Calibration Improves Bayesian Optimization

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Abstract
Bayesian optimization is a procedure that allows obtaining the global optimum of black-box functions and that is useful in applications such as hyper-parameter optimization. Uncertainty estimates over the shape of the objective function are instrumental in guiding the optimization process. However, these estimates can be inaccurate if the objective function violates assumptions made within the underlying model (e.g., Gaussianity). We propose a simple algorithm to calibrate the uncertainty of posterior distributions over the objective function as part of the Bayesian optimization process. We show that by improving the uncertainty estimates of the posterior distribution with calibration, Bayesian optimization makes better decisions and arrives at the global optimum in fewer steps. We show that this technique improves the performance of Bayesian optimization on standard benchmark functions and hyperparameter optimization tasks.

1 Introduction
Designing a complex system requires tuning multiple knobs or parameters to ensure good performance. In particular, machine learning models require tuning their hyperparameters in order to maximize predictive accuracy and other performance metrics [Snoek et al., 2012]. Selecting such parameters by hand is challenging and requires considerable time and expertise, which motivates the need for specialized algorithms.

Bayesian optimization has recently emerged as a powerful tool for hyperparameter search [Shahriari et al., 2016; Thornton et al., 2013; Bergstra et al., 2011; Snoek et al., 2012]. In its general form, Bayesian optimization optimizes a black-box objective function — i.e., a function that is initially unknown and that can be learned via a sequence of evaluation queries — by forming a probabilistic model that encodes our beliefs about the shape of the function and then iteratively selecting query points in order to strike a balance between learning the unknown shape of the function and finding its minimum.

Evaluating the objective function at each step of Bayesian hyperparameter optimization can be very expensive — it may involve training a machine learning model to measure its performance. Bayesian optimization aims to minimize the
number of objective function queries via its probabilistic model, whose predicted uncertainty envelopes help guide exploration and exploitation efforts [Frazier, 2018].

Despite their importance in guiding the optimization process, uncertainty estimates coming out of probabilistic models may not always be reliable [Guo et al., 2017]. In practice, they are often miscalibrated [Kuleshov et al., 2018], which impacts performance on downstream decision-making tasks, such as planning with a probabilistic model [Malik et al., 2019].

This paper takes a similar angle to that of Malik et al. [2019], and studies the role of calibration in Bayesian optimization. We argue that uncertainty estimates in Bayesian optimization models should be calibrated — this allows us to better balance exploration and exploitation and reach the optimum in a smaller number of steps. Specifically, we adapt the methods of Kuleshov et al. [2018] and Malik et al. [2019] and propose a simple calibration algorithm that improves the performance of Bayesian optimization. We show that this technique can result in faster convergence to higher quality optima in a range of benchmark functions and hyperparameter optimization tasks.

Contributions: This paper proposes a simple algorithm to calibrate the uncertainty estimates given by a probabilistic model in Bayesian optimization. This method results in better decisions while choosing the datapoints that are evaluated through the course of optimization. We show that our method finds optimal function values in a smaller number of steps in real-world hyperparameter optimization tasks as well as standard benchmark functions used to evaluate Bayesian optimization techniques, accelerating search by up to 50%.

2 Background

2.1 Bayesian Optimization

Notation. Bayesian optimization is a technique for finding the global minimum $x^* = \arg\min_{x \in \mathcal{X}} f(x)$ of an unknown black-box objective function $f : \mathcal{X} \to \mathbb{R}$ over an input space $\mathcal{X} \subseteq \mathbb{R}^D$. We assume there exists a data distribution $P$ over the features and labels $X, Y \in \mathcal{X} \times \mathbb{R}$, and we are given an initial labeled dataset $x_t, y_t \in \mathcal{X} \times \mathbb{R}$ for $t = 1, 2, ..., N$ of i.i.d. realizations of random variables $X, Y \sim P$.

Computing $f(x)$ is usually expensive in terms of computational resources, and we may not have access to the gradient of $f$. A classical application area of Bayesian optimization is hyperparameter search, where $x \in \mathcal{X}$ are choices of hyperparameters, and $f(x)$ is the resulting performance of a machine learning model.

