A Comparative study of Hyper-Parameter Optimization Tools

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Abstract—Most of the machine learning models have associated hyper-parameters along with their parameters. While the algorithm gives the solution for the model, its utility for model performance is highly dependent on the choice of hyper-parameters. For a robust performance of a model, it is necessary to find out the right hyper-parameter combination. Hyper-parameter optimization (HPO) is a systematic process that helps in finding the right values for them. The conventional methods for this purpose are grid search and random search and both methods create issues in industrial-scale applications. Hence a set of strategies have been recently proposed based on Bayesian optimization and evolutionary algorithm principles that help in runtime issues in a production environment and robust performance. In this paper, we compare the performance of four python libraries, namely Optuna, Hyper-opt, Optunity, and sequential model-based algorithm configuration (SMAC) that has been proposed for hyper-parameter optimization. The performance of these tools is tested using two benchmarks. The first one is to solve a combined algorithm selection and hyper-parameter optimization (CASH) problem. The second one is the NeurIPS black-box optimization challenge in which a multilayer perceptron (MLP) architecture has to be chosen from a set of related architecture constraints and hyper-parameters. The benchmarking is done with six real-world datasets. From the experiments, we found that Optuna has better performance for CASH problem and HyperOpt for MLP problem.

Index Terms—hyper-parameter optimization, bayesian optimization, evolutionary computing

I. INTRODUCTION

Machine learning algorithms for the learning tasks such as classification, regression, clustering, etc., are associated with parameters and hyper-parameters. The parameters associated with the algorithm are those that can be learned through optimization of a loss function or through the gradients. For example, the weights and bias associated with a linear regression can be learned by optimizing a squared loss function. On the other hand, the hyper-parameters are the ones that control the learning process, and they cannot be inferred like the parameters during the model fitting or loss function optimization. As an example, the regularization constant in ridge regression is a term that makes a trade-off between the empirical error and the generalization capability of the model. It cannot be learned via the gradients like the parameters of the regression rather it exerts control over the entire learning process. Hence, we can see that learning the parameters alone is not good enough for the model performance, but it is also dependent on the right choice of hyper-parameters. There have been studies that have shown that the set of optimal hyper-parameters improves the performance of the model [1] [2].

Different algorithms may have different sorts of hyper-parameters and their influence on model performance can also be in different ways. For example, in the case of random forest algorithm, number of estimators, and depth of the trees are hyper-parameters that can have a profound influence in the model performance while minimal cost complexity pruning parameter can have its effect depending on the noise content in the data. In this context, the selection of hyper-parameters in most of the algorithms is done by putting the analyst in the loop. But this can be a costly process if we have to select the models from a collection of algorithms as they are highly sensitive to the selection of hyper-parameters. To carry out the tuning process in a systematic manner considering the cost of time and performance guarantee, we have different hyper-parameter optimization techniques.

In this paper, we compare the hyper-parameter optimization techniques based on Bayesian optimization (Optuna [3], HyperOpt [4] and SMAC [5], and evolutionary or nature-inspired algorithms such as Optunity [6]. As part of the experiment, we have done a CASH [7] benchmarking and the replication of NeurIPS black box optimization challenge of 2020 [8]. In the CASH problem, 12 different classifier models are chosen for solving large-scale machine learning problems, and to get the best classifier from that when applied to real-world datasets. A total of 58 hyper-parameters of 12 classifier models are tuned for the selection of the best model. For evaluation, we take accuracy and time consumption. NeurIPS black-box optimization challenge was a competition conducted to find out the best hyper-parameter optimization methods. The task was to find out an optimal architecture of a multi-layer perceptron by optimizing the hidden layer sizes, learning parameter, batch size, etc.

