AutoML: Interpretability

Global Hyperparameter Importance

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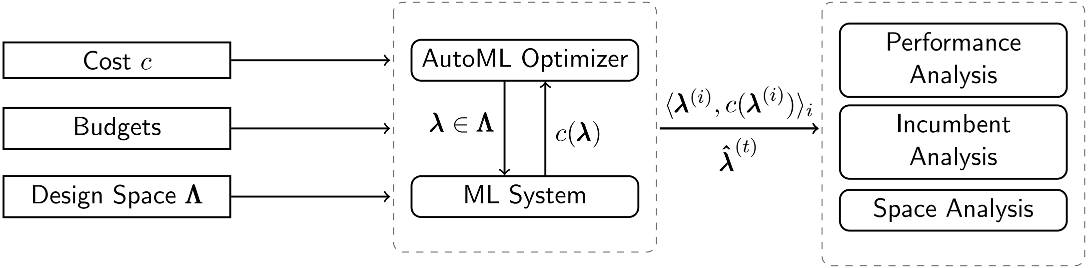
Idea



$\rightsquigarrow$ focus on which hyperparameters are important across the entire search space

Importance Analysis of Surrogate Model

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- Potential drawback:
  - The surrogate model might overfit to different subsets of the hyperparameters (if we don't provide sufficient data)

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fANOVA [Sobobl. 1993]

Write performance predictions as a sum of components:

$$\hat{y}(\boldsymbol{\lambda}_1, \ldots, \boldsymbol{\lambda}_n) = \hat{f}_0 + \sum_{i=1}^{n} \hat{f}_i(\boldsymbol{\lambda}_i) + \sum_{i \neq j} \hat{f}_{ij}(\boldsymbol{\lambda}_i, \boldsymbol{\lambda}_j) + \ldots$$

$$\hat{y}(\boldsymbol{\lambda}_1, \ldots, \boldsymbol{\lambda}_n) = \text{average response} + \text{main effects} + \text{2-D interaction effects} + \text{higher order effects}$$

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Variance Decomposition

$$\mathrm{V} = \frac{1}{||\boldsymbol{\Lambda}||} \int_{\boldsymbol{\lambda}_1} \dots \int_{\boldsymbol{\lambda}_n} [(\hat{y}(\boldsymbol{\lambda}) - \hat{f}_0)^2] d\boldsymbol{\lambda}_1 \dots d\boldsymbol{\lambda}_n$$

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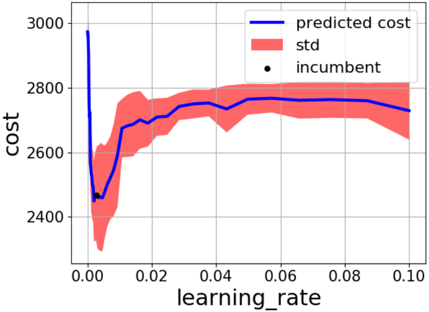

Source: [Lindauer et al. 2019]

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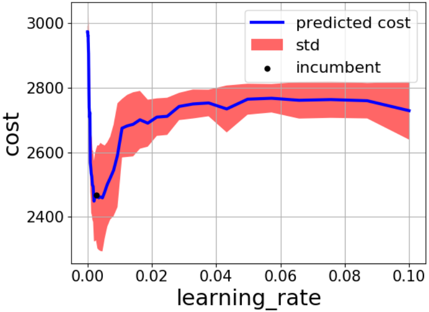

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- Warning: The optimum on these curves does not have to be the global optimum across all hyperparameters

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- How much of the variance can be explained by a hyperparameter (or combinations of hyperparamaters) marginalized over all other parameters?

Table: Exemplary analysis of PPO on cartpole

Hyperparameter	Explained Variance
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$\rightsquigarrow$ You should run both to get a good understanding of why an AutoML tool chose a configuration