Algorithm. We optimize $f$ iteratively. At each step, we form a probabilistic model $\mathcal{M} : \mathcal{X} \to (\mathbb{R} \to [0,1])$ of $f$. We use uncertainty estimates from this probabilistic model to pick an $x_{next}$ and update $\mathcal{M}$ iteratively. Algorithm 1 describes the basic Bayesian optimization loop.
Algorithm 1: Bayesian Optimization

Initialize base model $M$ with data $D = \{x_t, y_t\}_{t=0}^N$;
for $n = 1, 2, ..., T$ do
  $x_{next} = \arg \max_{x \in X} \text{Acquisition}(x, M);$  
  $y_{next} = f(x_{next});$
  $D = D \cup \{(x_{next}, y_{next})\};$
  Update model $M$ with data $D;$
end

Acquisition Functions. Expected Improvement, Probability of Improvement and UCB (Upper Confidence Bound) are common choices for the acquisition function [Frazier, 2018].

Let $f(x^*)$ be the maximum value found so far. The Probability of Improvement (PI) function is specified by $\text{Acquisition}_{PI}(x, M) = \arg \max_x P(f(x) \geq (f(x^*) + \epsilon))$. Expected Improvement (EI) can be written as $\text{Acquisition}_{EI}(x, M) = \arg \max_x E(f(\max(0, f(x) - f(x^*))))\{x_t, y_t\}_{t=0}^N$. Finally the Upper Confidence Bound (UCB) function is given by $\text{Acquisition}_{UCB}(x, M) = \mu(x) + \gamma \sigma(x)$ where $\gamma$ itself is a hyperparameter, and $\mu(x), \sigma(x)$ are the posterior mean and variance of $f(x)$ given by the probabilistic model. We use lower confidence bound (LCB) when considering minimization.

2.2 Calibration of Probabilistic Models

A desirable property of forecasts from a probabilistic model is calibration. Intuitively, calibration means that a 90% confidence interval for the output $y$ contains $y$ approximately 90% of the time.

Formally, suppose we have a model $H : X \rightarrow (\mathbb{R} \rightarrow [0, 1])$ that outputs a probabilistic forecast $F_x$ given an input $x$. We take $F_x$ to be a cumulative distribution function (CDF) and we use $F_X^{-1}(p) = \inf\{y : F_X(y) = p\}$ to denote its inverse, the quantile function. We say that $H$ outputs calibrated forecasts if $P(Y \leq F_X^{-1}(p)) = p \forall p \in [0, 1]$. Equivalent formulations used in this paper include $P(Y \leq y | F_X(Y) = p) = p, \forall p \in [0, 1]$.

Most machine learning models are not calibrated out-of-the-box. However, given a forecaster $H : X \rightarrow (Y \rightarrow [0, 1])$, we may use a technique called recalibration to learn a helper model $R : [0, 1] \rightarrow [0, 1]$ such that the forecasts $R \circ F$ are calibrated [Kuleshov et al., 2018]. We compute CDF $F_t$ for each output data-point $y_t$ and use this to estimate the empirical fraction of data-points below each quantile. Algorithm 2 outlines this procedure.

3 Calibrated Uncertainties in Bayesian Optimization

The probabilistic model $M$ of $f$ is a crucial ingredient of the Bayesian optimization process. This naturally raises the question of what type of probabilistic model is best suited for running an effective optimization process.
Algorithm 2: Calibrated Regression [Kuleshov et al., 2018]

\textbf{Input:} Dataset of probabilistic forecasts and outcomes \( \{F_t, y_t\}_{t=1}^N \)

1. Form recalibration set \( D = \{F_t, \hat{P}(F_t)\}_{t=1}^N \) where \( \hat{P}(p) = |\{y_t|F_t \leq p, t = 1, \ldots, N\}|/N \).