The contribution of this work is a comparative study of the different tools for hyper-parameter optimization on real-world problems in terms of the performance and runtime characteristics.
II. HYPER-PARAMETER OPTIMIZATION – THE FORMAL DEFINITION

Consider a machine learning model \( \mathcal{M} \). We assume that the corresponding learning algorithm \( \mathcal{A} \) associated with \( \mathcal{M} \) is parameterized by a set of hyper-parameters \( x = (h_1, h_2, \ldots, h_n) \) where each \( h_i \in \mathcal{X}_i \). Let \( \lambda = \mathcal{X}_1 \times \mathcal{X}_2 \times \cdots \times \mathcal{X}_n \) be the hyper-parameter space from which the algorithm \( \mathcal{A} \) chooses its hyper-parameters. We denote this model as \( \mathcal{M}_\lambda \). The dataset available for the training the model is assumed to be \( D = (D_{\text{train}}, D_{\text{test}}) \) where \( D_{\text{train}} \) is the training data using which the model is trained and \( D_{\text{test}} \) is the testing data in which the model performance is evaluated. For defining the hyper-parameter optimization problem, \( \mathcal{M}_\lambda \) is assumed to be optimizing a loss function as part of its training.

With this setting, the hyper-parameter optimization problem is to maximize the function,

\[
 f(x) = l(\mathcal{A}_\lambda, D_{\text{train}}, D_{\text{test}}).
\]  

(1)

Note that here \( f \) is a black box function where we do not have knowledge about its analytical form.

A. Challenges in Hyper-parameter tuning

Time consumption: If the modeling problem has the time or scalability constraints, we shall have an efficient mechanism for hyper-parameter tuning that process only through those configurations that are likely to give better performance. The conventional methods like grid search and random search may not guarantee this behavior but the Bayesian optimization strategies have inbuilt capabilities to make use of the posterior probability for selecting a feasible configuration.

Variety and inter-dependency: The hyper-parameters can be of the continuous type that gets values in a range, categorical type, or a discrete setting of fixing the number of layers in a neural network. Apart from this, a choice of hyper-parameter can be dependent on another one. They put additional constraints on the optimization problem.

III. BACKGROUND AND RELATED WORKS

In this section, we review the hyper-parameter optimization techniques and other related works.

A. Grid Search

The grid search is a technique that has been applied classically by checking all the possible parameter combinations. In grid search, the entire parameter space is considered and the space is divided as in the form of a grid. Then each of the points in the grid is evaluated as hyper-parameters. The method can be implemented easily and simply [9].

Limitations: The method can be used only in the case of a low dimensional hyper-parameter space, that is, 1-D, 2-D, etc. The method is time-consuming for a larger number of parameters. The method cannot be applied for model selection as it can be used only for tuning a single model.

B. Random Search

Random search is another commonly used approach in which the hyper-parameters are selected at random, independent of other choices. The method is simple to implement and it is well suited for learning gradient-free function. Compared to the grid search, the random search method converges faster. The method finds an optimal model by effectively searching a larger, less promising hyper-parameter space [9].

Limitations: It is a time-consuming method as the evaluation of the function gets expensive. The method does not have the capability of model selection as it is used only with a single model. Compared to Bayesian optimization, this method does not exploit the knowledge of well-performing search space [10] [11].

C. Bayesian Hyper-parameter Optimization

In this section, we describe briefly the techniques involved in Bayesian hyper-parameter optimization.

1) Overview: The hyper-parameter optimization problem given in [1] involves a black-box function \( f \) whose analytical form is not known. We do not have the knowledge about its derivatives with respect to the hyper-parameters and it may not be convex. Due to these reasons, it is very difficult to apply the classical optimization problems. It is in this context we go for Bayesian optimization [12].

We assume that we have certain samples from the function \( f \), that is, we know for certain hyper-parameter combination what is their performance as a prior information. We denote \( D_t = \{(x_1, f(x_1)), (x_2, f(x_2)), \ldots, (x_t, f(x_t))\} \) as \( t \) number of such samples. Note that here each \( x_t \) corresponds to a particular hyper-parameter configuration. It is also assumed that \( f \) follows a prior distribution which is \( P(f) \). Hence the posterior distribution can be written as,

\[
 P(f|D_t) \propto P(D_t|f)P(f).
\]  

(2)

This posterior distribution helps to make a better estimate of the hyper-parameter configuration given the performance of observed ones [13]. In practice, the objective function \( f \) is evaluated with a surrogate function. The next point at \( t+1 \) to be evaluated is found out using an acquisition function. The process is graphically visualized in Figure 1. The acquisition function adheres to the property of exploring in the regions where the objective function is uncertain and exploiting the values of \( \lambda \) where the objective function has the minimum. Hence it is likely to provide a new candidate configuration that is better than the previous ones by finding a balance between exploration and exploitation.

