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

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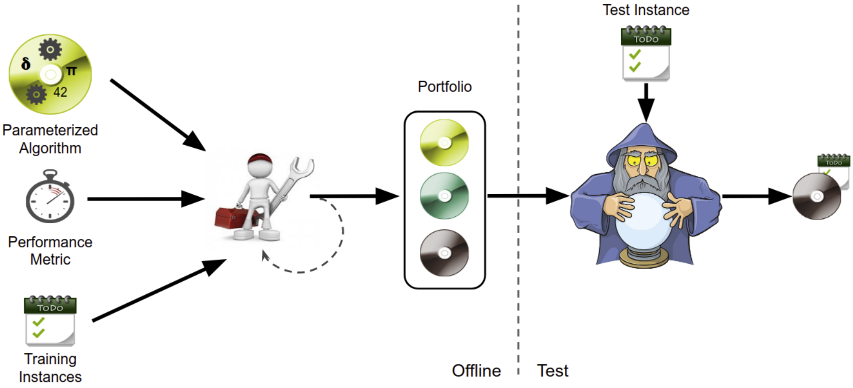
    2. The underlying task or business case might change
2. We don't want to do algorithm configuration always from scratch
3. An adaptive configuration system would be the holy grail
    - $\rightsquigarrow$ hard to achieve

PIAC: Per-Instance Algorithm Configuration



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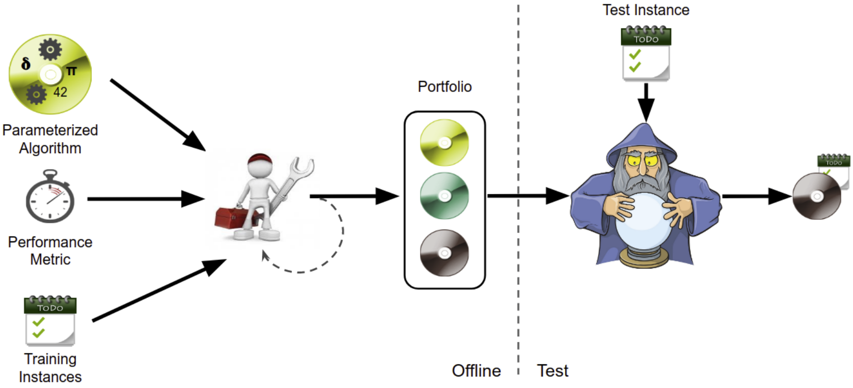

- You can use whichever kind of algorithm selection (wizard) you want
- Challenge: Building a portfolio
- Use case: Instances are heterogeneous

PIAC: Manual Expert Approach

Basic Assumption

Heterogeneous instance set can be divided into homogeneous subsets

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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

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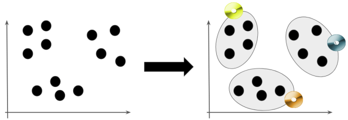
Test:

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 $\mathbf{P}$
  - $\leadsto$ 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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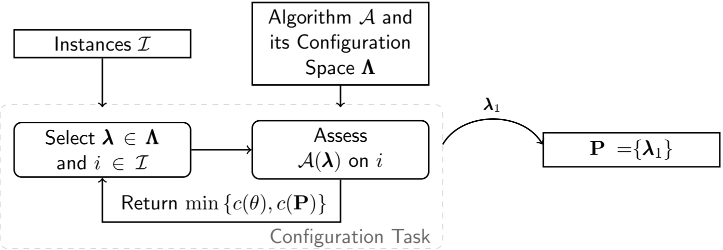

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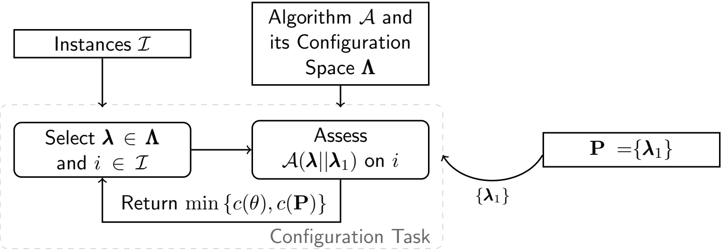

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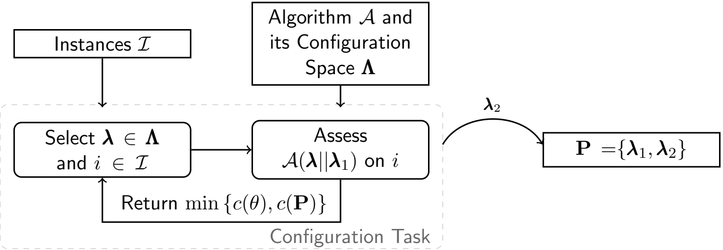

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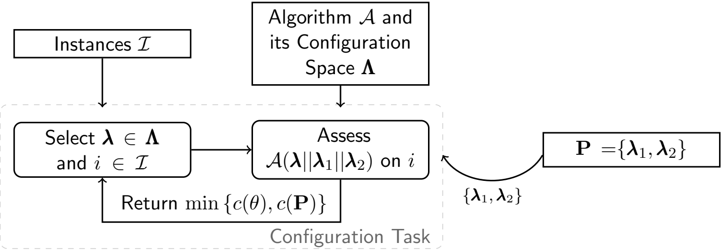
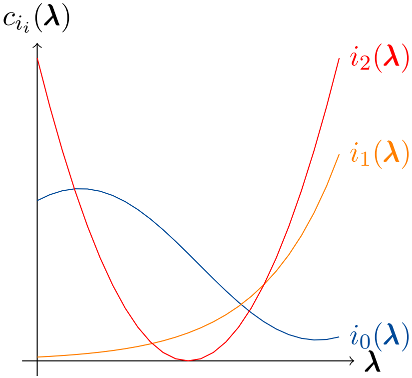


