Bayesian Optimization with Missing Inputs *

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Abstract. Bayesian optimization (BO) is an efficient method for optimizing expensive black-box functions. In real-world applications, BO often faces a major problem of missing values in inputs. The missing inputs can happen in two cases. First, the historical data for training BO often contain missing values. Second, when performing the function evaluation (e.g. computing alloy strength in a heat treatment process), errors may occur (e.g. a thermostat stops working) leading to an erroneous situation where the function is computed at a random unknown value instead of the suggested value. To deal with this problem, a common approach just simply skips data points where missing values happen. Clearly, this naive method cannot utilize data efficiently and often leads to poor performance. In this paper, we propose a novel BO method to handle missing inputs. We first find a probability distribution of each missing value so that we can impute the missing value by drawing a sample from its distribution. We then develop a new acquisition function based on the well-known Upper Confidence Bound (UCB) acquisition function, which considers the uncertainty of imputed values when suggesting the next point for function evaluation. We conduct comprehensive experiments on both synthetic and real-world applications to show the usefulness of our method.

Keywords: Bayesian optimization · Missing data · Matrix factorization · Gaussian process.

1 Introduction

Bayesian optimization (BO) [20] is a powerful tool to optimize expensive blackbox functions. Typically, at each iteration BO first models the black-box function via a statistical model e.g. a Gaussian process (GP) based on historical data (*observed data*) and then seeks out the next point (*suggestion*) for function evaluation by maximizing an *acquisition function*. BO has been successfully applied to a wide range of practical applications such as hyper-parameter tuning, automated machine learning, material design, and robot exploration [22,15,6,16].

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Fig. 1: Four main steps in BO: (1) build a GP from the historical data $[\mathbf{X}, \mathbf{y}]$, (2) maximize an acquisition function α to get a suggested point x_t , (3) evaluate the suggested point x_t with the true black-box function and obtain a function value y, and (4) augment the historical data with the new observed point. With the presence of missing values in (M1) historical data and (M2) new observed *point*, BO faces two significant problems: it cannot build the GP at Step-1 and it cannot use the new observed point at Step-4.

In real-world applications, BO often faces a significant problem that is missing values in inputs. As shown in Figure 1, missing values in input can happen in two cases. First, similar to other machine learning models, the historical data for training BO may contain missing values (missing values in historical data). Without imputing these missing values, we cannot model the black-box function using GP. Second, when performing the function evaluation at the suggested point, if an error happens (e.g. failure of devices), we obtain the function value at an unknown random point (missing values in new observed point). Missing values in input can lead to many crucial failures in BO optimization such as erroneous calculation, and difficulties in interpretation and representation of information [21].

To address the missing input problem in BO, one approach is to apply imputation methods e.g. mean/mode imputation and k-nearest neighbors (KNN) [1,3] to fill missing values first and then apply a traditional BO method. Although these imputation methods can predict missing values, their performance is non-optimal since mean/mode methods do not consider the correlation between missing values and non-missing values while KNN strongly depends on the current available data and distance metric [5]. Recently, more complex imputation methods have been introduced, including using random forest [24] and deep neural network [26]; however, these methods require extensive training data, which is unrealistic in the BO context where the historical data is quite limited. Another approach is to simply apply BO to non-missing data where points with

 $\mathbf{2}$

missing values are removed [11]. As mentioned before, this approach does not use the data efficiently, leading to poor performance in optimization. Oliveira et. al proposed a BO method for uncertain inputs [16], where they observe the difference between the actual input value and the one recommended by BO, and they estimate the variance needed to build the probability distribution of input values. However, in the case of missing values, this variance is unknown (i.e. the noise level added to the actual input value is unknown), their method cannot approximate missing values well. To the best of our knowledge, there is no BO method that can directly handle missing values in input.

Our method. To overcome the disadvantages of existing methods, we propose a novel method (named **BOMI**) for optimizing black-box functions with missing values in input. In particular, we first adapt the idea of Bayesian probabilistic matrix factorization (BPMF) [19] to find the distribution of each missing value for imputation. Note that none of the imputation methods discussed above use the distributions of missing values for imputation even though these distributions are essential since they represent a certain level of noise in the actual values. By adapting the idea of BPMF, these distributions are built using one of the collaborative filtering technique so that the correlation between values in the data is taken into account. We then propose a new acquisition function, based on the widely used UCB acquisition function [23], to achieve greater confidence in modeling the black-box function. Our new acquisition function differs from a traditional acquisition function in a sense that it does not use one single GP built from imputed data but leverages multiple GPs to take into account the uncertainty of predicted values. By doing this, our method achieves an agreement on the imputed values that results in a higher confidence in the posterior predictive distribution. As a result, it improves the optimization performance when the black-box functions involve missing inputs.

