Bayesian Optimization for Cascade-type Multistage Processes

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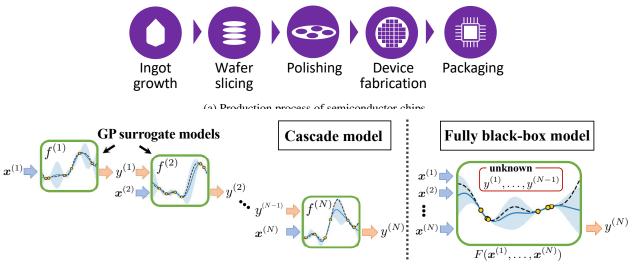
Abstract

Complex processes in science and engineering are often formulated as multistage decision-making problems. In this paper, we consider a type of multistage decision-making process called a cascade process. A cascade process is a multistage process in which the output of one stage is used as an input for the subsequent stage. When the cost of each stage is expensive, it is difficult to search for the optimal controllable parameters for each stage exhaustively. To address this problem, we formulate the optimization of the cascade process as an extension of the Bayesian optimization framework and propose two types of acquisition functions based on credible intervals and expected improvement. We investigate the theoretical properties of the proposed acquisition functions and demonstrate their effectiveness through numerical experiments. In addition, we consider an extension called suspension setting in which we are allowed to suspend the cascade process at the middle of the multistage decision-making process that often arises in practical problems. We apply the proposed method in a test problem involving a solar cell simulator, which was the motivation for this study.

1 Introduction

A complex process in science and engineering problems is often formulated as a multistage *cascade* process. For example, the production process of semiconductor chips consists of hundreds of process steps such as ingot growth, wafer slicing, and polishing, device fabrication, and packaging as shown in Figure 1 (a). Similarly, most manufacturing processes, including garment manufacturing, automobile manufacturing, and building construction are multi-stage processes. These multistage processes are often formulated as a cascade process in which the output of one stage is used as a part of the input for the subsequent stage.

Figure 1 (b) shows a schematic illustration of a cascade process. Each stage of a cascade process is formulated as a function with two types of inputs: the controllable parameters of that stage and the output of the previous stage. The former is controllable, whereas the latter is uncontrollable because of the uncertainty in the previous stage. The



(b) Schematic illustration of a cascade process.

Figure 1: (a) Example of the cascade manufacturing process for semiconductor chips. (b) The left part shows a cascade process with N stages, where the function $f^{(n)}$ is the black-box function representing the n^{th} stage for $n \in [N]$. The function $f^{(n)}$ considers two types of inputs: the controllable parameters of that stage $\boldsymbol{x}^{(n)}$ and the output of the previous stage. The goal of the cascade process optimization is to identify the controllable parameters of all the stages $\{\boldsymbol{x}^{(n)}\}_{n\in[N]}$ that optimize the output of the final stage. The right part shows the fully black-box model view of the problem, where the function F collectively considers all the controllable parameters $\{\boldsymbol{x}^{(n)}\}_{n\in[N]}$ as the inputs. By properly modeling each stage and incorporating the observable outputs in the middle of the cascade process $y^{(1)},\ldots,y^{(N-1)}$, more efficient optimization than that of the fully black-box model F is possible.

optimization of the entire cascade process can be formulated as a joint optimization problem by collectively considering the controllable parameters of all the stages as the inputs. Nevertheless, more efficient optimization is possible by properly modeling each stage and incorporating the observable outputs in the middle of the cascade process.

In this study, we consider the problem of optimizing a cascade process composed of black-box functions with expensive evaluation costs within the framework of Gaussian process-based (GP-based) Bayesian optimization (BO). Each stage is modeled as a GP, whose inputs consist of controllable parameters and the outputs from the previous stage. To optimize the output of the final stage, we consider the identification of the controllable parameters for each stage by considering the uncertainties of the GP models. The difficulty with this problem is that when setting the controllable parameters for each stage, decisions are made by considering the influence of the output of that stage on the subsequent stages.