2. Train recalibrator model \( \mathcal{R} \) on dataset \( D \).

3.1 What Uncertainties Are Useful for Bayesian Optimization?

A natural property of good forecasts is calibration. However, many types of models, including recent methods based on deep neural networks, are not calibrated out of the box [Guo et al., 2017]. Gaussian processes may also be uncalibrated if their underlying Gaussian assumptions like stationarity of the objective function are not met [Snelson et al., 2004] [Rasmussen and Williams, 2005]. In this section, we examine whether calibration can improve Bayesian optimization.

The Role of Calibration. Recently, Malik et al. [2019] studied the role of probabilistic models in model-based reinforcement learning. They argued that probabilistic transition models should be calibrated, since this improves the estimation of future reward and leads to better decisions during planning.

This paper starts with the observation that Bayesian optimization is also a decision-making process similar to model-based planning. At each step, we make a decision about which \( x \in \mathcal{X} \) to query next based on a probabilistic model. On the basis of this intuition, we make a series of arguments for why these models should be calibrated in Bayesian optimization as well.

Formally, we define calibration in Bayesian optimization analogously to Kuleshov et al. [2018] and Malik et al. [2019]. We say that a Bayesian optimization model \( \mathcal{M} : \mathcal{X} \rightarrow (\mathbb{R} \rightarrow [0, 1]) \) is calibrated if \( P(Y \leq F_X^{-1}(p)) = p \ \forall p \in [0, 1] \), where \( F_X : \mathbb{R} \rightarrow [0, 1] \) is the forecast \( \mathcal{M}(X) \).

Balancing Exploration vs. Exploitation. A key challenge faced by Bayesian optimization algorithms is balancing exploration within the space of \( x \in \mathcal{X} \) — i.e., the process of learning the shape of the unknown function \( f \) — against exploitation — the process of selecting points \( x \) at which \( f \) takes small values. This tradeoff is analogous to that of a reinforcement learning agent that needs to explore its environment.

Crucially, exploration-exploitation decisions are made using a probabilistic model. In regions that are unexplored, the confidence interval around the value of \( f(x) \) is large, which increases the value of the acquisition function and makes it likely for us to select this point. For example, the UCB acquisition function directly corresponds to the value of a large (e.g., 80%) confidence interval.

In this setting, calibration is useful as it ensures that the width of the intervals accurately reflects our uncertainty about the function being modeled. Conversely,
an uncalibrated model is likely to be over-confident in certain regions, which will prevent the optimization process from exploring them well.

**Expectations Under Quantile-Calibrated Models.** Another benefit of calibrated models in reinforcement learning is accurate computation of expected values of future rewards [Malik et al., 2019]. Expectations also play a role in Bayesian optimization, particularly in certain types of acquisition functions.

We can formalize the intuition that calibration helps better compute expectations using the following proposition.

**Proposition 1.** Let $Q(Y|X)$ be a calibrated model over $X, Y \sim P$ such that $P(Y \geq y \mid Q(Y \geq y \mid X) = p) = p$. Then the expectation of $Y$ is the same under $P$ and $Q$: $E_{y \sim P(Y)}[y] = E_{x \sim P(X)}[E_{y \sim Q(Y \mid X=x)}[y]].$

This proposition is a direct analogue of Lemma 1 in Malik et al. [2019], with a few crucial differences. Unlike the lemma of Malik et al. [2019], ours applies to continuous variables, such as the output of a function $f$ optimized via Bayesian optimization. It only assumes that the calibration model $Q$ is quantile-calibrated, rather than making a stronger distribution calibration assumption. Note that the condition $P(Y \geq y \mid Q(Y \geq y \mid X) = p) = p$ is equivalent to quantile calibration.

Although the conditions of our proposition are more general, its conclusion is also weaker: we only consider expectations over $Y$, not functions of $Y$. However, in the context of Bayesian optimization, we are typically interested in the target variable $y = f(x)$ directly, and this formulation is sufficient, as we will discuss below.

### 3.2 Calibrated Bayesian Optimization

Based on the intuition outlined above, we propose a formal extension of Bayesian optimization that leverages calibrated models obtained using the recent technique of Kuleshov et al. [2018].

**General Procedure.** We aim to improve the decisions made at every step in Bayesian optimization by calibrating the underlying model $M : \mathcal{X} \to (Y \to [0, 1])$. The base model is commonly chosen to be a Gaussian Process, but can be anything in general (e.g., a neural network) that can represent a distribution over possible objective functions. We use the following general procedure.