The Bayesian optimization technique takes only a few evaluations in the optimization problem. This is particularly useful in the case where the cost of the function evaluation is very high. In the following sections, we briefly discuss the surrogate and acquisition functions which are the key components in Bayesian optimization.
where $K_f$ values shall now estimate $f$ evaluation returned by the acquisition function. A GP is a distribution over Gaussian Process (GP):

$$\mathcal{N}(0, K)$$

A common choice for the covariance function is the squared exponential function, $k(x_i, x_j) = \exp(-\frac{1}{2} \|x_i - x_j\|^2)$ where $\beta$ is a hyper-parameter.

Considering the prior observations from $D_t$, the function values $f$ are drawn from a normal distribution $\mathcal{N}(0, K)$, where $K$ is the covariance matrix. Let the new point of evaluation returned by the acquisition function be $x_{t+1}$. We shall now estimate $f_{t+1}$ using the posterior described by $f_1:t$. In that case, by the properties of GP,

$$f_{t+1} \sim \mathcal{N}(0, [K - k^T k_{(x_{t+1}, x_{1:t})}^{-1}])$$

where $f_{1:t} = [f(x_1), f(x_2), \ldots, f(x_t)]$, and $k = [k(x_{t+1}, x_1), k(x_{t+1}, x_2), \ldots, k(x_{t+1}, x_t)]$.

Now the posterior distribution can be written as:

$$P(f_{t+1}|D_t, x_{t+1}) = \mathcal{N}(\mu_{t+1}, \sigma^2_{t+1})$$

where $\mu_{t+1} = k^T K^{-1} f_{1:t}$ and $\sigma^2_{t+1} = k(x_{t+1}, x_{1:t}) - k^T K^{-1} k$.

The choices for covariance function are Automatic relevance determination (ARD) kernels and Matern kernels. The alternatives for GP are random forest and tree parzen estimators.

3) Acquisition functions: The purpose of the acquisition function is to choose the next point of evaluation of the function $f$ such that the optimization shall progress towards the maxima. This is accomplished by finding the argument point that maximizes the acquisition function.

One of the popular choices is to maximize the expected improvement (EI) with respect to $f(x^*)$ where $x^* = \arg \max_{x \in D_t} f(x)$. The improvement function is defined as, $I(x) = \max\{0, f_{t+1}(x) - f(x^*)\}$. Now the new point for evaluation is found out by maximizing the EI, $x = \arg \max_{x \in D_t} E[I(x)|D_t]$.

The likelihood of $I$ is computed from the normal density function as, 

$$\frac{1}{\sqrt{2\pi \sigma(x)}} \exp\left(-\frac{(\mu(x) - f(x^*))^2}{2\sigma^2(x)}\right)$$

With this setting, the expected improvement can be evaluated as follows,

$$EI(x) = \begin{cases} 
\frac{(\mu(x) - f(x^*))\Phi(Z) + \sigma(x)\phi(Z)}{\sigma(x)} & \text{if } \sigma(x) > 0 \\
0 & \text{if } \sigma(x) = 0
\end{cases}$$

where $Z = (\mu(x) - f(x^*))/\sigma(x)$, $\phi$ and $\Phi$ denote the probability distribution function and cumulative distribution function of the standard normal distribution respectively.

The discussion about the evolutionary algorithms is omitted for brevity.

IV. HYPER-PARAMETER OPTIMIZATION TOOLS

This section briefly describes the tools we have used.

A. HyperOpt

HyperOpt [4][15] is a python library that works based on the sequential model-based optimization (SMBO) [6] associated with the Bayesian optimization defined in the previous section. It provides an interface where the user can configure the search space of the variables, customizing an evaluation function and assigning the loss function for evaluating the points in search space. It can also facilitate to set up a single large hyperparameter optimization problem in which a variety of algorithms, data pre-processing modules and their hyper-parameters are combined.

