# BOAH: A Tool Suite for Multi-Fidelity Bayesian Optimization & Analysis of Hyperparameters

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#### Abstract

Hyperparameter optimization and neural architecture search can become prohibitively expensive for regular black-box Bayesian optimization because the training and evaluation of a single model can easily take several hours. To overcome this, we introduce a comprehensive tool suite for effective multi-fidelity Bayesian optimization and the analysis of its runs. The suite, written in Python, provides a simple way to specify complex design spaces, a robust and efficient combination of Bayesian optimization and HyperBand, and a comprehensive analysis of the optimization process and its outcomes.

## 1. Introduction

Finding well-performing hyperparameter settings for a machine learning method often makes the difference between achieving state-of-the-art or quite weak performance. While many prominent methods, such as Bayesian optimization (BO, Shahriari et al. 2016) or random search (Bergstra and Bengio, 2012) formulate hyperparameter tuning as a black-box optimization problem, the long training time and the demand for large computational power of contemporary machine learning methods, such as deep neural networks, limit the usefulness of these methods: when single function evaluations require days or weeks, black-box optimization becomes computationally infeasible. Recent advances in hyperparameter optimization therefore go beyond this limiting blackbox formulation and consider cheap, approximate function evaluations (a.k.a. evaluation budgets), such as performance when running on a subset of data, optimizing a deep neural network for only a few epochs or down-sampled images in computer vision (cf Feurer and Hutter 2019).

Here, we present the first comprehensive tool suite for such multi-fidelity optimization, called BOAH, allowing users to not only optimize their hyperparameters much more effectively, but to also automatically analyze the optimization process and the importance of the various hyperparameters. This automatic analysis provides much-needed insights into

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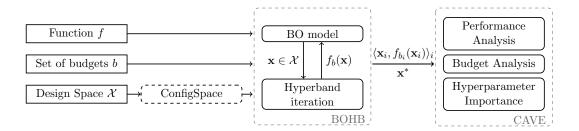


Figure 1: Workflow of BOAH

the algorithm being optimized that is not available from executing any other multi-fidelity hyperparameter optimization package we are aware of.

## 2. Related Work

While there are many available tools for standard BO, e.g., Spearmint (Snoek et al., 2012), SMAC (Hutter et al., 2011), HyperOpt (Bergstra et al., 2011), GPyOpt and BOTorch, the same cannot be said for multi-fidelity BO; we are only aware of RoBO (Klein et al., 2017), BOHB (Falkner et al., 2018), and Dragonfly (Kandasamy et al., 2019). Out of these, RoBO and Dragonfly use Gaussian Processes (GPs), which scale cubically in the number of data points and are thus problematic for multi-fidelity settings in which it is possible to gather many cheap data points. GPs also require carefully chosen hyperpriors and typically struggle to perform well in high-dimensional, categorical design spaces. In contrast, BOHB uses kernel density estimators (KDEs), similar to Tree Parzen Estimators as used in HyperOpt (Bergstra et al., 2011), which work well across a wide range of problems. We therefore include BOHB as part of the BOAH tool suite; we also strive to integrate other state-of-the-art optimization tools into BOAH. We emphasize that all existing open-source hyperparameter optimization tools we are aware of only focus on yielding good performance, not on aiding intuition and scientific understanding by means of automated analyses.

#### 3. The BOAH Tool Suite

BOAH<sup>1</sup> consists of three modular packages that interact as shown in the workflow in Figure 1. In the following, we describe the individual packages in turn.

## 3.1 ConfigSpace: Definition of the Design Space

To specify the design space  $\mathcal{X}$ , we provide a package dubbed ConfigSpace. It supports all common hyperparameter types, such as *categorical*, *ordinal*, *integer-valued* and *continuous* hyperparameters. Furthermore, users can define *conditional constraints* between hyperparameters (e.g., hyperparameters of the RBF kernel are only active if a RBF kernel is chosen) or whether or not a continuous hyperparameter should be sampled on a logarithmic scale (such as the learning rate for gradient descent algorithms). This package can also be used

<sup>1.</sup> https://www.automl.org/BOAH. We provide at BOAH's website also a links to all packages and to a repository with many examples as Jupyter notebooks on how to combine these packages.

on its own and is already used by other AutoML packages, such as SMAC3 (Lindauer et al., 2017) or Auto-Sklearn (Feurer et al., 2015).