Note that Algorithm 3 is effectively standard Bayesian optimization, except that we recalibrate $M$ at every step. We can represent the calibrated model as a combination of a base model $M$ and the recalibrator model $R$ that takes a forecast $F$ from $M$ and transforms it into a calibrated $R \circ F$. By a slight abuse of notation, we denote this by $F = R(M(x))$.

Note that this procedure treats $M$ as a black box. This makes our approach compatible with any baseline $R$ that can be interpreted as outputting a CDF. The inputs explored during Bayesian optimization are not i.i.d. in general, but we see that this algorithm works in practice.
Algorithm 3: Calibrated Bayesian Optimization

Initialize base model $M$ with data $D = \{x_t, y_t\}_{t=0}^M$;
$R \leftarrow \text{CALIBRATE}(M, D)$;

for $n = 1, 2, ..., T$ do
  $x_{next} = \arg\max_{x \in X} (\text{Acquisition}(x, R \circ M))$;
  $y_{next} = f(x_{next})$;
  $D = D \cup \{(x_{next}, y_{next})\}$;
  Update model $M$ with data $D$;
  $R \leftarrow \text{CALIBRATE}(M, D)$;
end

Recalibrating a Bayesian Optimization Model. A particular challenge faced by recalibration algorithms in the context of Bayesian optimization is that the dataset $D$ is small, and it is expensive to acquire more datapoints by evaluating $f$. In particular, we may not have enough data for a separate recalibration set. To address this challenge, we develop a recalibration procedure specialized for Bayesian optimization that can deal with small dataset sizes and that is based on cross-validation.

Algorithm 4: CALIBRATE

Input: Base model $M$, Dataset $D = \{x_t, y_t\}_{t=0}^N$

1. Initialize recalibration dataset $D_{\text{recal}} = \phi$

2. $S = \text{CREATE SPLITS}(D)$

3. For each $(D_{\text{train}}, D_{\text{test}})$ in $S$:
   (a) Train base model $M'$ on dataset $D_{\text{train}}$
   (b) Compute CDF dataset $\{(M'(x_i))(y_i)\}_{i=1}^M$ from dataset $D_{\text{test}}$
   (c) $D_{\text{recal}} = D_{\text{recal}} \cup \{(M'(x_i))(y_i), y_i\}_{i=1}^M$

4. Train recalibrator model $R$ on the recalibration dataset $D_{\text{recal}}$ using Algorithm 2

5. Return $(R)$

Algorithm 4 builds a recalibration dataset $D_{\text{recal}}$ via cross-validation on $D$. At each step of cross-validation, we train a base model $M'$ on the training folds and compute forecasts on the test folds. The union of all the forecasts on the test folds produces the final calibration dataset on which the recalibrator is trained. We have used the concept of quantile calibration from Algorithm 2 since the training dataset in this setup is small.

In our experiments, we used leave-one-out cross-validation within CREATE SPLITS.
Formally, given a dataset $\mathcal{D} = \{x_i, y_i\}_{i=1}^N$, \textsc{CreateSplits}(\mathcal{D}) produces $N$ train-test splits of the form \{($\mathcal{D} \setminus \{x_i, y_i\}, \{x_i, y_i\}$) | $i = 1, 2, ..., N$\}. Thus, the base model $\mathcal{M}'$ is trained on $(N-1)$ data-points in the train split and used to generate predicted output CDF for the only data-point $\{x_i, y_i\}, 1 \leq i \leq N$ within the test split. This process is repeated for each split, so that we have the output CDF for each of the $N$ data-points from our original training dataset. The time complexity of Algorithm 4 depends linearly on the number of splits. The choice of model $\mathcal{M}$ also influences the run-time of this algorithm.

4 Understanding the Role of Calibration in Bayesian Optimization

Having provided the formal definition of our algorithm, we can now examine in more detail the role of calibration in Bayesian optimization.