To summarize, we make the following contributions.

- Develop <u>Bayesian Optimization with Missing Inputs</u> (BOMI) to optimize black-box functions with missing values in input.
- Propose a new acquisition function that takes into account the distributions of missing values when suggesting the next point for function evaluation.
- Demonstrate the usefulness of BOMI in both synthetic and real-world applications, and show that it outperforms well-known state-of-the-art baselines.

2 Background

2.1 Bayesian optimization

Bayesian optimization (BO) is an efficient method for automatically finding the optimum of an expensive black-box function within a small number of function evaluations [13,4]. Given an unknown function $f: \mathcal{X} \to \mathbb{R}$, our goal is to find the optimal input $x^* = \operatorname{argmax}_{x \in \mathcal{X}} f(x)$, where \mathcal{X} is a bounded domain in \mathbb{R}^d . Since the objective function f is expensive to evaluate, BO attempts to model f via a surrogate model e.g. Gaussian process (GP) [17]. The function f is assumed

to be drawn from the GP, i.e. $f(x) \sim \mathcal{GP}(\mu(x), k(x, x'))$, where $\mu : \mathcal{X} \to \mathbb{R}$ and $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ are mean and covariance functions. Normally, $\mu(x)$ is assumed to be zero and k is the squared exponential kernel (Equation (1)):

$$k(x, x') = \sigma^2 exp(-\frac{1}{2l^2} ||x - x'||^2)$$
(1)

where σ^2 is a parameter dictating the uncertainty in f, and l is a length scale parameter which controls how quickly f can change.

Given the historical data up to iteration t, $\mathcal{D}_t = \{(x_i, y_i)\}_{i=1}^t$ that contains inputs x_i and their evaluations $y_i = f(x_i) + \epsilon_i$ for i = 1, 2, ..., t where $\epsilon_i \sim \mathcal{N}(0, \sigma_{\epsilon}^2)$, we obtain the predictive distribution $f(x) \mid \mathcal{D}_t \sim \mathcal{N}(\mu_t(x), \sigma_t^2(x))$ with $\mu_t(x)$ and $\sigma_t^2(x)$ as:

$$\mu_t(x) = \mathbf{k}^T (\mathbf{K} + \sigma_\epsilon^2 \mathbf{I})^{-1} \mathbf{y}$$
(2)

$$\sigma_t^2(x) = k(x, x) - \mathbf{k}^T (\mathbf{K} + \sigma_\epsilon^2 \mathbf{I})^{-1} \mathbf{k}$$
(3)

where $\mathbf{y} = (y_1, ..., y_t)$ is a vector of function evaluations, $\mathbf{k} = [k(x_i, x)]_{\forall x_i \in \mathcal{D}_t}$ is the covariance between a new input x and all observed inputs x_i , $\mathbf{K} = [k(x_i, x_j)_{\forall x_i, x_j \in \mathcal{D}_t}]$ is the covariance matrix between all inputs, \mathbf{I} is an identity matrix with the same dimension as \mathbf{K} , and σ_{ϵ}^2 is a measurement noise.

BO uses the predictive mean and standard deviation in Equations (2) and (3) in an *acquisition function* $\alpha(x)$ to find the next point to evaluate. The acquisition function uses the predictive distribution to balance two contrasting goals: sampling where the function is expected to have a high value vs. sampling where the uncertainty about the function value is high. Some well-known acquisition functions are *Probability of Improvement* (PI) [12], *Expected Improvement* (EI) [10], *Upper Confidence Bound* (UCB) [23], and *Predictive Entropy Search* (PES) [9].

Since we use UCB as a base to develop a new acquisition function (see Section 3.3) for the optimization problem with missing inputs, we describe it in detail in the next section.