Considering the main contribution of this study, we propose a method that deals with the intractable predictive distribution and develop two acquisition functions (AFs) based on the expected improvement (EI) and credible interval (CI). The proposed AFs can quantify the uncertainties of the subsequent stages in the cascade process using techniques developed in a multistep look-ahead strategy (Ginsbourger and Le Riche, 2010; Lam et al., 2016). The validity of the AFs was clarified through theoretical analysis, and their effectiveness was demonstrated using numerical experiments. Furthermore, as generalizations, we consider extensions of a cascade process optimization problem, such as the case where suspensions and resumes are possible in the middle of the cascade process and where the cost of each stage is different. Finally, we apply the proposed method to a test problem involving a solar cell simulator, which is the

motivation for this study.

Related Studies GP-based BO has been intensively studied as an efficient way to optimize black-box functions with high evaluation costs (Shahriari et al., 2015; Frazier, 2018). Various types of AFs were proposed for BO, such as Gaussian process upper confidence bound (GP-UCB) (Srinivas et al., 2010) and expected improvement (Močkus, 1975; Jones et al., 1998). The GP-based BO framework was extended to various problem settings, such as constrained optimization (Gardner et al., 2014; Takeno et al., 2022b), multiobjective optimization (Couckuyt et al., 2014; Suzuki et al., 2020), and multifidelity optimization (Swersky et al., 2013; Takeno et al., 2020, 2022a).

However, the only existing studies on cascade process optimization using a GP-based BO framework can be found in (Dai Nguyen et al., 2016) and (Astudillo and Frazier, 2021). In CBO (Dai Nguyen et al., 2016), the controllable parameters for each stage are determined in a reverse order (i.e., starting from the controllable parameters for the last stage, the second last stage, etc). That is, CBO selects the controllable parameters that are likely to produce the desired output, which is defined through the inverse function of the predictive mean function of the GP model in the subsequent stage. Importantly, since this desired output does not depend on the outputs from the previous stages, incorporating the observed outputs of the previous stages is difficult in CBO. Furthermore, if the earlier stages cannot achieve the desired output (which typically occurs when the range of each stage is unknown), the algorithm can become stuck. In addition, the exploration-exploitation trade-off cannot be considered in their method because the uncertainty of each stage is ignored when the desired output is predetermined by the predictive mean functions. Recently, a modified version of CBO was proposed in material science (Nakano et al., 2022). However, their approach is to address the practical application issues of CBO with some heuristics and does not fundamentally solve the drawbacks of CBO. EI-FN (Astudillo and Frazier, 2021) focuses on the optimization of a function network represented as a directed acyclic graph (DAG). Whereas their problem settings include the cascade structure as one of the DAGs, decision-making at each middle stage is not incorporated. In addition, noisy observations and suspension settings are not considered in their study. Furthermore, their approach is based on EI with full sampling (even the final stage), whereas our EI-based approach uses partial sampling, and we also provide a CI-based AF. Thus, our proposed method is clearly different from EI-FN.

One important related study is the study on multistep forward time-series prediction based on GP (Quinonero-Candela et al., 2002). In their study, the output of the GP at a time point becomes the input of the GP at the subsequent time point. This can be interpreted as a cascade process without controllable parameters. They introduced an iterative Gaussian approximation method to approximate the predictive distribution for the multistep forward time points. However, their method cannot be directly extended to cases with controllable parameters at each stage. Cascade process optimization is partially related to BO under input uncertainty because the output of the previous stage with uncertainty becomes the input of the subsequent stage. Recently, BO under input uncertainty was intensively studied (Beland and Nair, 2017; Oliveira et al., 2019; Iwazaki et al., 2021; Inatsu et al., 2021, 2022). However, these existing methods cannot be easily extended to our problem because the uncertainties in multiple stages are accumulated in a complicated manner in a cascade process. For example, an approach using the Bayesian quadrature framework (O'Hagan, 1991; Beland and Nair, 2017) cannot model the same cascade process correctly (see Appendix B for details). In our proposed method, the expected improvement in the cascade process is computed based on a multistage look-ahead strategy. Therefore, the BO methods for multistep look-ahead (Ginsbourger and Le Riche, 2010; Lam et al., 2016) are closely related to our method. In general, the exact evaluation of a look-ahead AF is difficult owing to its computational complexity. Our proposed method is based on several computational analyses developed in look-ahead type AFs, especially batch-type approximations (Jiang et al., 2020).