4.1 Empirical Analysis

In order to obtain an initial intuition about how calibration improves, we compare runs of calibrated and plain Bayesian optimization on a toy 1D task — the Forrester function (Figures 1 and 2). The full definition of our setup can be found in the Experiments section, but it is not essential to follow this example.

Both functions start at the same three points, which miss the global optimum in $[0.6, 0.9]$. The base function is overconfident, and never explores that region. However, the calibrated method learns around iteration 4 that its confidence intervals are uncalibrated and too narrow, and expands them. This leads it to immediately explore in $[0.6, 0.9]$ and find the global optimum. The uncalibrated method gets forever stuck at a local minimum near 0.2.

We observed similar behavior on many repetitions of this experiment. On some repetitions, the initial points were sampled sufficiently close to the global optimum, and the two methods performed similarly. Nonetheless, this experiment provides a concrete example for why calibration can improve Bayesian optimization.

4.2 Examining Acquisition Functions

Next, we analyze more closely the role of calibration for various common acquisition functions used in Bayesian optimization.

Probability of Improvement. The probability of improvement is given by $P(f(x) \geq (f(x^+) + \epsilon)$, where $\epsilon > 0$ and $x^+$ is the previous best point. Note that this corresponds to $1 - F_x(f(x^+) + \epsilon)$, where $F_x$ is the CDF at $x$ that is predicted by the model. In a quantile-calibrated model, these probabilities on average correspond to the empirical probability of observing an improvement event. This leads to acquisition function values that more accurately reflect the value of exploring specific regions; furthermore, if the model is calibrated, we
Figure 1: Eight steps of uncalibrated Bayesian optimization on the Forrester function (green) using the UCB acquisition function (red). The global minimum lies near 0.8; however, after sampling 3 initial points at random, the model is constant in [0.6, 0.9], while the true function has a large dip. Since confidence intervals in [0.6, 0.9] are fairly narrow, and the optimization algorithm never explores it, the global minimum is missed by a large margin.

Expected Improvement. The expected improvement can be defined as \( E[\max(f(x) - f(x^+), 0)] \). This corresponds to computing the expected value of the random variable \( R = \max(Y - c, 0) \), where \( Y \) is the random variable that we are trying to model by \( \mathcal{M} \), and \( c \in \mathbb{R} \) is a constant. If we have a calibrated distribution over \( Y \), it is easy to derive from it a calibrated distribution over \( R \). By Proposition 2, we can estimate \( E[R] \) under the calibrated model, just as we can estimate the probability of improvement in expectation.

Upper Confidence Bounds. The UCB acquisition function for a Gaussian process is defined as \( \mu(x) + \gamma \cdot \sigma(x) \) at point \( x \). For non-Gaussian models, this naturally generalizes to a quantile \( F^{-1}_x(\alpha) \) of the predicted distribution \( F \). In this context, recalibration adjusts confidence intervals such that \( \alpha \in [0, 1] \) corresponds to an interval that is above the true \( y \) a fraction \( \alpha \) of the time. This makes it easier to select a hyper-parameter \( \alpha \). Moreover, as \( \alpha \) or \( \gamma \) are typically annealed, calibration induces a better and smoother annealing schedule.
Figure 2: Eight steps of calibrated Bayesian optimization on the Forrester function (green) using the UCB acquisition function (red), starting from the same three initial points as the uncalibrated method. The recalibrator learns after iteration 4 that the model is overconfident, expanding its confidence intervals. This leads the model to explore in [0.6, 0.9] and find the global minimum. Thus, the calibrated method arrives at the global minimum in less number of steps.

5 Experiments

We perform experiments on several benchmark objective functions that are standard in the Bayesian optimization literature, as well as on a number of hyperparameter optimization tasks.

Setup. We use the Gaussian Process (GP) as our base model in the following experiments. However, our method can be applied to any probabilistic model underlying Bayesian optimization in general [Snoek et al., 2015] [Springenberg et al., 2016]. We implement our method on top of the GPyOpt library [authors, 2016] (BSD 3 Clause License) in Python. The output values of objective function are normalized before training the base GP model. The GP uses Radial Basis Function (RBF) kernel. In our implementation, we calibrate by mapping the standard deviation predicted by base model $\sigma$ to $\sigma_{\text{new}}$ such that the new CDF is calibrated according to Algorithm 2. Specifically, the standard deviation is increased or decreased to make sure that the uncertainty estimates derived from the resulting distribution are better calibrated. Leave-one-out cross-validation splits are used in the CREATESPLITS function in Algorithm 4. We use another GP as our recalibrator model $\mathcal{R}$. 