2.2 Upper Confidence Bound acquisition function

The UCB acquisition function is a weighted sum of predictive mean and variance from Equations (2) and (3), computed as:

$$\alpha_t^{UCB}(x) = \mu_t(x) + \sqrt{\beta_t}\sigma_t(x) \tag{4}$$

where β_t is the exploitation-exploration trade-off factor. Following [23], β_t is calculated as $\beta_t = 2 \log (t^2 2\pi^2/3\delta) + 2d \log (t^2 dbr \sqrt{\log (4da/\delta)})$ to guarantee an upper bound on the cumulative regret with probability greater than $1 - \delta$ in the search space $\mathcal{X} \subseteq [0, r]^d$, where r > 0 and a, b > 0 are constants.

To suggest a next point for the black-box objective function evaluation, we maximize the UCB acquisition function in Equation (4) as follows:

$$x_{t+1} = \underset{x \in \mathcal{X}}{\operatorname{argmax}} \ \alpha_t^{UCB}(x)$$
(5)

3 Framework

3.1 Problem definition

Before formally defining the problem of Bayesian optimization (BO) with missing inputs, we provide two cases when missing values occur in inputs.

Case 1. (Missing values in historical data) Given a point $\boldsymbol{x} = \{x_1, \ldots, x_d\}$ in historical data, \boldsymbol{x} contains missing values if $\exists x_i \in \boldsymbol{x} \ (i \in \{1, \ldots, d\} \text{ and } d \text{ is the input dimension})$ such that x_i is unobserved (i.e. missing), and we denote x_i by a question mark '?'.

Case 2. (Missing values in the next suggested point) At iteration t, when we intend to evaluate the black-box function f at a suggested point $\mathbf{x}_t = \{x_1, \ldots, x_d\}_t$ to obtain the function value y_t , two scenarios may arise. (1) Due to an error in the evaluation, the function may actually be evaluated at \mathbf{x}'_t instead of intended point \mathbf{x}_t . In general, we denote an element x'_i of \mathbf{x}'_t using the corresponding element of \mathbf{x}_t as $x'_i = x_i \pm \eta$ where η is an unknown noise amount. (2) In case of no error, \mathbf{x}'_t is same as \mathbf{x}_t .

We present the problem of BO with missing inputs. Given a historical data $[\mathbf{X}, \mathbf{y}]$ and a *black-box* function $f : \mathcal{X} \to \mathbb{R}$ (\mathcal{X} is the input domain), \mathbf{X} may contain missing values as mentioned in Case 1, and if we query a point $\mathbf{x}_t \in \mathcal{X}$ to compute the function value $y_t = f(\mathbf{x}_t)$, then we may obtain $y_t = f(\mathbf{x}_t')$ as mentioned in Case 2. Our goal is to find the optimal point \mathbf{x}^* that maximizes the black-box function f, as follows:

$$\boldsymbol{x}^* = \arg \max_{\boldsymbol{x} \in \mathcal{X}} f(\boldsymbol{x}) \tag{6}$$

3.2 Building a probability distribution for each missing value

Let \boldsymbol{x}_o and \boldsymbol{x}_m be non-missing and missing values. An observation is denoted as $\boldsymbol{x} = \{\boldsymbol{x}_o, \boldsymbol{x}_m\}$. To solve the optimization problem in Equation (6), one simple approach is to omit observations having missing values \boldsymbol{x}_m and then apply a standard BO to observations containing only non-missing values. As discussed in Section 1, this method may perform poorly since it has too few data points to build a good model. To overcome this, we propose to use the distribution of a missing value so that we can both impute it as well as utilize the uncertainty in its prediction. Therefore, instead of directly substituting $\boldsymbol{x} = c$ ($\boldsymbol{x} \in \boldsymbol{x}_m$ and c is a single constant value), we assume that $\boldsymbol{x} \sim p(\boldsymbol{x})$, where $p(\boldsymbol{x})$ is an unknown probability distribution of \boldsymbol{x} , and our goal is to find $p(\boldsymbol{x})$ for each $\boldsymbol{x} \in \boldsymbol{x}_m$.