### 3.2 BOHB: Bayesian Optimization with Hyperband

As optimizers, BOAH supports BOHB (Falkner et al., 2018) and its components, including successive halving (Jamieson and Talwalkar, 2016), HyperBand (Li et al., 2018), a hyperoptlike optimizer (Bergstra et al., 2011) and the combination of BO and HyperBand. The main idea of the latter is to use BO to suggest new configurations  $\mathbf{x} \in \mathcal{X}$  and to efficiently determine the best  $\mathbf{x}^*$  with the help of HyperBand evaluating  $f_b(\mathbf{x})$  on different budgets b.

Due to its flexibility and strong anytime performance, BOHB is a well-suited optimizer for several settings, including DNN architectures with number of epochs being the budgets (e.g., Auto-PyTorch), hyperparameters of RL algorithms with episode length being the budgets and hyperparameters of machine learning algorithms (e.g., SVMs) with number of validated cross validation folds being the budgets. Another advantage of BOHB compared to other BO-tools is its efficient parallelization. To make BOHB as easy to use as possible, we added a new high-level *fmin* interface, inspired by the well-known *fmin* interface of scipy.

#### 3.3 CAVE: Visualization of Results

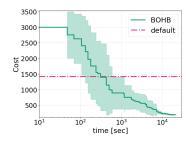
For analyzing the data collected by BOHB, we integrated CAVE Biedenkapp et al. (2018) into BOAH. To this end, we extended CAVE to be able to analyze multi-fidelity data and to help users to gain a better understanding of how BOHB searched a given design space. On each budget and across budgets, CAVE provides extended analyses of:

- Hyperparameter importance using local parameter importance (Biedenkapp et al., 2018) and fANOVA (Hutter et al., 2014) to analyze which hyperparameters were the most important ones to achieve high performance. To be applicable to BOHB, CAVE provides analyses for each budget and adds uncertainty estimates for each budget.
- Rank correlation between the budgets to verify that the observations on the individual budgets are highly correlated. Multi-fidelity optimizers, such as BOHB, perform best if similar configurations perform best across the various budgets. Therefore, the degree to which this is the case is important to keep track of.
- Optimizer footprint plots to study how BOHB sampled the design space. For example, these plots help to identify general promising areas in the design space. CAVE uses multi-dimensional scaling to project the n-dimensional space into a 2-dimensional space under consideration of a distance metric in complex design spaces.

## 4. Show Case: Hyperparameter Optimization for Reinforcement Learning

To showcase BOAH's flexibility and the usefulness of its automated analyses, we ran it on a rarely studied AutoML problem: hyperparameter optimization for reinforcement learning (Falkner et al., 2018).<sup>2</sup> The goal is to obtain well-performing hyperparameters of Proximal Policy Optimization (PPO) (Schulman et al., 2017) such that PPO on average solves

<sup>2.</sup> https://github.com/automl/BOAH/blob/master/examples/icml\_2018\_experiments/cartpole.ipynb



	fANOVA	LPI
discount	19.32	38.88
learning rate	3.70	35.4
batch size	15.77	21.5
# units 1	1.86	0.07
# units 2	0.39	0.01

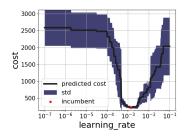


Figure 2: Left: Performance of incumbent configuration found by BOHB over time. As a baseline we show the final cost of the PPO's default configuration. Cost refers to the number of epochs PPO needed to solve the cartpole problem. Middle: Hyperparameter importance with fANOVA and LPI as percentages on the largest budget. Because of space limitations, we do not show uncertainty estimates. Right: Estimated local hyper-parameter importance (LPI) analysis of the learning rate.

the cartpole problem within a minimal number of epochs. As budgets for BOHB, we used the number of PPO runs, since individual PPO runs provide a very noisy performance estimate and thus multiple repetitions yield a clearer signal. We ran BOAH 10 times for 128 iterations using 10 workers on a compute cluster with nodes equipped with two Intel Xeon E5-2630v4 and 128GB memory running CentOS 7. We set the lowest budget to be 1 repetition and allow 9 repetitions for the highest budget.

