Automated Hyperparameter Optimization Challenge at CIKM 2021 AnalyticCup

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ABSTRACT
In this paper, we describe our method for tackling the automated hyperparameter optimization challenge in QQ Browser 2021 AI Algorithm Competition (ACM CIKM 2021 AnalyticCup Track 2). The competition organizers provide anonymized realistic industrial tasks and datasets for black-box optimization. Based on our open-sourced package OpenBox, we adopt the Bayesian optimization framework for configuration sampling and a heuristic early stopping strategy. We won first place in both the preliminary and final contests with the results of 0.938291 and 0.918753, respectively.

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1 INTRODUCTION
The automated hyperparameter optimization challenge of ACM CIKM 2021 AnalyticCup is an annual contest that evaluates automated hyperparameter optimization algorithms on 30 anonymized realistic tasks. The data is constructed on industrial recommendation scenarios, which aims at improving the practical performance of machine learning models and strategies and reducing human effort in choosing hyperparameters based on experts’ experience.

In general, the contest can be viewed as a black-box optimization problem, in which the performance of a set of hyperparameters can only be obtained via a specific function $f$ without analytical forms. The problem can be formulated as,

$$\arg \min_{x \in X} f(x),$$

(1)

where $X$ is the hyperparameter space and $x$ is a choice from the space. The goal is find the best choice that minimizes the given function $f$.

Bayesian optimization (BO) [1, 2, 6] is a typical framework for solving black-box optimization tasks shown in Equation 1. It contains two core components that allow for improved exploration over the search space. The first component is the probabilistic surrogate model that approximates $f(x)$ based on historical evaluations and outputs uncertainty estimates to guide exploration. The other component is the acquisition function that measures the utility by trading off exploration and exploitation.

In this contest, we elaborately select each component for Bayesian optimization and design a heuristic early stopping strategy. The solution is implemented based on OpenBox [5], a generalized service for black-box optimization. In the following sections, we first give a brief introduction to the Bayesian optimization framework, and then introduce our solutions for the preliminary and final contest.

2 BAYESIAN OPTIMIZATION FRAMEWORK
In this section, we briefly introduce the framework of Bayesian Optimization (BO). We denote a configuration $x$ as a choice of hyperparameters from their value ranges and observations $D$ as the collection of configurations and their corresponding performance. Since evaluating the objective function $f$ for a given configuration $x$ is very expensive, BO approximates $f$ using a probabilistic surrogate model $M : p(f | D)$ that is much cheaper to evaluate. Given a configuration $x$, the surrogate model $M$ outputs the posterior predictive distribution at $x$, that is, $f(x) \sim N(\mu_M(x), \sigma_M^2(x))$. In the $n^{th}$ iteration, BO methods iterate the following three steps: 1) use the surrogate model $M$ to select a configuration that maximizes the acquisition function $x_n = \arg \max_{x \in X} a(x; M)$, where the acquisition function is used to balance the exploration and exploitation; 2) evaluate the configuration $x_n$ to get its performance $y_n = f(x_n) + \epsilon$ with $\epsilon \sim N(0, \sigma^2)$; 3) add this measurement $(x_n, y_n)$ to observations $D = \{(x_1, y_1), \ldots, (x_{n-1}, y_{n-1})\}$, and refit the surrogate model on the augmented $D$.

3 PRELIMINARY CONTEST
The preliminary contest is a typical black-box optimization problem. In each iteration, the optimizer should suggest 5 configurations from a given search space in a synchronous manner. Rewards will return afterward for the next round of suggestion. The objective is to maximize the reward within 100 hyperparameter evaluations. We will introduce our method for the preliminary contest in detail in this section.