We represent the observed data $[\mathbf{X}, \mathbf{y}]$ as a matrix $R = [\mathbf{X}, \mathbf{y}] \in \mathbb{R}^{N \times M+1}$, where N is the number of rows (data points) and M is the number of columns (features). Let x_{ij} be a missing value at row *i* and column *j*, and x_{ij} is assumed to be sampled from a normal distribution $p(x_{ij}) = \mathcal{N}\left(\mu_{x_{ij}}, \sigma_{x_{ij}}^2\right)$. To find the distribution $p(x_{ij})$, we adapt the idea of Bayesian probabilistic matrix factorization (BPMF) [19].

Our goal is to decompose the partially-observed matrix $R \in \mathbb{R}^{N \times M+1}$ into a product of two smaller matrices $U \in \mathbb{R}^{N \times K}$ and $V \in \mathbb{R}^{K \times M+1}$ such that $R \approx UV$ i.e. we find two matrices U and V whose product is as close as possible to the original matrix R.

We first construct the prior distributions on U and V as follows:

$$p(U \mid \mu_U, \Lambda_U) = \prod_{i=1}^{N} \mathcal{N} \left(U_i \mid \mu_U, \Lambda_U^{-1} \right) p(V \mid \mu_V, \Lambda_V) = \prod_{i=1}^{M+1} \mathcal{N} \left(V_i \mid \mu_V, \Lambda_V^{-1} \right)$$
(7)

where $\Theta_U = \{\mu_U, \Lambda_U\}$ and $\Theta_V = \{\mu_V, \Lambda_V\}$ are hyper-parameters of the priors. We learn them using Gibbs sampling [14].

Next, we sample U and V from their distributions, as in Equation (8):

$$U_i^{l+1} \sim p\left(U_i \mid R, V^l, \Theta_U^l\right) \text{ for } i = 1, \dots, N \text{ rows}$$

$$V_j^{l+1} \sim p\left(V_i \mid R, U^{l+1}, \Theta_V^l\right) \text{ for } j = 1, \dots, (M+1) \text{ columns}$$
(8)

where l is the number of iterations used in Gibbs sampling.

Finally, we reconstruct $R \approx UV$ and the missing value $x_{ij} = R_{ij}$ is filled by a linear combination of matrix product, i.e. $x_{ij} = U_{i,:}V_{:,j}$, where $U_{i,:}$ is the row *i* of *U* and $V_{:,j}$ is the column *j* of *V*.

Although we can impute a missing value using $x_{ij} = U_{i,:}V_{:,j}$, using a single predicted value is not effective. Thus, we go a step further to obtain the distribution $p(x_{ij})$ of x_{ij} . In particular, following [19] we use the Monte Carlo approximation [14] to approximate $p(x_{ij})$ as:

$$p(x_{ij}) \approx p(x_{ij} \mid U_{i,:}V_{:,j},\xi),$$

where $\xi = \sigma_{R_{ij}}^2$ (called *precision factor*) is the "width" of distribution covering the actual value of x_{ij} . To fill/predict a missing value x_{ij} , we simply draw a sample from its distribution $\tilde{x}_{ij} \sim p(x_{ij})$ and set $x_{ij} = \tilde{x}_{ij}$.

3.3 Bayesian optimization with missing inputs (BOMI)

In Section 3.2, we find a distribution $p(x_{ij})$ for each missing value x_{ij} . To optimize the black-box function $f(\mathbf{x})$, we can simply draw a sample $\tilde{x}_{ij} \sim p(x_{ij})$ to fill the missing value x_{ij} , and then apply a standard BO to the new non-missing data. We call this method *Imputation-BPMF*. However, the performance of this approach heavily depends on the quality of $\tilde{x}_{ij} \sim p(x_{ij})$. In other words, it does not consider the uncertainty of \tilde{x}_{ij} .

We propose a novel BO method to optimize black-box functions with missing inputs, called <u>Bayesian Optimization with Missing Inputs</u> (BOMI). Our method has three main steps, which illustrated in Figure 2. Step 1: from the observed data with missing values, BOMI learns a distribution for each missing value (see Section 3.2), then uses these distributions to impute and generate Qnew non-missing data. Step 2: for each new non-missing data, BOMI builds a GP and computes the acquisition function UCB (see Equation (4)). Step 3: **BOMI** aggregates the information from Q acquisition functions to come up with a new acquisition function that takes into account the uncertainty of imputed values. The new acquisition function (called **UCB-MI**) is described next.