5.1 Forrester, Alpine and Six-Hump Camel functions

We run experiments on some commonly used functions that benchmark the performance of Bayesian optimization.

Forrester function is a simple 1-dimensional function with one local minimum and one global minimum, which we can use to visualize the progress of our algorithm. We have used the Lower Confidence Bound (LCB) as our acquisition function. The results for this function are shown in Figure 3(a). We can see that the calibrated method was able to search the global minimum before the uncalibrated method. The uncalibrated method was stuck in the local minimum and calibration allowed our method to escape it.

Alpine function is another benchmark function used to evaluate Bayesian optimization. This function has many local minima and one global minimum. It can be evaluated for any number of input dimensions. We experiment on Alpine function in 7 input dimensions, where \( x_i \in [-10, 10] \) for \( i \in \{1, 2, ..., 7\} \). We used LCB acquisition function here. We also compare this with Alpine function in 15 input dimensions. Figure 3(b) and Figure 3(c) show that the calibrated method continues to stay ahead of the uncalibrated method while finding the minima. In Figure 3(b), calibrated method was about 2x faster in searching the minimum at 10.

Six-hump camel back function has 6 local minima and two of them are global. The input is 2-dimensional and we consider the domain \( x_1 \in [-2, 2], x_2 \in [-1, 1] \). The comparative performance of Bayesian optimization with calibrated and uncalibrated method under Lower Confidence Bound (LCB) acquisition is shown in Figure 4(a). We also compare the performance of this function under Expected Improvement (EI) and Probability of Improvement (PI) acquisition functions in Figure 4(c) and Figure 4(b) respectively.

In all these examples, we see that the calibrated method finds the minimum before the uncalibrated method on an average. Each of these experiments is repeated 5 times and the results are averaged over these runs.

5.2 Hyperparameter optimization tasks

We consider three hyperparameter optimization tasks: Online Latent Dirichlet Allocation (LDA), SVHN dataset classification and CIFAR10 dataset classification. All these experiments use Expected Improvement as acquisition function. For all these experiments, we use 5 randomly chosen data-points to initialize the base GP and run Bayesian optimization for 30-50 steps. This is repeated 5 times and the results are averaged over these 5 runs. We ran these experiments on a GPU cluster.

5.2.1 Online LDA

In the Online LDA algorithm, we have three hyperparameters: \( \tau_0 \) and \( \kappa \) which control the learning rate and minibatch size \( s \) used while running the algorithm \cite{Hoffman2010}. We use the grid of parameters mentioned in Table 2 in
the Appendix as the input domain while running Bayesian optimization. We run this algorithm on the 20 Newsgroups dataset which contains 20,000 news documents partitioned evenly across 20 different newsgroups. We train the algorithm on 11,000 randomly chosen documents. A test-dataset of 2200 articles is used to assess the perplexity. Thus, the objective function in this experiment takes as its input hyperparameters ($\kappa, \tau_0, s$), runs the online LDA algorithm on the training set and outputs perplexity on the test dataset after running the Online LDA algorithm to convergence. The results are shown in Figure 5(a). We see that the calibrated method achieves a configuration of hyperparameters giving lower perplexity on an average. In Figure 5(a) we see that the error bars around the averaged runs are intersecting significantly as there was more variation across experiment repetitions. Hence, we add a separate plot showing the average of improvement made by the calibrated method over uncalibrated method during individual runs of the experiment. Formally, the improvement at any given iteration of Bayesian optimization is the difference between the best minimum found by uncalibrated method and the best minimum found by calibrated method. We see that the average improvement made by the calibrated method and the error bars surrounding it are positive most of the time in Figure 5(a).

