new incumbent: $\hat{\boldsymbol{\lambda}} \leftarrow \boldsymbol{\lambda}''$
- Perform an additional run for new $\hat{\boldsymbol{\lambda}}$ to increase confidence over time

Racing achieves the best of both worlds

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

Test performance



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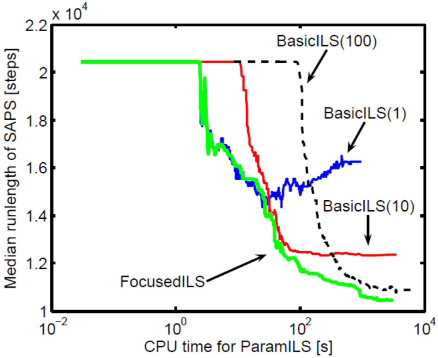

Overview of Racing

Input : candidate configurations $\boldsymbol{\Lambda}_{new}$, cutoff κ_{max}, previously evaluated runs $\mathcal{D}_{\mathsf{Hist}}$, budget T, incumbent $\hat{\boldsymbol{\lambda}}$

while $\boldsymbol{\Lambda}_{new}$ *not empty* **do**

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    - $\hat{\boldsymbol{\lambda}} \leftarrow \boldsymbol{\lambda}^{(t)}$;
- **if** *time spent exceeds* T *or* $\boldsymbol{\Lambda}_{new}$ *is empty* **then**
  - **return** $\hat{\boldsymbol{\lambda}}, \mathcal{D}_{\textit{Hist}}$

AutoML: Beyond AutoML

Best Practices for Algorithm Configuration

Bernd Bischl Frank Hutter Lars Kotthoff
Marius Lindauer Joaquin Vanschoren

Pitfalls & Best Practices

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BUT:

1. algorithm configuration can lead to over-tuning
2. using algorithm configuration requires (at least some) expertise in algorithm configuration

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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

Setting up AC

9 Steps to your well-performing algorithm:

1. Define your performance metric

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9. Validate the eventually returned configuration on your test instances

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We have encountered algorithms that

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Best Practice 1: Never trust your algorithm

Explicitly check and use external software to:

1. ensure resource limitations
2. terminate your algorithm
3. verify returned solutions
4. measure performance

Pitfall 2: File System

Algorithm configurators ...

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

To relieve the file system of 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 overtune to different aspects, incl.:

- training instances
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In practice, it can be hard to prevent over-tuning, e.g., by

- using larger instance sets
- tuning on the target hardware

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
- a different hardware

Pitfall 4: Heterogeneous Instance Sets

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Best Practice 4: Ensure Homogeneity

Algorithm configurators should only run on homogeneous instance sets.
Different degrees of homogeneity:

- Strong homogeneity: all instances agree on the ranking of configurations
- Weak homogeneity: all instances agree on the top-performing configurations

More Pitfalls and Best Practices

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

AutoML: Beyond AutoML

Overview: Algorithm Configuration

Bernd Bischl Frank Hutter Lars Kotthoff
Marius Lindauer Joaquin Vanschoren

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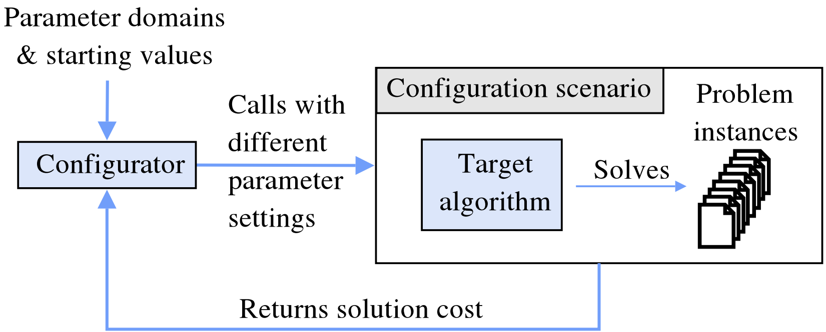
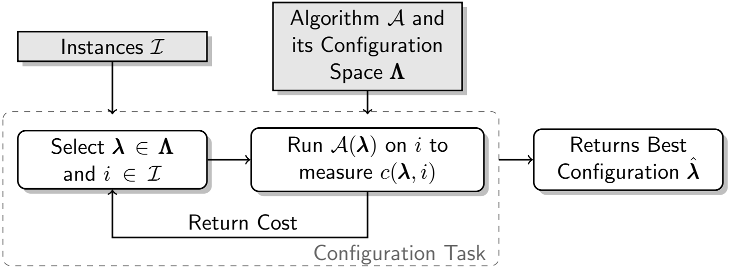
$\rightsquigarrow$ Algorithm configuration

Algorithm Configuration Visualized



Algorithm Configuration – in More Detail



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Given a parameterized algorithm $\mathcal{A}$ with possible (hyper-)parameter settings $\boldsymbol{\Lambda}$,

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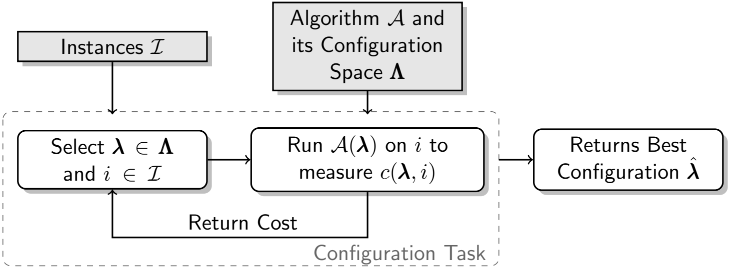

