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
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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
- What should we do with heterogeneous instance distributions?

Why are systems for heterogeneous instance distributions important?

- We cannot guarantee homogeneity in practice
 - Instances might get larger and harder
 - The underlying task or business case might change

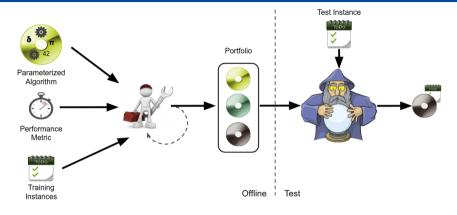
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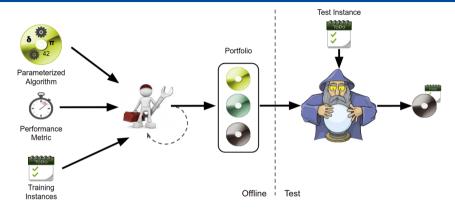
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- We don't want to do algorithm configuration always from scratch
- An adaptive configuration system would be the holy grail
 - → hard to achieve

PIAC: Per-Instance Algorithm Configuration



PIAC: Per-Instance Algorithm Configuration



- 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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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:

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

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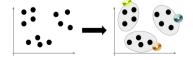
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Test:

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



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

 \leadsto Maximize marginal contribution to ${f P}$

Idea

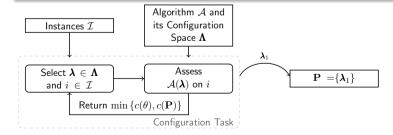
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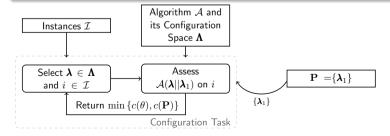
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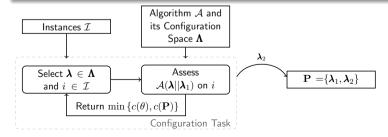
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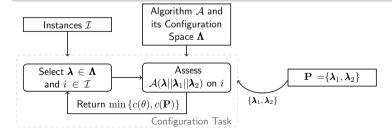
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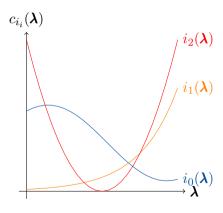


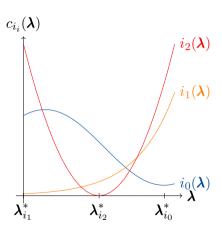
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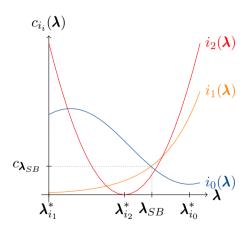
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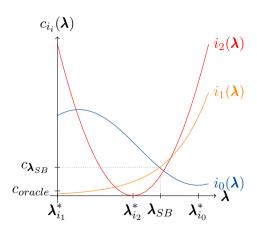
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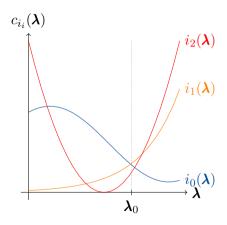




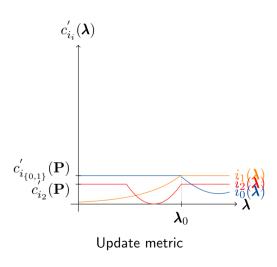


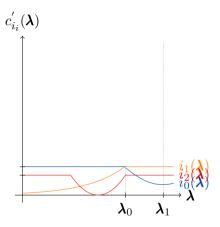




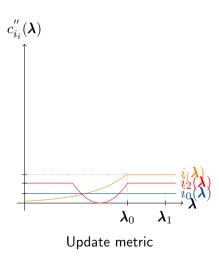


Search initial well performing configuration. Add ${oldsymbol \lambda}_0$ to ${f P}$





Search well performing configuration complementary to ${\bf P}.$ Add λ_1 to ${\bf P}.$



Cedalion [Seipp et al 2015]

Idea

• Optimize a schedule of configurations with algorithm configuration

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Approach

• 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 $\mathcal{S} \oplus \langle \pmb{\lambda}, t \rangle$
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- 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 $\mathcal{S} \oplus \langle \pmb{\lambda}, t \rangle$
- 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 & Golovin '08])

Dynamic Instance Grouping [Liu et al. 2019]

Idea

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

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Main Idea

- Group instances randomly into clusters
- 2 run AC on each cluster
- Update clusters based on performance (estimates)
- Go to 2. if budget is not empty
- Onsider all configurations ever found to create final portfolio

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- Group instances randomly into clusters
- 2 run AC on each cluster
- 3 Update clusters based on performance (estimates)
- Go to 2. if budget is not empty
- Onsider all configurations ever found to create final portfolio
- increase the configuration budget in each iteration
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 - ightharpoonup later clusterings will be better ightarrow more configuration time