Heterogeneous example



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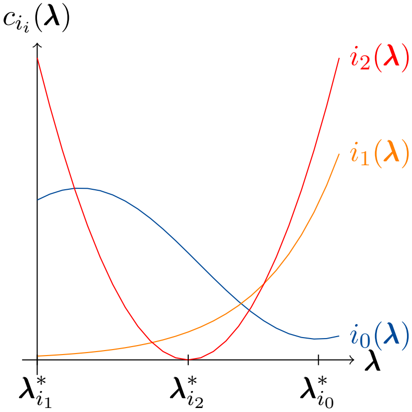

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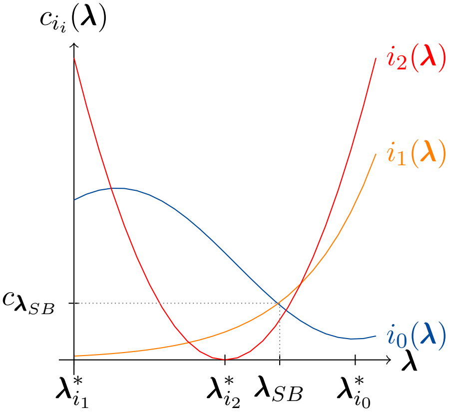

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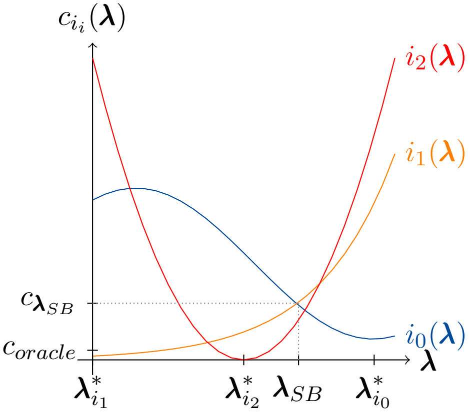
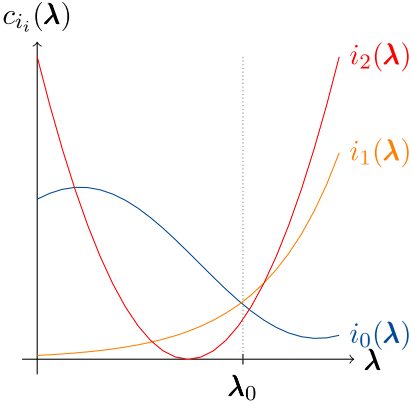


Hydra: Iteration 1



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

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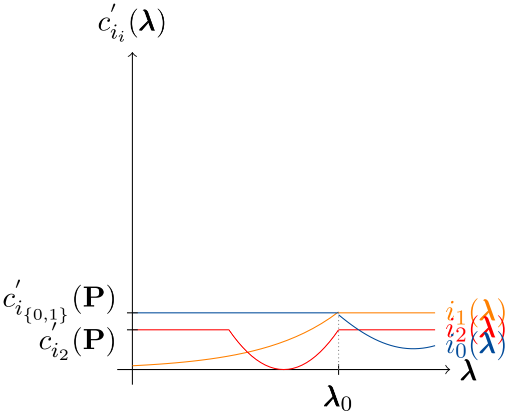
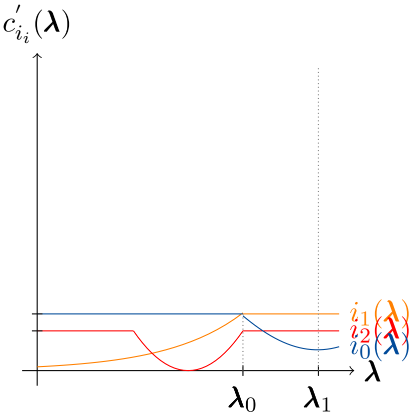


Update metric

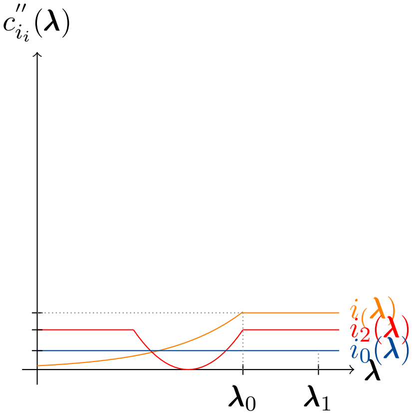
Hydra: Iteration 2



Search well performing configuration complementary to $\mathbf{P}$.

Add $\boldsymbol{\lambda}_1$ to $\mathbf{P}$.

Hydra: Iteration 2



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Cedalion [Seipp et al. 2015]

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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 $\mathcal{S} \oplus \langle \boldsymbol{\lambda}, t \rangle$
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- The time slot is a further parameter in the configuration space

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- 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
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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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- 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