Practical Bayesian Optimization with Threshold-Guided Marginal Likelihood Maximization

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Abstract

We propose a practical Bayesian optimization method, of which the surrogate function is Gaussian process regression with threshold-guided marginal likelihood maximization. Because Bayesian optimization consumes much time in finding optimal free parameters of Gaussian process regression, mitigating a time complexity of this step is critical to speed up Bayesian optimization. For this reason, we propose a simple, but straightforward Bayesian optimization method, assuming a reasonable condition, which is observed in many practical examples. Our experimental results confirm that our method is effective to reduce the execution time. All implementations are available in our repository.

1 Introduction

Bayesian optimization is a global optimization method with an acquisition function induced by a surrogate function. Because we usually assume that a function is unknown in Bayesian optimization setting, the acquisition function instead of original function is optimized. The selection of surrogate function and acquisition function is a design choice that should be carefully considered, in order to converge to global optimum quickly. Even though there is a rule of thumb for choosing both functions, Gaussian process (GP) regression [Rasmussen and Williams, 2006] is mainly taken into account as surrogate function for the reason why its complexity and model capacity are sufficient [Snoek et al., 2012], and we usually choose a simple acquisition function such as expected improvement [Mockus et al., 1978] and GP upper confidence bound [Srinivas et al., 2010] because of their powerful performance [Snoek et al., 2012; Sui et al., 2015; Springenberg et al., 2016; Kim and Choi, 2018].

For the perspective of time consumed in a single round of Bayesian optimization, Bayesian optimization with GP regression spends most of execution time in two individual steps: (i) building a GP regression model with optimal kernel free parameters and (ii) optimizing an acquisition function to find a next query point. The main interest of this paper is to alleviate the time complexity for the issue on GP regression, assuming a generic condition and its circumstance. To be precise, a step for model selection of GP accounts for a large portion of the consumed time, which is originated from matrix inverse operations (i.e., the

https://github.com/jungtaekkim/practical-bo-with-threshold-guided-mlm
time complexity of which is $O(n^3)$ where $n$ is the number of data points). Therefore, in this paper we tackle this problem, proposing the method to reduce the model selection step.

Since a surrogate function produces similar outputs as query points are accumulated, optimal free parameters of kernel in GP regression are not changed dramatically. Thus, in practice we might skip the model selection step where sufficiently enough data points have been observed. This observation encourage us to suggest our method. From now, we introduce backgrounds and main idea.

2 Background

In this section, we briefly introduce GP regression and model selection techniques for GP regression, which are discussed in this work.

2.1 Gaussian Process Regression

GP regression is one of Bayesian nonparametric regression methods, which provides function estimates and uncertainty estimates. The outputs of GP regression are used to balance exploration and exploitation in the perspective of Bayesian optimization. To compute a posterior mean function and a posterior covariance function, we need to set appropriate kernel free parameters in GP regression, using model selection which is described in Section 2.2. Due to a space limit, we omit the detailed explanation of GP regression. See [Rasmussen and Williams 2006] for the details.

2.2 Model Selection of Gaussian Process Regression

We usually choose one of two popular model selection techniques of GP regression: (i) marginal likelihood maximization (MLM) and (ii) leave-one-out cross-validation (LOO-CV), to find an optimal model that expresses the given dataset well. The marginal likelihood over function values $y \in \mathbb{R}^n$ conditioned on inputs $X \in \mathbb{R}^{n \times d}$ and kernel free parameters $\lambda$ (in this paper $\lambda \in \mathbb{R}^{d+1}$, but it can be differed as a type of kernel) is

$$L_{ML} = \log p(y|X, \lambda) = -\frac{1}{2} y^T (K(X, X) + \sigma^2_n I)^{-1} y - \frac{1}{2} \log \det (K(X, X) + \sigma^2_n I) - \frac{n}{2} \log 2\pi \tag{1}$$

where $K(X, X) \in \mathbb{R}^{n \times n}$ is a covariance function that maps from two matrices to all pairwise comparisons in two matrices, and $\sigma_n$ is an observation noise. (1) is maximized to choose an optimal kernel free parameters in the MLM.

