AutoML: Introduction

Overview of AutoML Problems

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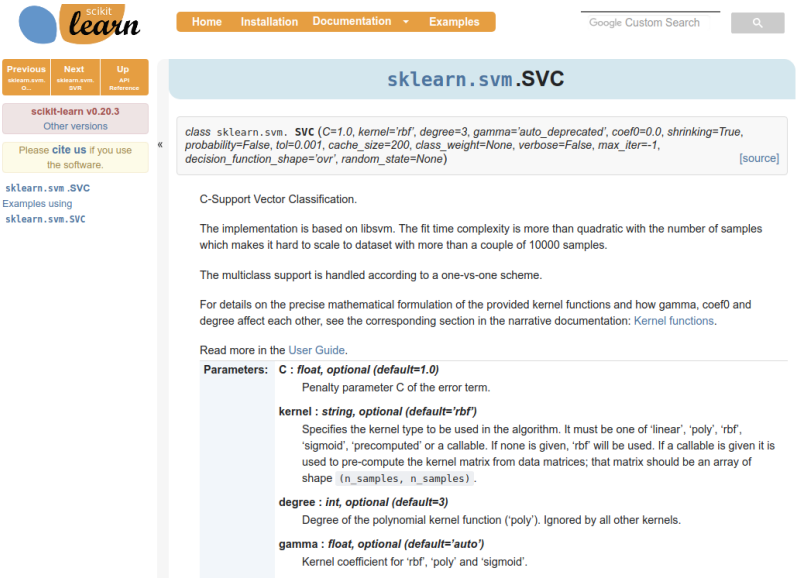
Hyperparameters of an SVM



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- Sometimes, we want to optimize for different metrics, instead of one
  - $\rightsquigarrow$ multi-objective optimization and Pareto fronts

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- In practice, we actually want to jointly choose the best ML-algorithm and its hyperparameters

CASH: Combined Algorithm Selection and Hyperparameter Optimization

Definition

Let

- $\mathbf{A} = \{\mathcal{A}_1, \mathcal{A}_2, \ldots, \mathcal{A}_k\}$ be a set of algorithms (a.k.a. portfolio)
- $\mathbf{\Lambda}$ be a set of hyperparameters of each machine learning algorithm $\mathcal{A}_i$
- $\mathcal{D}_{opt}$ be a dataset which is split into $\mathcal{D}_{train}$ and $\mathcal{D}_{valid}$
- $c(\mathcal{A}_{\boldsymbol{\lambda}}, \mathcal{D}_{train}, \mathcal{D}_{valid})$ denote the cost of $\mathcal{A}_{\boldsymbol{\lambda}}$ trained on $\mathcal{D}_{train}$ and evaluated on $\mathcal{D}_{valid}$.

we want to find the best combination of algorithm $\mathcal{A} \in \mathbf{A}$ and its hyperparameter configuration $\boldsymbol{\lambda} \in \mathbf{\Lambda}$ minimizing:

$$(\mathcal{A}^*, \boldsymbol{\lambda}^*) \in \underset{\mathcal{A} \in \mathbf{A}, \boldsymbol{\lambda} \in \mathbf{\Lambda}}{\arg\min}\, c(\mathcal{A}_{\boldsymbol{\lambda}}, \mathcal{D}_{train}, \mathcal{D}_{valid})$$

Architectures of Neural Networks

- Many architecture were proposed
- Differences in
  - Depth
  - Resolution
  - Width
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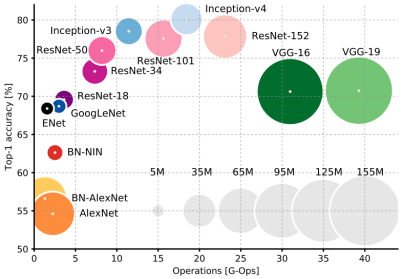

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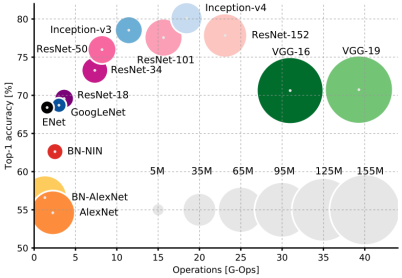

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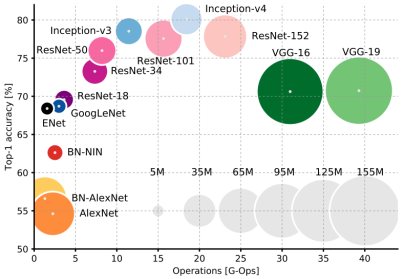

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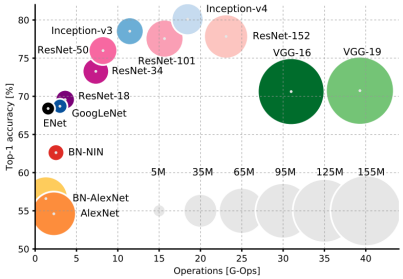

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  - For similar datasets, you might use scaled versions of known architectures (e.g., CIFAR10 and Imagenet)

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- $\boldsymbol{\lambda}$ be an architecture for a deep neural network N with domain $\boldsymbol{\Lambda}$,
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- In practice, you want jointly optimize HPO and NAS [Zela et al. 2018]

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the *per-instance algorithm selection problem* is to obtain a mapping $s : \mathcal{D} \mapsto \mathcal{A}$ such that

$$\arg\min_{s} \int_{\mathbf{D}} c(s(\mathcal{D}), \mathcal{D}) p(\mathcal{D}) \, \mathrm{d}\mathcal{D}$$

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the *dynamic algorithm configuration problem (DAC)* is to obtain a configuration policy $\pi^* : s_t \times \mathcal{D} \mapsto \boldsymbol{\lambda}$ by optimizing its cost across a distribution of datasets:

$$\pi^* \in \arg\min_{\pi \in \mathbf{\Pi}} \int_{\mathbf{D}} p(\mathcal{D}) c(\pi, \mathcal{D}) \, \mathrm{d}\mathcal{D}$$

Summary

HPO	Search for the best hyperparameter configuration of a ML algorithm
CASH	Search for the best combination of algorithm and hyperparameter configuration
NAS	Search for the architecture of neural network
Selection	Predict the best algorithm (and its hyperparameter configuration)
DAC	Predict the best hyperparameter configuration for an algorithm state at a given time point