AutoML: Beyond AutoML

Overview: Algorithm Configuration

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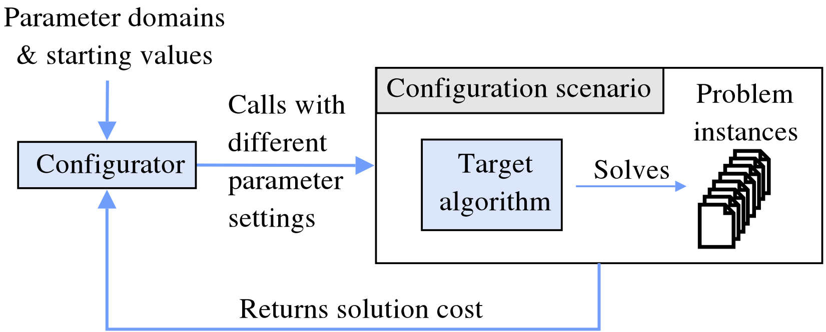
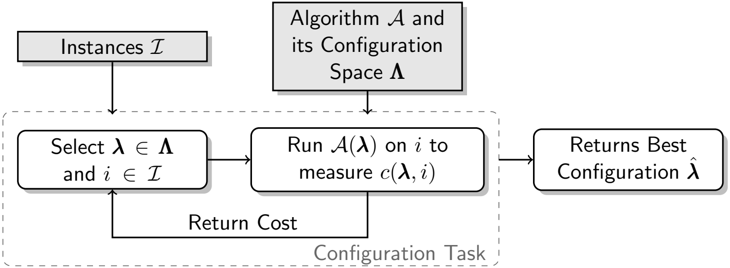
$\rightsquigarrow$ Algorithm configuration

Algorithm Configuration Visualized



Algorithm Configuration – in More Detail



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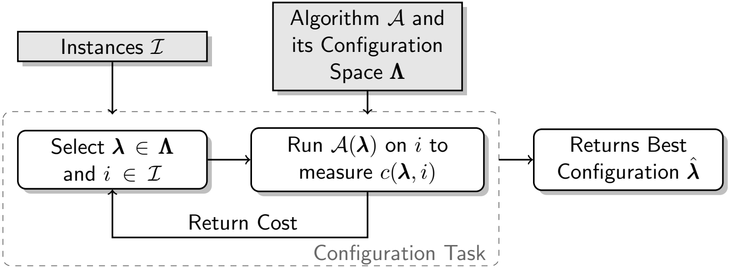

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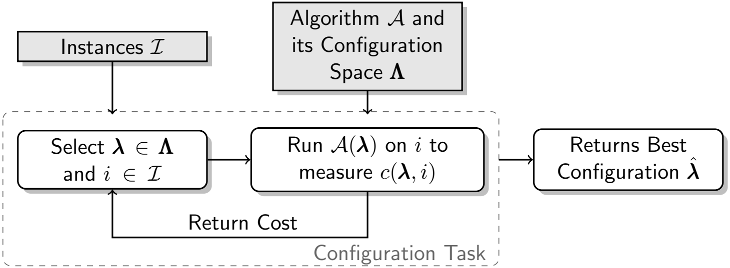

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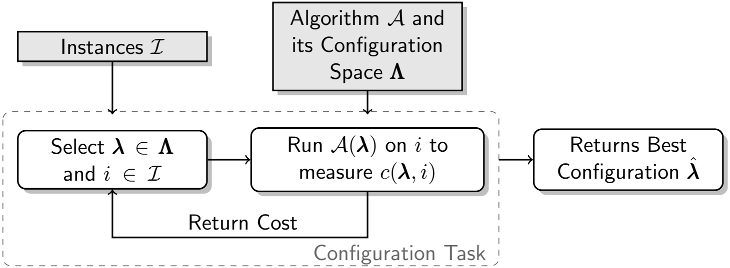

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Given a parameterized algorithm $\mathcal{A}$ with possible (hyper-)parameter settings $\boldsymbol{\Lambda}$, a set of training problem instances $\mathcal{I}$, and a cost metric $c : \boldsymbol{\Lambda} \times \mathcal{I} \to \mathbb{R}$, the algorithm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

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 $\boldsymbol{\lambda}^* \in \arg\min_{\boldsymbol{\lambda} \in \mathbf{\Lambda}} f(\boldsymbol{\lambda})$.

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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

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

[Eggensperger et al. 2019]