AutoML: Introduction

Overview of AutoML Problems

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$\rightsquigarrow$ AutoML optimizes an arbitrary cost function, denoted as c.

$\rightsquigarrow$ $c(\cdot)$ can also return several cost metrics

Hyperparameters of an SVM

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scikit-learn v0.20.3
Other versions

Please **cite us** if you use the software.

`sklearn.svm`.SVC
Examples using `sklearn.svm.SVC`

`sklearn.svm`.SVC

class `sklearn.svm.` **SVC** (*C=1.0, kernel='rbf', degree=3, gamma='auto_deprecated', coef0=0.0, shrinking=True, probability=False, tol=0.001, cache_size=200, class_weight=None, verbose=False, max_iter=-1, decision_function_shape='ovr', random_state=None*) [source]

C-Support Vector Classification.

The implementation is based on libsvm. The fit time complexity is more than quadratic with the number of samples which makes it hard to scale to dataset with more than a couple of 10000 samples.

The multiclass support is handled according to a one-vs-one scheme.

For details on the precise mathematical formulation of the provided kernel functions and how gamma, coef0 and degree affect each other, see the corresponding section in the narrative documentation: Kernel functions.

Read more in the User Guide.

Parameters:

C : *float, optional (default=1.0)*
Penalty parameter C of the error term.

kernel : *string, optional (default='rbf')*
Specifies the kernel type to be used in the algorithm. It must be one of 'linear', 'poly', 'rbf', 'sigmoid', 'precomputed' or a callable. If none is given, 'rbf' will be used. If a callable is given it is used to pre-compute the kernel matrix from data matrices; that matrix should be an array of shape `(n_samples, n_samples)`.

degree : *int, optional (default=3)*
Degree of the polynomial kernel function ('poly'). Ignored by all other kernels.

gamma : *float, optional (default='auto')*
Kernel coefficient for 'rbf', 'poly' and 'sigmoid'.

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The *hyper-parameter optimization (HPO)* problem is to find a hyper-parameter configuration that minimizes this cost:

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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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  - naïve Bayes
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  - random forest
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- [Fernández-Delgado et al. 2015] studied 179 classifiers on 121 datasets
- 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:

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

Architectures of Neural Networks

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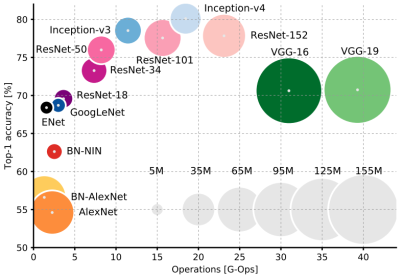

on Imagenet [Canzian et al. 2017]

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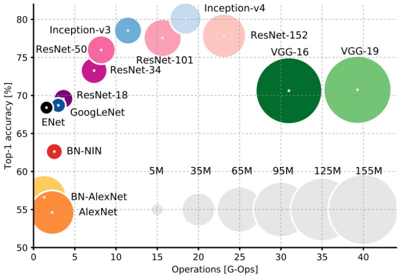

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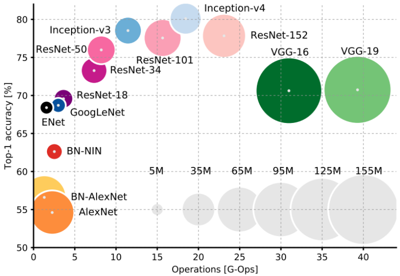

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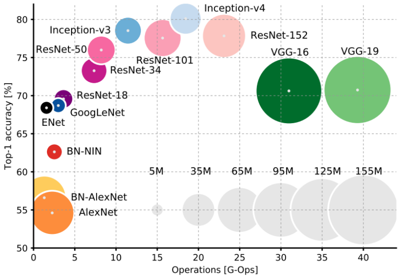

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- For other datasets, you might need different architectures to achieve top-performance
  - For similar datasets, you might use scaled versions of known architectures (e.g., CIFAR10 and Imagenet)

Neural Architecture Search (NAS)

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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