Reinforcement learning (RL) (Sutton and Barto, 2018; Bertsekas, 2019) is also formulated as a multi-stage decision-making problem, which often involves several uncertainties similar to the output of each stage in the cascade process. Thus, RL can be casted into the optimization of the cascade process by setting the state and action as the output from the previous stage and the input of the current stage, respectively. On the other hand, it is difficult to directly apply the RL algorithm to our cascade optimization problem because the problem setup differs in many aspects. For example, while the goal of RL is to maximize cumulative rewards, the goal of cascade process optimization is to find optimal input conditions for multiple stages. Furthermore, cascade process optimization has the limitation that function evaluation is costly and cannot be performed many times, making it difficult to apply the RL algorithm under such a limitation.

2 Preliminaries

2.1 Cascade Process Optimization

We consider a cascade process with N stages. Let $x^{(n)} \in \mathcal{X}^{(n)} \subset \mathbb{R}^{D^{(n)}}$ be a $D^{(n)}$ -dimensional controllable input and $y^{(n)} \in \mathcal{Y}^{(n)} \subset \mathbb{R}$ be a scalar output of the stage $n \in [N] := \{1, \dots, N\}$. Each stage is formulated as a function $f^{(n)}: \mathcal{Y}^{(n-1)} \times \mathcal{X}^{(n)} \to \mathcal{Y}^{(n)}$ and is written as

$$y^{(n)} = f^{(n)}(y^{(n-1)}, \boldsymbol{x}^{(n)}), n \in [N], \tag{1}$$

where we define $y^{(0)} = 0$ and $\mathcal{Y}^{(0)} = \{0\}$ for notational simplicity.

Combining all the inputs $\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N)}$, the entire cascade process can be represented as $y^{(N)}=F(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N)})$, where $F:\mathcal{X}^{(1)}\times\cdots\times\mathcal{X}^{(N)}\to\mathcal{Y}^{(N)}$ is recursively defined using (1). The goal of a cascade process optimization is to solve the following optimization problem:

$$x_*^{(1)}, \dots, x_*^{(N)} = \underset{(x_*^{(1)}, \dots, x_*^{(N)}) \in \mathcal{X}}{\arg \max} F(x_*^{(1)}, \dots, x_*^{(N)})$$
 (2)

with a number of function evaluations as small as possible, where $\mathcal{X} := \mathcal{X}^{(1)} \times \cdots \times \mathcal{X}^{(N)}$.

For simplicity, we consider the case in which the output of each stage is scalar. Furthermore, we assume that the output $y^{(n)}$ is observed without noise. Extensions to the case of multidimensional output and noisy observation settings are described in the Appendix.

2.2 GP Models

In this study, we employed GP models as surrogate models for black-box functions. One simple way to model the cascade process is the *fully black-box model* view, where we regard F as a single black-box function that outputs $y^{(N)}$ for a collected input $(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N)})$. However, regarding the fully black-box model view, the outputs observed in the intermediate stages of the cascade process cannot be effectively used. Therefore, we employ a *cascade model*, in which all stages are modeled by independent GP surrogate models. We assume that the prior distribution for $f^{(n)}$ is $\mathcal{GP}(0,k^{(n)})$, where $\mathcal{GP}(\mu,k)$ denotes a GP with mean and kernel functions μ and k, respectively. From the properties of a GP, given the observed data, the posterior distribution of $f^{(n)}$, $n \in [N]$ is also represented as a GP, and its mean and variance functions can be obtained in a closed form (Rasmussen and Williams, 2005).

3 Proposed Method

In this section, we consider the sequential observations of a cascade process from stage 1 to N. For each iteration $t \in \{0, N, 2N, \ldots\}$, users determine $\boldsymbol{x}_{t+1}^{(1)}$, a controllable parameter of stage 1, and observe an output $y_{t+1}^{(1)} = f^{(1)}(0, \boldsymbol{x}_{t+1}^{(1)})$. Subsequently, users choose $\boldsymbol{x}_{t+2}^{(2)}$, a controllable parameter of stage 2, and observe $y_{t+2}^{(2)} = f^{(2)}(y_{t+1}^{(1)}, \boldsymbol{x}_{t+2}^{(2)})$. By repeating this operation, users obtain $y_{t+N}^{(N)} = f^{(N)}(y_{t+N-1}^{(N-1)}, \boldsymbol{x}_{t+N}^{(N)})$.