Fig. 2: Three main steps in our method **BOMI**: (1) sample missing values from their distributions, (2) build GPs and compute UCB acquisition functions (Equation (4)), and (3) develop a new acquisition function based on aggregated information.

<u>Upper Confidence Bound acquisition function for Missing Inputs (UCB-MI)</u>. Our new acquisition function UCB-MI aggregates the information from Q standard UCB acquisition functions computed at Step-2, as follows:

$$U^{CB-MI}(x) = \mu_{\alpha} \left(\boldsymbol{\alpha}^{UCB}(x) \right) + \beta_{\alpha} \sigma_{\alpha} \left(\boldsymbol{\alpha}^{UCB}(x) \right)$$
(9)
$$= \frac{1}{Q} \sum_{q=1}^{Q} \left(\alpha_{q}^{UCB}(x) \right) + \beta_{\alpha} \sqrt{\frac{\sum_{q=1}^{Q} \left(\alpha_{q}^{UCB}(x) - \frac{1}{Q} \sum_{q=1}^{Q} \alpha_{q}^{UCB}(x) \right)^{2}}{Q-1}}$$

where α^{UCB} is the UCB acquisition function (see Equation (4)).

α

Our acquisition function α^{UCB-MI} is based on the commonly used UCB acquisition function, but it incorporates the posterior predictive information from different GPs. It is described as a summation of the mean of Q acquisition values $\mu_{\alpha}(\alpha)$ and their standard deviation $\sigma_{\alpha}(\alpha)$ multiplied by a trade-off factor β_{α} . This acquisition function quantifies the level of agreement between Q individual acquisition functions to determine the confidence in predicting the outcome of an input. As a result, we have more information about the variance of one point \boldsymbol{x} and more certainty about its outcome. To suggest a next point for evaluation, we maximize the acquisition function α^{UCB-MI} :

$$x_{t+1} = \operatorname*{argmax}_{x \in \mathcal{X}} \alpha^{UCB-MI}(x)$$
(10)

Discussion. We can see that when Q is set to a small value, our acquisition function α^{UCB-MI} is close to the standard acquisition function UCB α^{UCB} . For example, with Q = 1, the standard deviation $\sigma_{\alpha} \left(\boldsymbol{\alpha}^{UCB} \right) = 0$ and $\alpha^{UCB-MI}(x) = \alpha_1^{UCB}(x) + \beta_{\alpha} 0 = \alpha^{UCB}(x)$.

When Q > 1, the first term $\frac{1}{Q} \sum_{q=1}^{Q} (\alpha_q^{UCB}(x))$ in Equation (9) represents the average among different acquisition functions, which can be considered as an agreement on different acquisition functions. In contrast, the second term represents the disagreement on acquisition values since it is the standard deviation measuring how much acquisition functions differ from their mean (agreement). The trade-off factor β_{α} is used to control the balance between agreement and disagreement.

Our proposed method **BOMI** is summarized in Algorithm 1.

```
Algorithm 1: The proposed BOMI algorithm.
    Input: Observed data D_0, # iterations T, # new non-missing data Q
 1 begin
         for t = 0, ..., T do
 \mathbf{2}
             for q = 1, ..., Q do
 3
                  Sample U_{(q)} \sim p\left(U \mid R, V, \Theta_U\right) and V_{(q)} \sim p\left(V \mid R, U, \Theta_V\right)
 4
                   Generate new non-missing data R_{(q)} = U_{(q)}V_{(q)}
 5
                  Build GP GP_{(q)} \leftarrow R_{(q)}
 6
                  Compute acquisition function \alpha_q^{UCB} \leftarrow \text{Acquisition}(GP_{(q)})
 7
              \mathbf{end}
 8
              Compute \alpha^{UCB-MI} using Equation (9)
 9
             Suggest a next point x_{t+1} = \operatorname{argmax}_{x \in \mathcal{X}} \alpha^{UCB-MI}(x)
10
              Evaluate the objective function y_{t+1} = f(x_{t+1})
11
             if missing event then
12
                  x_{t+1} \to x'_{t+1} (see Case 2)
13
                  y_{t+1} = f(x_{t+1}')
14
              end
15
              Augment D_{t+1} = \{D_t, (x_{t+1}, y_{t+1})\}
16
17
         end
18 end
```

4 Experimental Results

We evaluate our proposed method **BOMI** in both synthetic and real-world applications. For synthetic experiments, we test our method with four benchmark synthetic functions to show its optimization performance and stability. For real-world experiments, we test the performance of our method in two real-world applications, namely, a robot exploration simulation and a heat treatment process. In these two applications, missing inputs often occur since the failures of robots and thermostat are unmanageable.