### 5.2.2 Image Classification Using Neural Networks

The Convolutional Neural Network (CNN) architecture is commonly used for image classification. In our experiment, we define a CNN with 6 tunable hyperparameters – batch-size, learning-rate, learning-rate decay, l2-regularization, number of convolutional filters and number of neurons in the fully connected layer. The exact range of values used for these parameters is mentioned in
We compare the effect of calibration under different acquisition functions. On an average, we continue to see that the calibrated method (blue) dominates the uncalibrated method (yellow) by achieving the minimum value of function using less number of steps in Bayesian optimization. The blue and orange lines show the value of best minimum found at a given iteration, averaged over 5 repetitions of the experiment, for calibrated and uncalibrated method respectively. The shaded regions represent confidence interval equal to two standard deviations in both directions over multiple repetitions of the experiment.

With these hyperparameter values as input, our objective function trains the CNN and returns the classification error on test dataset. We use Bayesian optimization to search for an optimum configuration of hyperparameters that results in lower classification error. We run our experiments on CIFAR10 [Krizhevsky 2009] and SVHN datasets [Netzer et al., 2011]. The results appear in Figure 5(b) and Figure 5(c).

Figure 5(b) shows experimental results on the CIFAR10 dataset. Here, we see that the calibrated method achieves a lower classification error on an average at the end of 50 iterations of Bayesian optimization. The calibrated method also achieves this minimum using about 50% less number of steps. In the SVHN experiment, we see that the calibrated method does not show any significant improvement, but is also not worse on an average.

6 Discussion

Limitations. We demonstrate that calibrated Bayesian optimization helps us search the optima of an objective function in less number of steps on an average, but there can be situations where calibration does not improve performance. The image classification experiment on SVHN dataset is an example of this. It is important to further understand the situations where calibration does not give significant benefits and if we can modify our algorithm to improve the performance in such cases. Studying the properties of objective functions where calibrated Bayesian optimization produces more benefits can be useful.
Figure 5: Comparison of Bayesian optimization in Hyperparameter Optimization tasks. The top plots in red show the average of improvement made by the calibrated method over uncalibrated method during individual runs of the respective experiment. In the plots on the bottom, the blue and orange lines correspond to average of the best minimum found by Bayesian optimization at a given iteration, for calibrated and uncalibrated method respectively. The shaded region surrounding these lines represent confidence interval equal to two standard deviations of the corresponding value over multiple repetitions of the experiment.

Extensions and new applications. Bayesian optimization can use various underlying base models including neural networks [Snoek et al., 2015]. It would be interesting to understand the benefits of calibration in a greater variety of underlying models and acquisition functions. Gómez-Bombarelli et al. [2018] use Bayesian optimization to search within latent space of the Variational Auto-Encoder (VAE) for proposing chemical structures with desirable properties. It would be interesting to apply our method to such novel applications. The recalibration dataset is small due to which the design of calibration algorithm is important. We have used the idea of calibration for regression given by Kuleshov et al. [2018] in this paper. However we would also like to understand if other calibration methods like distribution calibration [Song et al., 2019] could help Bayesian optimization. Finally, it would be interesting to understand how the performance of our calibration algorithm changes under varying acquisition functions.

7 Related Work

Bayesian Optimization. Bayesian optimization is commonly used for optimizing black-box objective functions in applications like robotics [Calandra et al., 2016].
reinforcement learning [Brochu et al., 2010], hyperparameter optimization [Bergstra et al., 2011], recommender systems [Vanchinathan et al., 2014], automatic machine learning, [Thornton et al., 2013] and materials design [Frazier and Wang, 2015]. The choices like acquisition function [Snoek et al., 2012], kernel function [Duvenaud et al., 2013] and transformation of input spaces [Snoek et al., 2014] are important in making sure that the optimization works efficiently.