The main components of HyperOpt are a search domain, an objective function, and an optimization algorithm. The search domain provides greater flexibility in the optimization process as it can be characterized by continuous, ordinal, or categorical variables. The objective function can be a user-defined python function that accepts the variables and return a loss function corresponding to that variable combination. The search algorithm stands for the surrogate function defined in the previous section. The choices provided by the tool are random search, TPE, and adaptive TPE. The tool also provides the facility for parallel implementation utilizing Apache Spark and MongoDB.
B. Optuna

The features of Optuna as quoted by the authors are "(1) define-by-run API that allows users to construct the parameter search space dynamically, (2) efficient implementation of both searching and pruning strategies, and (3) easy-to-setup, versatile architecture that can be deployed for various purposes, ranging from scalable distributed computing to light-weight experiment conducted via interactive interface." 

The define-by-run API is unique to Optuna whereas, in the case of HyperOpt, the users have to specify the search spaces for each hyper-parameters explicitly. The objective function of Optuna receives a trial object that is embedded with the parameter space and function to optimize instead of the hyper-parameter values. The define-by-run API also gives the ability for modular programming.

In the hyper-parameter optimization problem, it is required to deal with relational sampling as well as independent sampling. Relational sampling refers to the correlation that exists between the parameters while the other refers to the sampling process that performs independently. Optuna has the ability to identify the experiment runs that contain these concurrence relations.

Optuna provides the pruning feature that helps to prematurely terminate the runs that are not optimal. For this purpose, the intermediate objective values are monitored and those that do not meet predefined conditions are terminated. This is enabled by an asynchronous successive halving algorithm. It also provides the distributed computing capabilities.

C. Optunity

Optunity is a framework for CASH problem [7] with a set of different solvers. Optunity provides a collection of solvers - basic solver, grid search, random search, evolutionary methods such as particle swarm optimization (PSO) and covariance matrix adaption evolutionary strategy (CMA-ES). In the experiments related to this paper, only PSO is used. The features of Optunity are it can be configured with minimal efforts, number of evaluations can be set to an upper limit and the hyper-parameters can be given box constraints [5].

D. Sequential model based algorithm configuration (SMAC)

SMAC is [6] introduced as an improvement to the classical sequential model-based optimization (SMBO). SMAC has an efficient sampling mechanism in which multiple instances can be processed by considering their performance into account. It has also introduced the mechanism to incorporate categorical parameters into the optimization procedures.

A model to predict the runtime of the algorithm for different parameter configurations is embedded in SMAC. It helps to reduce the number of runs of the algorithms. SMAC also has the capabilities to select promising configurations in large mixed numerical/categorical configuration spaces.

V. Experiments

In this section, we describe the details of the experiments, datasets used, system setup, implementation details and metrics used for the classification tasks.

A. Datasets

We have taken six publicly available datasets from OpenML [16] machine learning repository. The details of the datasets are described in Table I. The datasets are chosen in a way that they cover the probable real-world scenarios that commonly occur.

B. System setup and Implementation

We built a model of classifiers in the Python3 framework. The system configuration is 3.50 GHz Intel Xeon i7-4771 CPU with 32GB RAM. We use K-fold cross-validation (K = 3) and compute the f1-score as the performance metric. The methods are evaluated for 50 iterations.

C. Benchmark-I

The configuration space for the CASH algorithm contains 12 classifiers with a total number of 58 hyper-parameters. This configuration space is listed in Table II.

1) Results and Observations: The results are given in Table III. We can see that in terms of time, Optuna has the better performance in all the datasets except semeion. However, this pattern is not followed in terms of the performance score. In the case of dna, nomao, and pendigits, the score of all the methods is satisfactory. But in the case of electricity and gas drift, Optunity PSO has a high score although the
time taken is higher than Optuna. Note that these datasets have a high sample size and moderately high dimensional. On the other hand, the score of Optunity PSO is lower in the high dimensional semeion dataset although it has the least run time. In this case, Optuna has a high score with a slight increase in runtime compared with Optunity PSO.