The leave-one-out log predictive probability (a.k.a. log pseudo-likelihood) is

$$L_{LOO} = \sum_{i=1}^{n} \log p(y_i|X, y_{-i}, \lambda) \tag{2}$$

where $\log p(y_i|X, y_{-i}, \lambda) = -\frac{1}{2} \log \sigma_i^2 - \frac{(y_i - \mu_i)^2}{2\sigma_i^2} - \frac{1}{2} \log 2\pi$. Note that $y_{-i} \in \mathbb{R}^{n-1}$ is all function values except index $i$ and $\mu_i/\sigma_i^2$ are posterior mean/variance functions. Since we can preemptively compute the inverse of $K(X, X) + \sigma^2_n I$, the time complexity of (2) is almost similar to (1).
We propose a practical Bayesian optimization framework with threshold-guided MLM, which leads to speed up Bayesian optimization. As mentioned above, we assume that optimal kernel free parameters in GP regression are not significantly changed as Bayesian optimization procedure is iterated. To measure whether or not the model is converged, we can consider some metrics such as marginal likelihood and pseudo-likelihood. However, they are not appropriate to measure the discrepancy between two models we attempt to compare, because they are obtained from different data points and their corresponding observations (in practice two models are the models at iteration $t$ and iteration $t + 1$). For this reason, we simply compare the free parameters at iteration $t$ with the free parameters at the subsequent iteration, computing $l_2$ distance between them.

Our method is described in Algorithm 1. First of all, we provide four inputs: (i) a function domain $\mathcal{X} \in \mathbb{R}^d$ where $d$ is a domain dimension, (ii) the number of initial points $t \in \mathbb{Z} > 0$, (iii) iteration budget $\tau \in \mathbb{Z} > 0$, and (iv) a convergence threshold $\rho \in \mathbb{R} > 0$. Our method basically follows an ordinary Bayesian optimization procedure. After it finds $t$ initial points and their observations, iterate querying and observing steps $\tau$ times, as shown in Line 4 to 12 of Algorithm 1. The main difference between an ordinary Bayesian optimization and our method is presented in Line 4 to 10. We assess the distance between the last two kernel free parameters after obtaining at least two optimal free parameters, as shown in Line 4. If the distance is larger than $\rho$, new optimal free parameters are found by maximizing marginal likelihood. Otherwise, the previous kernel free parameters are used to build a surrogate function. Due to logical flow and space limit, we omit the detailed explanation of ordinary Bayesian optimization. See the details of Bayesian optimization in [Brochu et al. 2010], [Shahriari et al. 2016], [Frazier 2018].

Although it is a practical and simple algorithm to find a global optimum of black-box

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**Algorithm 1 Practical Bayesian Optimization with Threshold-Guided MLM**

**Input:** Function domain $\mathcal{X} \in \mathbb{R}^d$ where $d$ is a dimension of domain, the number of initial points $t \in \mathbb{Z} > 0$, iteration budget $\tau \in \mathbb{Z} > 0$, and a threshold for validating convergence $\rho \in \mathbb{R} > 0$

**Output:** Point $x^\dagger$ that has shown the best observation.

1. Sample $t$ initial points randomly $\{x_i\}_{i=1}^t$ where $x \in \mathcal{X}$.
2. Observe $t$ points from $y = f(x) + \epsilon$ where $\epsilon$ is an observation noise, $\{y_i\}_{i=1}^t$.
3. for $j = t + 1, \ldots, \tau$ do
4. \hspace{1em} if $j > t + 2$ and $||\lambda^*_j - \lambda^*_{j-2}||^2 < \rho$ then
5. \hspace{2em} Build a surrogate model via GP regression with the previous kernel free parameters $\lambda^*_{j-2}$, $f(\cdot|\{x_i, y_i\}_{i=1}^{j-1}, \lambda^*_{j-1})$.
6. \hspace{2em} Consider $\lambda^*_j$ as $\lambda^*_{j-1}$.
7. \hspace{1em} else
8. \hspace{2em} Build a surrogate model via GP regression with MLM over kernel free parameters, $f(\cdot|\{x_i, y_i\}_{i=1}^{j-1}, \lambda^*_j)$.
9. \hspace{1em} end if
10. Keep the kernel free parameters $\{\lambda^*_i\}_{i=1}^{j-1}$.
11. Query a point to sample $x^*$, optimizing an acquisition function $a(\cdot|\{x_i, y_i\}_{i=1}^{j-1})$.
12. Update historical points and their associated observations $\{(x_i, y_i)\}_{i=1}^{j-1}$.
13. end for
14. return the point that has shown the best observation $x^\dagger = \arg\min_{(x,y)\in\{(x_i,y_i)\}_{i=1}^{t}} y$.