3.1 Configuration Space Definition
We use the package ConfigSpace¹ to define the configuration (hyperparameter) space. Since the choices of all hyperparameters are

¹https://github.com/automl/ConfigSpace
We adopt the Expected Improvement (EI) function [3] as the acquisition function, which can be formulated as,

\[ EI(x; D) = \int_{-\infty}^{y_{\text{min}}} \max(0, y - y_{\text{min}}) p_D(y|x)dy, \]

where \(y_{\text{min}}\) is the best performance observed so far. Given observations \(D\), the EI function computes the expectation of improving the current best performance. To maximize the EI function, we further apply the L-BFGS-B algorithm [7], which is a popular algorithm for parameter estimation in machine learning. While the results of L-BFGS-B largely depend on the choice of initial points, we adopt the following two sampling strategies: 1) Randomly sample a large number of configurations via the Monte Carlo sampling from the entire space; 2) Sample a few points from the best-observed configurations by changing the value of only one hyperparameter. We combine the configurations sampled by the two strategies, and select 10 configurations with the largest EI value as the start points for L-BFGS-B. This method is provided in OpenBox as the “random_scipy” acquisition optimizer.

### 3.5 Other Techniques

To suggest multiple configurations in one iteration, we adopt a simple method. We restart the optimization of the acquisition function and obtain one configuration each time until a desired number of suggestions is reached. To increase the exploratory of Bayesian optimization and ensure the convergence of the algorithm, we set the probability of suggesting random configuration to 10%.

### 4 FINAL CONTEST

The final contest is a more challenging optimization problem. The evaluation process of each configuration is divided into 14 iterations, with partially evaluated rewards in the first 13 iterations and fully evaluated reward in the last iteration reported. The 95% confidence interval information for the reward is additionally provided. The optimizer should decide whether to early stop the evaluation process of a configuration to speed up optimization. The objective is kept the same, but only the configurations evaluated for 14 iterations will be recorded as valid ones. The time budget is reduced to half of the preliminary stage, which means at most 50 configurations could be fully evaluated. In this section, we will present our solution in detail.

#### 4.1 Data Analysis

To design a promising strategy for the final contest, we first look into the opened local datasets and find some interesting properties:

- Given any confidence interval reported in the first 13 iterations of a configuration, the probability that the final reward in the 14-th iteration of the same configuration is located in the interval is perfectly 95%.
- Given any reward in the first 13 iterations of a configuration, the probability that the final reward in the 14-th iteration of the same configuration is greater than the given reward is perfectly 50%.
- For any configuration, during the 14 iterations of evaluation, the confidence interval is reduced, however, the reward values show a random trend.

We also explore the order relation between configurations. Given any two configurations and their rewards of any iteration in the first 13 iterations, we compare the order of the given rewards with the order of their final rewards in the 14-th iteration and find that:

- Among all configurations, the consistency of the reward orders between partial evaluation and full evaluation is greater than 95%.
- Among configurations with top 1% final reward in search space, the consistency of order of rewards between partial evaluation and full evaluation is about 50% to 70%.

As shown in Figure 1, we plot the performance of the best 2 configurations and 8 random configurations over iteration. The median performance of the top-2 configurations outperforms the random ones at the 7-th iteration, which indicates we can pick out those badly-performing configurations in early iterations. However, by the same way, it is hard to identify the best configuration among
Figure 1: The upper bound (blue), median (red), lower bound (green) of the best 2 configurations and 8 random configurations. Well-performing configurations because of non-negligible noise in partial evaluations.

4.2 Early Stopping

Based on the observations, we consider a heuristic early stopping strategy. However, there is a trade-off on when to start early stopping. On one hand, early stopping speeds up evaluation and explores more configurations. On the other hand, full evaluation provides accurate reward information, which benefits the surrogate in Bayesian optimization. In our final implementation, we begin early stopping after 40 configurations are fully evaluated. Our early stopping strategy is inspired by ASHA [4], in which we compare the reward at the 7-th iteration of the running configuration with all rewards observed in the same iteration. If the reward is not in the top half, the evaluation is stopped and a new configuration should be suggested.

4.3 Value Imputation

Since the partial results involve non-negligible noises, we apply BO only on those fully evaluated configurations. However, if we early stop a configuration, the BO framework will not receive its feedback and may suggest a similar configuration in the next round. As a result, we assume that the stopped configuration is not a good one, and then we impute its final performance with the median of all the observed results.

5 CONCLUSION

In this technical report, we presented our winning solution for the automated hyperparameter optimization challenge at ACM CIKM 2021 AnalyticCup. We adopted the Bayesian optimization in the preliminary contest and added a heuristic early stopping strategy in the final contest. Our implementation for the preliminary contest has been integrated into OpenBox. Please refer to the Github repository ² for more details.

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