Regarding the cascade process optimization problem in (2), the following two points should be considered: First, because the optimization target is the output of the final stage, a multistep look-ahead is indispensable when a decision is made in the earlier stages. Second, the input at each stage can be determined after observing the output of the previous stage. Therefore, when designing the AF for stage n, we need to consider $F(\boldsymbol{x}^{(n:N)} \mid y^{(n-1)})$, where the output of the final stage is represented as a function of the remaining controllable parameters $\boldsymbol{x}^{(n:N)} := (\boldsymbol{x}^{(n)}, \dots, \boldsymbol{x}^{(N)})$ given the output of the previous stage $y^{(n-1)}$. If the predictive distribution of $F(\boldsymbol{x}^{(n:N)} \mid y^{(n-1)})$ is available, appropriate AFs can be easily derived for stage n. However, in the cascade model, the predictive distributions of $F(\boldsymbol{x}^{(n:N)}|y^{(n-1)})$ cannot be explicitly written because of the nested structure of the cascade process. To address this problem, we consider two approaches. First, by utilizing the property that is easy to sample from nested predictive distributions, we propose an EI-based AF in section 3.1. Second, by constructing the credible interval of $F(\boldsymbol{x}^{(n:N)}|y^{(n-1)})$, we propose a CI-based AF in section 3.2.

3.1 EI-based Acquisition Function

In this subsection, we assume that the true black-box function $f^{(n)}$ is sampled from the GP prior $\mathcal{GP}(0,k^{(n)})$ for each $n\in[N]$. Let $F_{\mathrm{best}}=\max_{1\leq t'\leq t}y_{t'}^{(N)}$ be the maximum value of the objective function F observed up to iteration t. Thereafter, we define the improvement $U_n(\boldsymbol{x}^{(n)}|y^{(n-1)})$ for the observation of stage n with input $(y^{(n-1)},\boldsymbol{x}^{(n)})$ as the expected improvement of F_{best} . First, in the case of n=N, F_{best} is improved when $f^{(N)}(y^{(N-1)},\boldsymbol{x}^{(N)})>F_{\mathrm{best}}$. Therefore, the expected improvement of F_{best} , $U_N(\boldsymbol{x}^{(N)}|y^{(N-1)})$, is given by:

$$U_N(\boldsymbol{x}^{(N)}|y^{(N-1)}) = \mathbb{E}_{f^{(N)}} \left[\left(F(\boldsymbol{x}^{(N)}|y^{(N-1)}) - F_{\text{best}} \right)^+ \right], \tag{3}$$

where $(\cdot)^+ := \max(0, \cdot)$. Equation (3) is the same formulation as in the ordinary EI, and its expectation can be calculated analytically.

With regard to the case of $n \neq N$, we define $U_n(\boldsymbol{x}^{(n)}|y^{(n-1)})$ as the maximum expected improvement of $F(\boldsymbol{x}^{(n:N)}|y^{(n-1)})$:

$$U_n(\boldsymbol{x}^{(n)}|y^{(n-1)}) = \mathbb{E}_{f^{(n)}} \left[\max_{\boldsymbol{x}^{(n+1)}} U_{n+1}(\boldsymbol{x}^{(n+1)}|y^{(n)}) \right]. \tag{4}$$

Equation (4) is a recursive expression that contains the max operator and expectation. Thus, it is difficult to calculate it analytically. In the context of multistep look-ahead approaches, methods to avoid this problem through approximation and sampling have been investigated (Lam et al., 2016; González et al., 2016b; Wu and Frazier, 2019; Jiang et al., 2020). We use the similar approach as in (Jiang et al., 2020) to approximate the lower bound of (4). Using the Monte Carlo integration with S samples and the exchange of expectation and max operators (note that (5a) contains the nested

max operators and expectation), (4) can be approximated as follows:

$$U_n(\boldsymbol{x}^{(n)}|y^{(n-1)}) = \mathbb{E}_{f^{(n)}} \left[\max_{\boldsymbol{x}^{(n+1)}} \cdots \mathbb{E}_{f^{(N-1)}} \left[\max_{\boldsymbol{x}^{(N)}} U_N(\boldsymbol{x}^{(N)}|y^{(N-1)}) \right] \right]$$
 (5a)