### 3 Main Algorithm

We propose a practical Bayesian optimization framework with threshold-guided MLM, which leads to speed up Bayesian optimization. As mentioned above, we assume that optimal kernel free parameters in GP regression are not significantly changed as Bayesian optimization procedure is iterated. To measure whether or not the model is converged, we can consider some metrics such as marginal likelihood and pseudo-likelihood. However, they are not appropriate to measure the discrepancy between two models we attempt to compare, because they are obtained from different data points and their corresponding observations (in practice two models are the models at iteration $t$ and iteration $t + 1$). For this reason, we simply compare the free parameters at iteration $t$ with the free parameters at the subsequent iteration, computing $l_2$ distance between them.
Figure 1: Results on Bayesian optimization of six benchmark functions. Horizontal and vertical axes stand for time (seconds) and model selection methods. LOO and tgMLM indicate LOO-CV and threshold-guided MLM, respectively. Ackley (4) is a four-dimensional Ackley function and the number of iterations for each round is described in each caption. All experiments are repeated 20 times.

function, it shows powerful performance according to our experimental results. Moreover, if we think over the implication of free parameters for the GP, this approach is intuitively reasonable. To show our method is effective, in the next section we demonstrate the results on six benchmark functions and two real-world problems. Furthermore, we will introduce the future directions to develop this idea to more theoretical and more sophisticated method.

4 Experiments

We conduct our method on six benchmark functions and two real-world problems. The baselines of our method is (i) MLM and (ii) LOO-CV with one of two local optimizers (i.e., BFGS and L-BFGS-B). The free parameter bounds of L-BFGS-B optimizer are $[10^{-2}, 10^3]$ for signal strength and $[10^{-2}, 10^3]$ for each dimension of length-scales. GP regression with Matérn 5/2 kernel and expected improvement criterion are used as surrogate function and acquisition function, respectively. Acquisition function is optimized by multi-started L-BFGS-B which is started from 100 uniformly sampled points [Kim and Choi, 2019]. Furthermore, $\rho$ is set by $5\%$ of $l_2$ norm of previous free parameter vector ($\rho = 0.05\|\lambda_{j-t-2}\|_2$ using the expressions in Algorithm 1), and $\tau$ is set by the number of iterations which is specified in each caption. All experiments given three initial points are repeated 20 times. To implement this work, bayeso [Kim and Choi, 2017] is used, and all codes are available in this repository.
Table 1: Quantitative results on Bayesian optimization of six benchmark functions. Arithmetic mean and standard deviation at the iteration where the fastest method reach the given budget $\tau$ are described. We use same settings and notations in Figure 1.

|                  | Ackley (4) | Branin | Eggholder |
|------------------|------------|--------|-----------|
| BFGS (MLM)       | 16.337 ± 2.047 | 0.414 ± 0.015 | -615.764 ± 127.834 |
| L-BFGS-B (MLM)   | 16.359 ± 2.051 | 0.422 ± 0.028 | -608.822 ± 137.141 |
| BFGS (LOO)       | 16.286 ± 2.167 | 0.456 ± 0.071 | -608.822 ± 137.141 |
| L-BFGS-B (LOO)   | 17.141 ± 1.936 | 0.482 ± 0.087 | -597.909 ± 136.818 |
| BFGS (tgMLM)     | 14.970 ± 1.782 | **0.413 ± 0.032** | -685.244 ± 99.999 |
| L-BFGS-B (tgMLM) | **14.968 ± 1.776** | 0.729 ± 0.649 | -676.851 ± 107.523 |