Baselines. We compare **BOMI** with six state-of-the-art baselines that use different ways to deal with missing values. They are categorized into two groups:

- Imputation-based methods: These methods first use imputation methods to predict missing values and then simply apply a standard BO method to optimize the black-box functions. Here, we use three well-known imputation methods in machine learning, namely, mean, mode, and KNN [3]. The mean method (called *Imputation-Mean*) replaces a missing value by the mean of its feature column. The mode method (called *Imputation-Mode*) replaces a missing value by the mode of its feature column. The KNN method (called *Imputation-KNN*) replaces a missing value by the mean value of its k nearest points. We also compare with *Imputation-BPMF*, where missing values are imputed using the BPMF method (see Section 3.3).
- **BO-based methods:** Since standard BO methods cannot directly deal with missing inputs, we consider two variants of BO. DropBO whenever a data point containing missing values occurs in historical data or new observed point, this method simply skips that data point and applies a standard BO method to non-missing data [11]. SuggestBO similar to DropBO this method removes data points containing missing values in historical data; however when a new observed point contains missing values, instead of skipping this new observation this method still uses it but substitutes missing values by the values suggested by the acquisition function. We also compare with BO-uGP [16] a recent BO method proposed for optimizing black-box functions with uncertain inputs. This method assumes that there is no missing values but all of them are noisy. It first maps all points into distributions and then builds a surrogate model over the distributions of points.

Implementation details. We implement our method **BOMI** and all baselines using GPyTorch [7] to accelerate matrix multiplication operations in GP inference. For a fair comparison, in our experiments we use the same kernel (*squared exponential* kernel) and identical initial points for all methods. For Imputation-KNN, we use the number of neighbors k = 5 and the Euclidean distance, following [2]. For BO-uGP, we use the same hyper-parameter setting, as mentioned in the paper. For our method **BOMI**, we set the dimension K of matrices U and V to 15, the precision $\xi=0.01$, the number of new non-missing data Q = 5, and the number of iterations in Gibbs sampling l = 40. We repeat each method 10 times and report the average result along with the standard error.

4.1 Synthetic experiments

We test our method and baselines with four benchmark synthetic functions where their characteristics are summarized in Table 1.

Performance comparison. The first experiment illustrates how our method **BOMI** outperforms other methods in terms of optimization result.

Experiment settings. We initialize 30 data points (historical data) for each function and keep them the same for all methods. To see the effect of missing values, we allow 80% of historical data to have missing values. When evaluating a suggested point, there is a probability ρ (called *missing rate*) that

Table 1: Characteristics of synthetic functions.

Function	Dimension	Range
Eggholder	2	$x_1, x_2 \in [-512, 512]$
Schubert	4	$x_i \in [-10, 10]$ for $i = 1, \dots, 4$
Alpine	5	$x_i \in [-10, 10]$ for $i = 1, \dots, 5$
Schwefel	5	$x_i \in [-500, 500]$ for $i = 1, \dots, 5$

the new observed point has missing values (i.e. an error occurs, see Case 2). With this probability ρ , an amount of noise η (called *missing noise*) is added to the suggested value, which is calculated as $x'_i = x_i \pm \eta r_i$, where x_i is the actual value suggested by the acquisition function, r_i is the value range of x_i , and x'_i is a random unknown value. In our experiments, we set $\rho = 0.25$ and $\eta = 0.05$ for all functions.



Fig. 3: Optimization results for four synthetic functions in Table 1.

Results and discussion. Figure 3 shows the optimization results for four synthetic functions in Table 1. We can see that our method **BOMI** generally outperforms other methods. On the 2d-function *Eggholder* (Figure 3(a)), **BOMI** and Imputation-BPMF are the two best methods, where they are slightly better than SuggestBO. When the dimension is increased up to 4 and 5 (Figure 3(b-d)), **BOMI** is always the best method, and especially it significantly outperforms other baselines on the 4d-function *Schubert* (Figure 3(b)).