The resulting CAVE report includes the following insights (Figure 2): (i) BOHB indeed improved the sample-efficiency of PPO substantially compared to the default settings of PPO; (ii) according to the global analysis of the hyperparameter importance based on fANOVA, the discount and the batch size are the most important hyperparameters; (iii) in addition to these, the learning rate is also very important according to the local hyperparameter importance analysis (LPI), also shown in the middle and right of Figure 2.

#### 5. Conclusion

We introduced BOAH, a comprehensive suite of tools that allow users to conveniently specify design spaces, efficiently search these spaces using multi-fidelity Bayesian optimization, and analyze the results in a wide variety of ways. We emphasize that these steps are integrated to work together seamlessly, and that the posthoc analysis of the optimization process with CAVE does not require any additional function evaluations. To the best of our knowledge, BOAH is the first tool suite which brings all these three important components together and therefore improves the usability of AutoML substantially.

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## References

- J. Bergstra and Y. Bengio. Random search for hyper-parameter optimization. *JMLR*, 13: 281–305, 2012.
- J. Bergstra, R. Bardenet, Y. Bengio, and B. Kégl. Algorithms for hyper-parameter optimization. In Proc. of NeurIPS'11, pages 2546–2554, 2011.
- A. Biedenkapp, J. Marben, M. Lindauer, and F. Hutter. Cave: Configuration assessment, visualization and evaluation. In *Proc. of LION'18*, 2018.
- S. Falkner, A. Klein, and F. Hutter. BOHB: robust and efficient hyperparameter optimization at scale. In *Proc. of ICML*, pages 1436–1445, 2018.
- M. Feurer and F. Hutter. Hyperparameter optimization. In *AutoML: Methods, Sytems, Challenges*, chapter 1, pages 3–38. Springer, 2019.
- M. Feurer, A. Klein, K. Eggensperger, J. T. Springenberg, M. Blum, and F. Hutter. Efficient and robust automated machine learning. In *Proc. of NeurIPS'15*, pages 2962–2970, 2015.
- F. Hutter, H. Hoos, and K. Leyton-Brown. Sequential model-based optimization for general algorithm configuration. In *Proc. of LION'11*, pages 507–523, 2011.
- F. Hutter, H. Hoos, and K. Leyton-Brown. An efficient approach for assessing hyperparameter importance. In *Proc. of ICML'14*, pages 754–762, 2014.
- K. Jamieson and A. Talwalkar. Non-stochastic best arm identification and hyperparameter optimization. In *Proc. of AISTATS'16*, 2016.
- K. Kandasamy, K. Vysyaraju, W. Neiswanger, B. Paria, C. Collins, J. Schneider, B. Poczos, and E. Xing. Tuning hyperparameters without grad students: Scalable and robust Bayesian optimisation with dragonfly. *arxiv:1903.06694*, 2019.
- A. Klein, S. Falkner, N. Mansur, and F. Hutter. RoBO: A flexible and robust Bayesian optimization framework in Python. In *NeurIPS Workshop: BayesOpt*, 2017.
- L. Li, K. Jamieson, G. DeSalvo, A. Rostamizadeh, and A. Talwalkar. Hyperband: A novel bandit-based approach to hyperparameter optimization. *JMLR*, 18:185:1–185:52, 2018.
- M. Lindauer, K. Eggensperger, M. Feurer, S. Falkner, A. Biedenkapp, and F. Hutter. SMACv3: Algorithm configuration in Python, 2017.
- J. Schulman, F. Wolski, P. Dhariwal, A. Radford, and O. Klimov. Proximal policy optimization algorithms. arXiv:1707.06347, 2017.
- B. Shahriari, K. Swersky, Z. Wang, R. Adams, and N. de Freitas. Taking the human out of the loop: A review of Bayesian optimization. *Procs. of the IEEE*, 104(1):148–175, 2016.
- J. Snoek, H. Larochelle, and R. Adams. Practical Bayesian optimization of machine learning algorithms. In *Proc. of NeurIPS'12*, pages 2960–2968, 2012.