$$\geq \max_{\boldsymbol{x}^{(n+1)},\dots,\boldsymbol{x}^{(N)}} \mathbb{E}_{f^{(n)},\dots,f^{(N-1)}} \left[U_N(\boldsymbol{x}^{(N)}|y^{(N-1)}) \right]$$
 (5b)

$$\approx \max_{\boldsymbol{x}^{(n+1)},\dots,\boldsymbol{x}^{(N)}} \frac{1}{S} \sum_{s=1}^{S} U_N(\boldsymbol{x}^{(N)}|y_s^{(N-1)}), \tag{5c}$$

where the inequality (5b) can be derived by (Jiang et al., 2020), and the sampling of $y_s^{(N-1)}$ is based on the GP model. First, we generate each $y_s^{(n)}$ from the predicted distribution of $f^{(n)}(y^{(n-1)}, \boldsymbol{x}^{(n)})$ independently. Then, we calculate the predicted distribution of $f^{(n+1)}(y_s^{(n)}, \boldsymbol{x}^{(n+1)})$ using the generated $y_s^{(n)}$, and we generate $y_s^{(n+1)}$ based on that. By repeating this process, $y_s^{(N-1)}$ can be generated. We propose the approximated utility function $\widetilde{U}_n(\boldsymbol{x}^{(n)}|y^{(n-1)})$, defined as (5c), as the EI-based AF. Therefore, given the observation $y_{t+n-1}^{(n-1)}$ of the previous stage, the observation point of the subsequent stage n is given by:

$$\boldsymbol{x}_{t+n}^{(n)} = \underset{\boldsymbol{x}^{(n)} \in \mathcal{X}^{(n)}}{\arg \max} \, \widetilde{U}_n(\boldsymbol{x}^{(n)}|y_{t+n-1}^{(n-1)}). \tag{6}$$

Although (5c) is the optimization problem for a stochastically determined function, deterministic gradient-based methods can be applied by applying the reparameterization trick (Kingma and Welling, 2014). Compared to EI-FN, which approximates all expectations by the Monte Carlo estimation, we analytically calculate the expectation with respect to $f^{(N)}$ in (5c). Furthermore, we select the controllable input in each stage depending on the output from the previous stage by using (6) in contrast to EI-FN which does not incorporate intermediate observations.

3.2 CI-based Acquisition Function

Thus far, we assume that each $f^{(n)}$ is sampled from the GP prior. Hereafter, we assume that each $f^{(n)}$ is an element of a reproducing kernel Hilbert space (RKHS). Under this RKHS setting, we propose a CI-based AF that can be interpreted as an optimistic improvement. First, we provide a credible interval of $F(\boldsymbol{x}^{(n:N)}|y^{(n-1)})$ and then, design the AF. To construct a valid CI, we assume the following regularity assumptions.

Regularity Assumptions We assume that $\mathcal{Y}^{(n-1)} \times \mathcal{X}^{(n)}$ is a compact set, and let $k^{(n)}$ be a positive definite kernel with $k^{(n)}((w, \boldsymbol{x}), (w, \boldsymbol{x})) \leq 1$ for any $n \in [N]$ and $(w, \boldsymbol{x}) \in \mathcal{Y}^{(n-1)} \times \mathcal{X}^{(n)}$. Furthermore, let $\mathcal{H}_{k^{(n)}}$ be an RKHS corresponding to the kernel $k^{(n)}$. Additionally, for each $n \in [N]$, we assume that $f^{(n)} \in \mathcal{H}_{k^{(n)}}$ and $\|f^{(n)}\|_{k^{(n)}} \leq B$, where B > 0 is a constant, and $\|\cdot\|_{k^{(n)}}$ denotes the RKHS norm on $\mathcal{H}_{k^{(n)}}$. There are several studies on BO using a GP model for the black-box function assumed as an element of an RKHS (Srinivas et al., 2010; Oliveira et al., 2019; Iwazaki et al., 2021).