|                  | Holder Table | Goldstein-Price | Six-hump Camel |
|------------------|--------------|-----------------|----------------|
| BFGS (MLM)       | -17.334 ± 1.041 | 37.054 ± 25.619 | -0.088 ± 1.047 |
| L-BFGS-B (MLM)   | -17.359 ± 1.329 | 33.634 ± 24.705 | -0.161 ± 0.537 |
| BFGS (LOO)       | -17.377 ± 1.182 | 71.180 ± 63.215 | 0.331 ± 1.053  |
| L-BFGS-B (LOO)   | -16.859 ± 1.345 | 54.592 ± 44.281 | -0.207 ± 0.682 |
| BFGS (tgMLM)     | **-17.537 ± 1.131** | **26.288 ± 21.871** | -0.215 ± 0.960 |
| L-BFGS-B (tgMLM) | -17.276 ± 1.192 | 28.520 ± 21.294 | **-0.272 ± 0.627** |

bayeso repository

4.1 Benchmark Functions

We test six benchmark functions: Ackley (4), Branin, Eggholder, Holder Table, Goldstein-Price, and Six-hump Camel functions.

As shown in Figure 1, our methods (i.e., BFGS (tgMLM) and L-BFGS-B (tgMLM)) are faster than other methods, and simultaneously their convergence qualities are preserved. In particular, as shown in Table 1, arithmetic mean and its standard deviation at the iteration where the fastest method finishes the optimization steps for the given iteration budget $\tau$.

4.2 Real-World Problems

We test two real-world problems: hyperparameter optimization for (i) classification using random forests (referred to as RW-1) and (ii) regression with elastic net regularization (referred to as RW-2).

RW-1 trained by the Olivetti face dataset has four hyperparameters to optimize: (i) the number of estimators, (ii) maximum depth, (iii) minimum samples to split, and (iv) maximum features used to train a single estimator. RW-2 trained by the California housing dataset has three hyperparameters: (i) coefficient for $l_1$ regularizer, (ii) coefficient for $l_2$ regularizer, and (iii) maximum iterations to train. scikit-learn [Pedregosa et al., 2011] is used to implement these real-world problems.

5 Future Work and Conclusion

In this article, we propose the practical and easy-to-implement Bayesian optimization method. By our empirical results, we demonstrate our method is practically effective in terms of
Figure 2: Results on Bayesian optimization of real-world problems. All settings follow the settings in Figure 1.

Table 2: Quantitative results on Bayesian optimization of real-world problems. All settings follow the settings in Figure 1.

| Method          | RW-1       | RW-2       |
|-----------------|------------|------------|
| BFGS (MLM)      | 0.107 ± 0.008 | 0.491 ± 0.044 |
| L-BFGS-B (MLM)  | 0.109 ± 0.007 | 0.491 ± 0.044 |
| BFGS (LOO)      | **0.106 ± 0.012** | **0.498 ± 0.046** |
| L-BFGS-B (LOO)  | 0.114 ± 0.018 | 0.498 ± 0.046 |
| BFGS (tgMLM)    | 0.117 ± 0.024 | **0.475 ± 0.038** |
| L-BFGS-B (tgMLM)| 0.116 ± 0.021 | 0.476 ± 0.038 |

execution time and convergence quality. However, our algorithm is not sophisticated and a theoretical analysis of our method is not provided. Thus, we can develop our method to more theoretical and more novel method in the future work. Similar to [Kim and Choi 2019], we can bound a discrepancy between Bayesian optimization optimized by MLM and tgMLM with the probability described by some related factors. Moreover, we can propose a method to select free parameters from historical free parameters. Because we keep all historical free parameters, those can be used to determine the current free parameters without time-consuming model selection procedure.

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