Comparing HyperOpt and SMAC, their performance score is similar in all datasets. But the runtime of SMAC is higher in most of the datasets. The performance score of HyperOpt and Optuna is similar in all datasets. Comparing the runtime, Optuna is better in most of the datasets except semeion although the difference is not significant.

Another useful comparison is about the random search and searches with TPE of HyperOpt and Optuna. We can see that the performance of TPE is slightly better compared to random search.

From the experiments, we can observe that considering the trade-off between the performance score and runtime, which is a common scenario in industry applications, Optuna is a better choice for HPO compared to other approaches. In the case of very large data, Optunity can also be a good choice and its runtime can be further optimized through parallel computation.

D. Benchmark-II

As part of the NeurIPS black-box optimization challenge, the task was to choose a multi-layer perceptron (MLP) architecture by optimizing through a set of hyper-parameters as described in Table IV.

1) Results and Observations: The performance score of Optuna is the highest for all datasets while in terms of runtime it is the HyperOpt. It can be noted that there is no considerable difference in the score between both the methods except in the case of gas drift and nomao. For a few datasets, SMAC also has a similar performance to Optuna but it has a comparatively higher runtime compared to other methods.

The performance score of Optunity PSO is the least among all the methods and its runtime performance is in between Optuna and HyperOpt and better than SMAC. From the experiments, we can observe that for neural network applications HyperOpt is the better option.

The plot of f1-score against iteration for the best performing model for each dataset are given in Fig.2 and Fig.3 for the benchmarks-I and II respectively. From the figures, we can see that the Optunity and HyperOpt shows an oscillatory behavior while Optuna is more stable.

VI. CONCLUSION

We compared the hyper-parameter optimization libraries HyperOpt, Optuna, Optunity, and SMAC on two benchmarks. Based on our experiments we found that for the CASH problem benchmark Optuna is the good option considering the trade-off between the runtime and performance score. On the other hand, for the MLP problem, it is the HyperOpt.

### Table III

| Dataset | Method         | Score      | Time  |
|---------|----------------|------------|-------|
| dna     | HyperOpt Random| 0.9538178  | 366   |
|         | HyperOpt TPE   | 0.9579369  | 322   |
|         | Optuna Random  | 0.9550853  | 94    |
|         | Optuna TPE     | 0.9602619  | 521   |
|         | Optunity PSO   | 0.925369   | 200   |
|         | SMAC           | 0.9595218  | 807   |
| electricity | HyperOpt Random | 0.8969229 | 546   |
|         | HyperOpt TPE   | 0.7011213  | 341   |
|         | Optuna Random  | 0.8942903  | 494   |
|         | Optuna TPE     | 0.7011213  | 167   |
|         | Optunity PSO   | 0.9074971  | 190   |
|         | SMAC           | 0.7011213  | 350   |
| gas drift | HyperOpt Random | 0.850121  | 23869 |
|         | HyperOpt TPE   | 0.88168    | 14105 |
|         | Optuna Random  | 0.868639   | 14549 |
|         | Optuna TPE     | 0.882114   | 4403  |
|         | Optunity PSO   | 0.982105   | 11923 |
|         | SMAC           | 0.825001   | 12986 |
| nomao   | HyperOpt Random| 0.926518   | 1771  |
|         | HyperOpt TPE   | 0.931569   | 1441  |
|         | Optuna Random  | 0.93677    | 1064  |
|         | Optuna TPE     | 0.937144   | 1124  |
|         | Optunity PSO   | 0.938943   | 1554  |
|         | SMAC           | 0.937003   | 2622  |
| pendigits | HyperOpt Random | 0.979188  | 1783  |
|         | HyperOpt TPE   | 0.987569   | 1012  |
|         | Optuna Random  | 0.982508   | 336   |
|         | Optuna TPE     | 0.983886   | 897   |
|         | Optunity PSO   | 0.958028   | 2980  |
|         | SMAC           | 0.984226   | 860   |
| semeion | HyperOpt Random| 0.901575   | 762   |
|         | HyperOpt TPE   | 0.915246   | 458   |
|         | Optuna Random  | 0.92832    | 895   |
|         | Optuna TPE     | 0.934616   | 1989  |
|         | Optunity PSO   | 0.700295   | 538   |
|         | SMAC           | 0.929794   | 1647  |