To construct the credible interval of $F(\boldsymbol{x}^{(n:N)}|y^{(n-1)})$, we first formally define a posterior mean and variance of a GP with independent Gaussian noise $\mathcal{N}(0,\sigma^2)$. Note that what we have just introduced is the noise model $\mathcal{N}(0,\sigma^2)$ of a GP, and the actual observations are still noiseless. For each $n \in [N]$, $(w,\boldsymbol{x}) \in \mathcal{Y}^{(n-1)} \times \mathcal{X}^{(n)}$ and $t \geq 1$, let $\mu_t^{(n)}(w,\boldsymbol{x})$ and $\sigma_t^{(n)2}(w,\boldsymbol{x})$ be the posterior mean and variance of $f^{(n)}(w,\boldsymbol{x})$, respectively. The interval $[\mu_t^{(n)}(w,\boldsymbol{x}) \pm \beta^{1/2}\sigma_t^{(n)}(w,\boldsymbol{x})]$ with an appropriate trade-off parameter β is the credible interval for $f^{(n)}(w,\boldsymbol{x})$ (Srinivas et al., 2010). We apply this interval to construct a valid credible interval for $F(\boldsymbol{x}^{(n:N)}|y^{(n-1)})$. However, it cannot be used directly because it has an uncontrollable variable w. To avoid this issue, we additionally consider the following assumptions.

Lipschitz Continuity Assumptions We assume that $f^{(n)}$ and $\sigma_t^{(n)}$ satisfy the following assumptions:

- (L1) Assume that $f^{(n)}$ is L_f -Lipschitz continuous with respect to L_1 -distance for any $n \in \{2, ..., N\}$, where $L_f > 0$ is a Lipschitz constant.
- (L2) Assume that $\sigma_t^{(n)}$ is L_{σ} -Lipschitz continuous with respect to L_1 -distance for any $n \in \{2, ..., N\}$ and $t \geq 1$, where $L_{\sigma} > 0$ is a Lipschitz constant.

This assumption enables us to give the CI of the output using the CI of the input. Since the output becomes the input of the next stage in the cascade process, CIs of the subsequent stages can be constructed in a chain reaction.

Under these assumptions, we introduce a credible interval of $F(x^{(n:N)}|y^{(n-1)})$ using a cascade model.

Theorem 3.1. Let

$$\begin{split} \tilde{\mu}_t^{(m)}(\boldsymbol{x}^{(n:m)}|\boldsymbol{y}^{(n-1)}) &= \mu_t^{(m)} \left(\tilde{\mu}_t^{(m-1)}(\boldsymbol{x}^{(n:m-1)}|\boldsymbol{y}^{(n-1)}), \ \boldsymbol{x}^{(m)} \right), \\ \tilde{\sigma}_t^{(m)}(\boldsymbol{x}^{(n:m)}|\boldsymbol{y}^{(n-1)}) &= \sigma_t^{(m)} \left(\tilde{\mu}_t^{(m-1)}(\boldsymbol{x}^{(n:m-1)}|\boldsymbol{y}^{(n-1)}), \ \boldsymbol{x}^{(m)} \right) + L_f \tilde{\sigma}_t^{(m-1)}(\boldsymbol{x}^{(n:m-1)}|\boldsymbol{y}^{(n-1)}), \end{split}$$

where $\tilde{\mu}_t^{(n)}(\boldsymbol{x}^{(n)}|y^{(n-1)}) = \mu_t^{(n)}(y^{(n-1)}, \boldsymbol{x}^{(n)})$ and $\tilde{\sigma}_t^{(n)}(\boldsymbol{x}^{(n)}|y^{(n-1)}) = \sigma_t^{(n)}(y^{(n-1)}, \boldsymbol{x}^{(n)})$. Assume that regularity assumptions and the Lipschitz continuity assumption (L1) hold. Also assume that $\tilde{\mu}_t^{(m)}(\boldsymbol{x}^{(n:m)}|y^{(n-1)}) \in \mathcal{Y}^{(n)}$ for all $m \in [N]$, $t \geq 1$ and $\boldsymbol{x}^{(n:m)}$. Define $\beta = B^2$. Then, the following holds:

$$|F(\boldsymbol{x}^{(n:N)}|y^{(n-1)}) - \tilde{\mu}_t^{(N)}(\boldsymbol{x}^{(n:N)}|y^{(n-1)})| \le \beta^{1/2}\tilde{\sigma}_t^{(N)}(\boldsymbol{x}^{(n:N)}|y^{(n-1)}).$$