**Calibrated Uncertainties** Platt scaling [Platt, 1999] and isotonic regression [Niculescu-Mizil and Caruana, 2005] are popular ways for calibrating uncertainties. This concept can be extended to regression calibration [Kuleshov et al., 2018], distribution calibration [Song et al., 2019], online learning [], and structured prediction [Kuleshov and Liang, 2015]. Accurate uncertainty representation has been studied for applications like model-based reinforcement learning [Malik et al., 2019], semi-supervised learning [Kuleshov and Ermon, 2017], neural networks [Guo et al., 2017], natural language processing, models [Nguyen and O’Connor, 2015], weak supervision [Ren et al., 2018], and neural machine translation [Kumar and Sarawagi, 2019].

8 Conclusion

Bayesian optimization is used for optimizing black-box functions with minimal number of steps. Accuracy of uncertainty envelopes is important for balancing exploration-exploitation decisions which guide the iterative optimization process. We show that we can calibrate the underlying probabilistic model without using additional function evaluations. Our approach results in improved average performance of Bayesian optimization in standard benchmark functions and hyperparameter optimization tasks.

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A  Hyperparameter Settings

| Name of HP                    | Bounds                  | Type of domain         |
|-------------------------------|-------------------------|------------------------|
| Batch size                    | [32, 512]               | Discrete (step size 32) |
| Learning rate                 | [0.0000001, 0.1]        | Continuous (log-scale) |
| Learning rate decay           | [0.0000001, 0.001]      | Continuous (log-scale) |
| L2 regularization             | [0.0000001, 0.001]      | Continuous (log-scale) |
| Outchannels in fc layer       | [256, 512]              | Discrete (step size=16) |
| Outchannels in conv layer     | [128, 256]              | Discrete (step size=16) |

Table 2: Hyperparameters for Online LDA

| Name of HP   | Bounds                  | Type of domain         |
|--------------|-------------------------|------------------------|
| Minibatch size | [1, 128]          | Discrete (log-scale)   |
| $\kappa$     | [0.5, 1]               | Continuous (step-size=0.1) |
| $\tau_0$     | [1, 32]                | Discrete (log-scale)   |

B  Mathematical Proofs

**Proposition 2.** Let $Q(Y|X)$ be a calibrated model over $X,Y \sim P$ such that $P(Y \geq y | Q(Y \geq y | X) = p) = p$. Then the expectation of $Y$ is the same under $P$ and $Q$:

$$E_{y \sim P(Y)} [y] = E_{x \sim P(X)} E_{y \sim Q(Y|X=x)} [y].$$

(1)

*Proof.* In this proof, we will use the well-known identity that for a non-negative $Y$,

$$E[Y] = \int_0^\infty F(Y \geq y)dy,$$

where $F$ is the CDF of $Y$.

Next, note that we can rewrite the expectation on the LHS of Equation 1 as:

$$E_{y \sim P(Y)} [y] = \int_0^\infty P(Y \geq y)dy$$

$$= \int_0^1 \int_0^\infty P(Y \geq y, Q(Y = y | X) = p)dydp$$

$$= \int_0^1 \int_0^\infty \left(P(Y \geq y | Q(Y \geq y | X) = p) \cdot P(Q(Y = y | X) = p)\right) dydp.$$
where we used the above identity in the first line, the law of total probability in the second line, and the chain rule in the third line.

Next, we can use our assumption on the calibration of $Q$ to replace one of the terms with $p$, further expanding the above into:

$$
\mathbb{E}_{y \sim P(Y)}[y] = \int_0^\infty \int_0^1 p \cdot P(Q(Y \geq y \mid X) = p) \, dp
$$

$$
= \int_0^\infty \int_0^1 p \cdot \sum_{x \in \mathbb{X}} I[Q(Y \geq y \mid X = x) = p] \cdot P(X = x) \, dp
$$

$$
= \int_0^\infty \sum_{x \in \mathbb{X}} Q(Y \geq y \mid X = x) \cdot P(X = x) \, dp
$$

$$
= \sum_{x \in \mathbb{X}} P(X = x) \int_0^\infty Q(Y \geq y \mid X = x) \, dy
$$

$$
= \mathbb{E}_{x \sim P(X)} \mathbb{E}_{y \sim Q(Y \mid X = x)}[y],
$$

where in the last line we again used the identity $E[Y] = \int_0^\infty F(Y \geq y)dy$. This completes the proof. \qed