AutoML: Interpretability

Global Hyperparameter Importance

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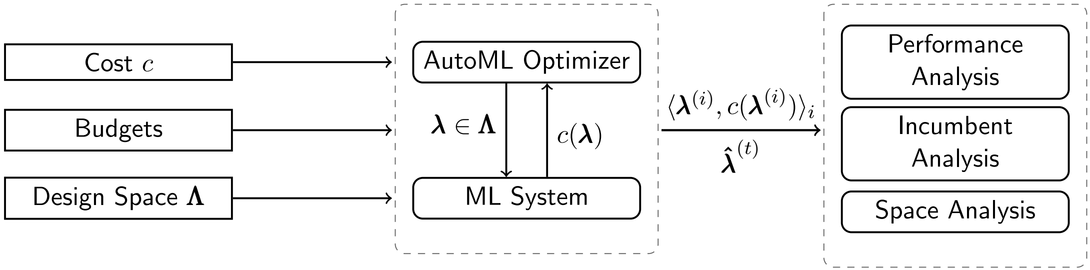
Idea



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

Importance Analysis of Surrogate Model

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- Advantages:
  - Very cheap to do, since we only have to query the surrogate model several times
- 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:

$$
\begin{aligned}
\hat{y}(\boldsymbol{\lambda}_1, \ldots, \boldsymbol{\lambda}_n) = &\quad \hat{f}_0 + \textstyle\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) = &\quad \text{average response} + \text{main effects} + \\
&\quad \text{2-D interaction effects} + \text{higher order effects}
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Variance Decomposition

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

fANOVA Analysis

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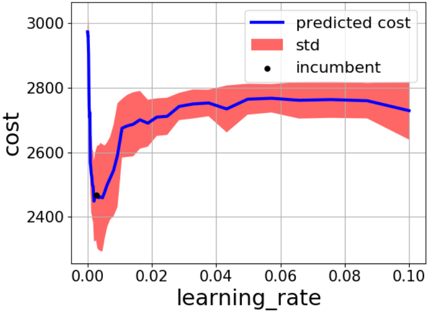

Source: [Lindauer et al. 2019]

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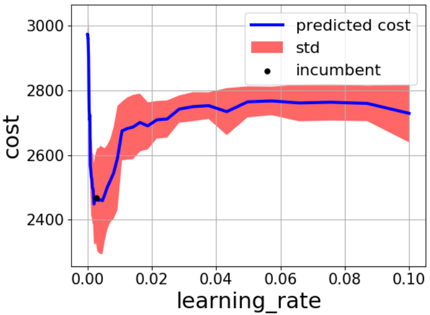

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- predicted cost is marginalized over all other hyperparameter effects
- Warning: The optimum on these curves does not have to be the global optimum across all hyperparameters

fANOVA Analysis

- 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
Discount rate	19.3 %
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discount rate & batch size	10.4%
discount rate & likelihood ration clipping	4.4%
...	

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