Imputation-based methods (mean, mode, KNN, and BPMF) work fairly well; however, their performance is not very consistent. Mean and mode imputations often fall behind KNN since they suffer from biases. Imputation-BPMF is often better or comparable with other imputation methods, which verifies our intuition about the importance of distributions of missing values, as mentioned in Section 3.2. **BOMI** is often better than Imputation-BPMF. This clearly proves that our proposal of using probability distributions to impute missing values along with the new acquisition function is more effective, as discussed in Section 3.3.

DropBO underperforms on most functions since it throws away many observations when they contain missing values, which leads to too few data to train a good GP model. In contrast, SuggestBO is always better than DropBO since it has more observations by replacing the missing value with the value of suggested point. On the *Eggholder* function (Figure 3(a)), SuggestBO achieves a very good performance, where it is the second-best method. However, on other functions SuggestBO only achieves fair results since these functions vary very quickly even with a small change in the input values. As expected, BO-uGP unsuccessfully optimizes most functions due to its lack of the ability to handle missing values.

Stability comparison. The second experiment illustrates how different values of three factors missing rate ρ , missing noise η , and maximum number of missing values v affect to our method and other baselines. Note that ρ and η were defined in the first experiment setting, while v indicates how many dimensions in a data point contain missing values.

Experiment settings. We show the optimization result on the 5d-function *Schwefel* as a function of one chosen factor while the others are fixed to their default values. We sequentially set up three separate settings as follows:

- 1. Missing Rate. We fix $\eta = 0.05$ and v = 1, then let $\rho \in [0.25, 0.65]$ with a step of 0.1.
- 2. Missing Noise. We fix $\rho = 0.25$ and v = 1, then let $\eta \in [0.1, 0.9]$ with a step of 0.1.
- 3. Maximum number of missing values. We fix $\rho = 0.5$ and $\eta = 0.05$, then allow v in a range of [1, d-1], where d = 5 is the dimension of function.

Results and discussion. From Figure 4(a), we can see that when ρ increases, the performance of DropBO drastically declines. This can be explained by the fact that the number of observations in DropBO is inversely proportional to ρ , which leads to too few data to train a good optimization model. Similarly, BO-uGP also faces the same problem as DropBO since it has no mechanism to handle missing values. Meanwhile, SuggestBO seems to be unstable, where its performance drops at $\rho = 0.35$ and 0.45 but increases at $\rho = 0.55$ before going down again at $\rho = 0.65$. In contrast, imputation-based methods and our method **BOMI** are stable and robust to the missing rate, where the performance is just slightly changed with different values for ρ .

From Figure 4(b), when η increases SuggestBO heavily drops since it imputation error increases in proportional to η . Interestingly, the performance of DropBO does not change since the noise is only applied to observations with missing values and DropBO does not consider these observations. BO-uGP is the worst method in this experiment since it computes wrong probability distributions of very noisy values. Imputation-based methods except KNN wiggles a lot, indicating that they suffer from an over-fitting. In contrast, our method **BOMI** can maintain a good performance even with very high values for missing noise (e.g. $\eta = 0.8, 0.9$).



Fig. 4: Optimization results of our method **BOMI** and other methods on the 5d-function *Schwefel* with different values for (a) missing rate ρ , (b) missing noise η , and (c) maximum number of missing values v.

Finally, when the number of missing values increases (Figure 4(c)), all methods trend to decrease, as expected. When more values are missing, the correlation vanishes that, in turn, reduces the optimization performance. Our method is still the best method, where it significantly outperforms other methods. Similar to Figures 4(a-b), DropBO and BO-uGP perform poorly in this experiment, where they are the two worst methods.

4.2 Real-world experiments

We also demonstrate the benefits of our method in two real-world applications, namely, robot exploration simulation [18] and heat treatment process [8].

Robot exploration simulation. We use the simulation software named CoppeliaSim¹ v.4 to simulate an environment for a robot to explore and measure the concentration of copper in the soil [18]. The environment is created by using the dataset Brenda Mines², which includes a textured terrain, trees, and bumps. Our goal is to find the best configuration for the robot to obtain the highest percentage of copper.