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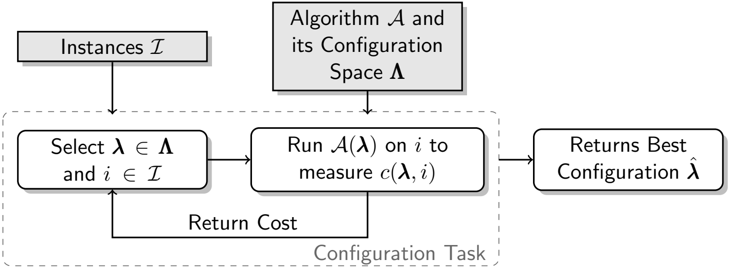

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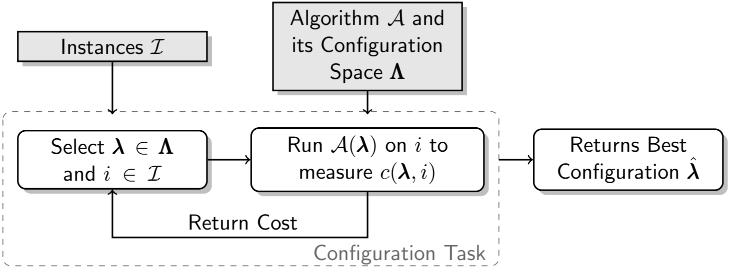

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Algorithm Configuration – Full Formal Definition

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

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

[Eggensperger et al. 2019]

AutoML: Beyond AutoML

Capping of Runtimes

Bernd Bischl Frank Hutter Lars Kotthoff
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Adaptive capping [Hutter et al. 2009]

- Assumptions
  - optimization of runtime
  - each configuration run has a time limit (e.g., 300 sec)

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$\leadsto$ To compare against $\hat{\boldsymbol{\lambda}}$ based on N runs,
we can terminate evaluation of $\boldsymbol{\lambda}'$ after time $\sum_{k=1}^{N} c(\hat{\boldsymbol{\lambda}}, i_k)$

Toy-Example: Adaptive capping

runtime cutoff $\kappa = 300$, comparison based on 2 instances

	i_1	i_2
$\hat{\boldsymbol{\lambda}}$	4	2

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$\rightarrow$ reject $\boldsymbol{\lambda}'$ (cost: 303)

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Note: To combine adaptive capping with BO, we need to impute the censored observations caused by adaptive capping. [Hutter et al. 2011]

Overview of Racing and Adaptive Capping

Input : candidate configurations $\mathbf{\Lambda}_{new}$, cutoff κ_{max}, previously evaluated runs $\mathcal{D}_{\text{Hist}}$, budget T, incumbent $\hat{\boldsymbol{\lambda}}$

while $\mathbf{\Lambda}_{new}$ *not empty* **do**

- $\boldsymbol{\lambda}^{(t)} \leftarrow$ getNext($\mathbf{\Lambda}_{new}$);
- [... add new run for incumbent ...];
- **while** *true* **do**
  - $\mathcal{I}^+, \mathbf{s}^+ \leftarrow$getAlreadyEvaluatedOn($\hat{\boldsymbol{\lambda}}, \mathcal{D}_{\text{Hist}}$);
  - $\mathcal{I}^{(t)}, \mathbf{s}^{(t)} \leftarrow$getAlreadyEvaluatedOn($\boldsymbol{\lambda}^{(t)}, \mathcal{D}_{\text{Hist}}$);
  - $i^{(t)}, s^{(t)} \leftarrow$ drawn uniformly at random from $\mathcal{I}_+ \setminus \mathcal{I}^{(t)}$ and $\mathbf{s}^+ \setminus \mathbf{s}^{(\mathbf{t})}$;
  - $\kappa^{(i)} \leftarrow$ AdaptCutoff($\kappa_{max}, \langle(\boldsymbol{\lambda}^{(j)}, c^{(j)})\rangle_{\boldsymbol{\lambda}^{(j)}=\boldsymbol{\lambda}^+}$) $\cdot\, \xi$;
  - $c_i \leftarrow$ EvaluateRun($\boldsymbol{\lambda}^{(t)}, i^{(t)}, s^{(i)}, \kappa^{(i)}$);
  - $\mathcal{D}_{\text{Hist}} \leftarrow \mathcal{D}_{\text{Hist}} \cup (\boldsymbol{\lambda}^{(t)}, i^{(t)}, s^{(t)}, c^{(t)})$;
  - **if** *average cost of* $\boldsymbol{\lambda}^{(t)} >$ *average cost of* $\hat{\boldsymbol{\lambda}}$ *across* $\mathcal{I}^{(t)}$ *and* $\mathbf{s}^{(t)}$ **then**
    - break;
  - **else if** *average cost of* $\boldsymbol{\lambda}^{(t)} <$ *average cost of* $\hat{\boldsymbol{\lambda}}$ *and* $\mathcal{I}^+ = \mathcal{I}^{(t)}$ *and* $\mathbf{s}^{(t)} = \mathbf{s}^+$ **then**
    - $\hat{\boldsymbol{\lambda}} \leftarrow \boldsymbol{\lambda}^{(t)}$;
- **if** *time spent exceeds* T *or* $\mathbf{\Lambda}_{new}$ *is empty* **then**
  - **return** $\hat{\boldsymbol{\lambda}}, \mathcal{D}_{Hist}$