From Theorem 3.1, a lower confidence bound $\mathrm{LCB}_t^{(F)}(\boldsymbol{x}^{(n:N)}|y^{(n-1)})$ and an upper confidence bound $\mathrm{UCB}_t^{(F)}(\boldsymbol{x}^{(n:N)}|y^{(n-1)})$ of $F(\boldsymbol{x}^{(n:N)}|y^{(n-1)})$ are given by:

$$LCB_{t}^{(F)}(\boldsymbol{x}^{(n:N)}|\boldsymbol{y}^{(n-1)}) = \tilde{\mu}_{t-1}^{(N)}(\boldsymbol{x}^{(n:N)}|\boldsymbol{y}^{(n-1)}) - \beta^{1/2}\tilde{\sigma}_{t-1}^{(N)}(\boldsymbol{x}^{(n:N)}|\boldsymbol{y}^{(n-1)}),$$

$$UCB_{t}^{(F)}(\boldsymbol{x}^{(n:N)}|\boldsymbol{y}^{(n-1)}) = \tilde{\mu}_{t-1}^{(N)}(\boldsymbol{x}^{(n:N)}|\boldsymbol{y}^{(n-1)}) + \beta^{1/2}\tilde{\sigma}_{t-1}^{(N)}(\boldsymbol{x}^{(n:N)}|\boldsymbol{y}^{(n-1)}).$$
(7)

Based on the above credible intervals, we define the pessimistic maximum estimator of $F(\boldsymbol{x}^{(1:n)})$ as $Q_t := \max_{\boldsymbol{x}^{(1:N)}} \mathrm{LCB}_t^{(F)}(\boldsymbol{x}^{(1:N)})$. In addition, given the observation $y_{t+n-1}^{(n-1)}$ in stage n-1, we define the pessimistic maximum estimator of $F(\boldsymbol{x}^{(n:N)}|y^{(n-1)})$ as follows:

$$LCB_{t+n}^{(F)}(y_{t+n-1}^{(n-1)}) = \max_{\boldsymbol{x}^{(n:N)}} LCB_{t+n}^{(F)}(\boldsymbol{x}^{(n:N)}|y_{t+n-1}^{(n-1)}), \tag{8}$$

where the \max operator is not necessary when n=N. Similarly, the optimistic maximum estimator of $F(\boldsymbol{x}^{(n:N)}|y_{t+n-1}^{(n-1)})$ is defined as follows:

$$\mathrm{UCB}_{t+n}^{(F)}(\boldsymbol{x}^{(n)}|y_{t+n-1}^{(n-1)}) \coloneqq \max_{\boldsymbol{x}^{(n+1:N)}} \mathrm{UCB}_{t+n}^{(F)}(\boldsymbol{x}^{(n:N)}|y_{t+n-1}^{(n-1)}).$$

Then, we define the optimistic improvement with respect to $(y^{(n-1)}, x^{(n)})$ as follows:

$$a_{t+n}^{(n)}(\boldsymbol{x}^{(n)}|y_{t+n-1}^{(n-1)}) = \text{UCB}_{t+n}^{(F)}(\boldsymbol{x}^{(n)}|y_{t+n-1}^{(n-1)}) - \max\left\{\text{LCB}_{t+n}^{(F)}(y_{t+n-1}^{(n-1)}), Q_{t+n}\right\}. \tag{9}$$

Furthermore, we define the maximum uncertainty

$$b_{t+n}^{(n)}(\boldsymbol{x}^{(n)}|y_{t+n-1}^{(n-1)}) = \max_{\boldsymbol{x}^{(n+1:N)}} \tilde{\sigma}_{t+n-1}^{(N)}(\boldsymbol{x}^{(n:N)}|y_{t+n-1}^{(n-1)}). \tag{10}$$