### Table IV

Configuration space for MLP tuning. The type, nature of search space and the range of values for searching are given as columns.

| Hyper-parameter | Type     | Space | Range          |
|-----------------|----------|-------|----------------|
| hidden layer size | integer  | linear | (50, 200)      |
| alpha           | real     | log   | (10^{-5}, 10)  |
| batch size      | integer  | linear | (10, 250)      |
| learning rate   | real     | log   | (10^{-5}, 10^{-1}) |
| tolerance       | real     | log   | (10^{-5}, 10^{-1}) |
| validation fraction | real | real | (0.1, 0.9) |
| beta 1          | real     | logit | (0.5, 0.99)    |
| beta 2          | real     | logit | (0.9, 1.0, 10^{-6}) |
| epsilon         | real     | log   | (10^{-9}, 10^{-6}) |

REFERENCES

[1] J. Bergstra, R. Bardenet, Y. Bengio, and B. Kégl, "Algorithms for hyper-parameter optimization," in 25th annual conference on neural information processing systems (NIPS 2011), vol. 24, Neural Information Processing Systems Foundation, 2011.

[2] J. Snoek, H. Larochelle, and R. P. Adams, "Practical bayesian optimization of machine learning algorithms," arXiv preprint arXiv:1206.2944, 2012.

[3] T. Akiba, S. Sano, T. Yanase, T. Ohta, and M. Koyama, "Optuna: A next-generation hyperparameter optimization framework," in Proceedings of the 25th ACM SIGKDD international conference on knowledge discovery & data mining, pp. 2623–2631, 2019.
Table V
RESULT OF BENCHMARK-II

| Dataset     | Method        | Score   | Time  |
|-------------|---------------|---------|-------|
| DNA         | HyperOpt Random | 0.942171 | 72    |
|             | HyperOpt TPE   | 0.946809 | 87    |
|             | Optuna Random  | 0.947759 | 267   |
|             | Optuna TPE     | 0.947453 | 415   |
|             | Optunity PSO   | 0.901858 | 243   |
|             | SMAC           | 0.950322 | 388   |
| Electricity | HyperOpt Random | 0.669953 | 366   |
|             | HyperOpt TPE   | 0.683778 | 229   |
|             | Optuna Random  | 0.692635 | 2042  |
|             | Optuna TPE     | 0.696458 | 1269  |
|             | Optunity PSO   | 0.583639 | 1550  |
|             | SMAC           | 0.685409 | 2844  |
| Gas Drift   | HyperOpt Random | 0.742839 | 257   |
|             | HyperOpt TPE   | 0.847971 | 173   |
|             | Optuna Random  | 0.89409  | 2798  |
|             | Optuna TPE     | 0.851657 | 706   |
|             | Optunity PSO   | 0.885599 | 1732  |
|             | SMAC           | 0.898836 | 3732  |
| Nomao       | HyperOpt Random | 0.909167 | 624   |
|             | HyperOpt TPE   | 0.920299 | 501   |
|             | Optuna Random  | 0.931145 | 3842  |
|             | Optuna TPE     | 0.931401 | 4933  |
|             | Optunity PSO   | 0.885599 | 1732  |
|             | SMAC           | 0.930689 | 12316 |
| Pendigits   | HyperOpt Random | 0.967597 | 205   |
|             | HyperOpt TPE   | 0.981328 | 182   |
|             | Optuna Random  | 0.985501 | 544   |
|             | Optuna TPE     | 0.980751 | 132   |
|             | Optunity PSO   | 0.72276  | 196   |
|             | SMAC           | 0.934178 | 12316 |
| Semeion     | HyperOpt Random | 0.918278 | 65    |
|             | HyperOpt TPE   | 0.922646 | 57    |
|             | Optuna Random  | 0.927138 | 254   |
|             | Optuna TPE     | 0.930875 | 132   |
|             | Optunity PSO   | 0.72276  | 196   |
|             | SMAC           | 0.931478 | 140   |