Figure 5(a) visualizes the copper percentage in the dataset Brenda Mines, where the highest copper percentage is 1.024. This map is matched with the area shown in Figure 5(b), where the robot needs to explore. Figure 5(b) shows the starting location of the robot, its target location (i.e. its *next location*), and also obstacles (e.g. trees and bumps). A 2-wheel robot is allowed 10 seconds to move along a pre-calculated path to a specific next location. If the robot is unable

¹ https://www.coppeliarobotics.com/

² http://www.kriging.com/datasets/



Fig. 5: (a) A visualization of copper density in the dataset Brenda Mines – the darker blue indicates a location with more copper, and the highest copper percentage is 1.024. (b) A screenshot of the robot simulation using CoppeliaSim v.4 software [18] – the figure shows the starting location of the robot, its target location (i.e. *the next location it needs to move to*), and obstacles in the environment, e.g. trees and bumps.

to reach the target location within 10 seconds, it takes the measurement at the current location before the simulation stops. On the way to the target location, many errors such as overturn or being stuck can happen and prevent the robot from reaching the target location. Whenever these errors occur, a certain noise is added to the current location of the robot by the simulation software.

In this experiment, we tune four parameters X, Y, Z, and *velocity* of the robot. $X \in [1899.94, 4301.51]$ and $Y \in [2177.37, 5400.19]$ are the coordinators of the next location where the robot needs to move to. $Z \in [4330.96, 5467.46]$ is the depth underground that the robot needs to drill to measure the copper percentage at the location (X, Y). *velocity* $\in [200, 700]$ is the speed of robot moving; the value range of velocity is chosen according to the simulation and path finding algorithm. We use the missing rate $\rho = 0.5$ and the number of missing variables v = 1 (i.e. one of two coordinators of the robot can be missing). We do not set value for the missing noise η since the noise is automatically added by the simulation when errors happen.

From the result in Figure 6(a), we can see our method **BOMI** performs the best, where it significantly outperforms other methods after 70 iterations. Two imputation-based methods Imputation-KNN and Imputation-Mode perform well in this experiment, where Imputation-KNN is the second-best method. Interesting, BO-uGP shows a good performance in this application, where it is better than SuggestBO and two other imputation-based methods. Again, the performance of DropBO is very poor.

Heat treatment process. This is a process of heating an alloy to achieve a desired strength. In particular, an Al-Sc alloy is posed to the heat in four stages,



Fig. 6: Optimization results on two real-world applications: (a) robot exploration simulation and (b) heat treatment process.

where each stage has a different temperature and a different time duration. Our goal is to choose which temperature and how long to heat the alloy at each stage to maximize its strength.

To simulate the heat treatment process for Al-Sc alloy, we use the Kampmann-Wagner model [25], same as in [8]. At each stage, there are two values to set, temperature te (in °C) and time ti (in second). In total, we tune eight parameters, including $te_1 \in [1, 100], te_2 \in [1, 1000], te_3 \in [1, 1000], te_4 \in [1, 1000]$, and the heating times $ti_k \in [1, 21600]$ for $k \in \{1, 2, 3, 4\}$. Since both temperature and heating time can be missing, we set the missing rate and missing noise $\rho_1 = 0.35$, $\eta_1 = 0.8$ for temperature and $\rho_2 = 0.25, \eta_2 \in [0.7, 0.9]$ for heating time.

Figure 6(b) shows the optimization result for the heat treatment process. We can see our method **BOMI** is the best method, where it slightly outperforms the second-best method Imputation-KNN. Two BO-based methods SuggestBO and BO-uGP perform well and become the third-best method. It can be seen that BO methods are generally better than imputation-based methods in this experiment. We also see DropBO performs very poorly; it can be concluded that this method is not favorable in practice.

The results in Figure 6 again confirm the real benefits of our method not only in synthetic applications but also in real-world applications when optimizing black-box functions with missing inputs.

5 Conclusion

We have presented a novel BO method **BOMI** to optimize expensive black-box functions with missing values in inputs. Our method computes the distributions of missing values for imputation and develops a new acquisition function that takes into account the uncertainty of imputed values to suggest the next point with more confidence. We demonstrate the efficiency of **BOMI** with several benchmark synthetic functions and two real-world applications in robot exploration simulation and heat treatment process. The empirical results show that **BOMI** has a better and more stable performance compared to state-of-the-art baselines, especially in experiments with high missing rates. Our future work will focus on improving the prediction of missing values, which can help to improve the performance of our method.

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