Using (9) and (10), we propose a CI-based AF $c_{t+n}^{(n)}(x^{(n)}|y_{t+n-1}^{(n-1)})$:

$$c_{t+n}^{(n)}(\boldsymbol{x}^{(n)}|y_{t+n-1}^{(n-1)}) = \max\left\{a_{t+n}^{(n)}(\boldsymbol{x}^{(n)}|y_{t+n-1}^{(n-1)}), \eta_t b_{t+n}^{(n)}(\boldsymbol{x}^{(n)}|y_{t+n-1}^{(n-1)})\right\},\tag{11}$$

where η_t is some learning rate and tends to zero. Therefore, the subsequent observation point is given by $\boldsymbol{x}_{t+n}^{(n)} \coloneqq \arg\max_{\boldsymbol{x}^{(n)} \in \mathcal{X}^{(n)}} c_{t+n}^{(n)}(\boldsymbol{x}^{(n)}|y_{t+n-1}^{(n-1)}).$

Equation (8) denotes the pessimistic maximum when we observe in the subsequent stages with the previous output, and Q_t represents the pessimistic maximum when the observation is performed from the first stage. Thus, the second term of (9) indicates a pessimistic maximum estimator in the current iteration, and $a_t^{(n)}$ optimistically evaluates how much the observed value exceeds the pessimistically estimated maximum value. Intuitively, CI-based AF selects the point that has high optimistic improvement, and if no optimistic improvement is expected (i.e., $a_t^{(n)}$ is small), it selects the point with the highest uncertainty of the cascade process.

The Lipschitz constant L_f is a new parameter derived from our proposed method. Since each $f^{(n)}$ is a black-box function, it is difficult to obtain the exact value of L_f . In practice, we have to estimate L_f , and one simple way is to determine it from prior knowledge. Another way is to estimate it from a GP surrogate model. For any Lipschitz continuous function f on a compact set $\mathcal{X} \subset \mathbb{R}^d$, $\bar{L} = \max_{x \in \mathcal{X}} \|\nabla f(x)\|_1$ satisfies the Lipschitz condition (González et al., 2016a). Additionally, it is known that if a GP is differentiable, its derivative is also a GP. Based on these facts, we can estimate L_f by constructing a GP surrogate model of ∇f and using its sample paths and predictive mean (Sui et al., 2015; González et al., 2016a). On the other hand, for the Lipschitz continuity assumption (L2), it depends on how the kernel function is chosen. If we use a kernel that does not consider any similarity between different points, i.e., a pathological kernel such as k(x, x') = 1 if x = x', and otherwise zero, the posterior standard deviation is discontinuous at the observed points, and (L2) does not hold. On the other hand, (L2) is shown to hold for commonly used kernels such as linear kernels, Gaussian kernels, and Matérn kernels with more than one degree of freedom (see Appendix E for details).

We discuss the multidimensional output setting and the noisy observation setting in the Appendix. Particularly in noisy situations, two different target functions can be considered. One is to maximize F through noisy observations, and the other is to maximize the expected final output with respect to the noise at each stage. We also propose the modified version of CI-based AFs for both target functions and show the theoretical analyses of them in Appendix D.

4 Theoretical Results

In this section, we provide the theoretical guarantee for the CI-based AF. First, we define the estimated solution $\hat{x}_t^{(1)}, \dots, \hat{x}_t^{(N)}$ and regret r_t at iteration t as follows:

$$\hat{\boldsymbol{x}}_{t}^{(1)}, \dots, \hat{\boldsymbol{x}}_{t}^{(N)} = \underset{\boldsymbol{x}^{(1:N)} \in \mathcal{X}, 1 \leq \tilde{t} \leq t}{\arg \max} \operatorname{LCB}_{\tilde{t}}^{(F)}(\boldsymbol{x}^{(1:N)}),$$

$$r_{t} = F(\boldsymbol{x}_{*}^{(1)}, \dots, \boldsymbol{x}_{*}^{(N)}) - F(\hat{\boldsymbol{x}}_{t}^{(1)}, \dots, \hat{\boldsymbol{x}}_{t}^{(N)}).$$
(12)

Then, the following theorem holds.

Theorem 4.1. Under the same assumptions as in Theorem 3.1, define the estimated solution $(\hat{x}_t^{(1)}, \dots, \hat{x}_t^{(N)})$ by (12). Then, for any positive number ξ , the following holds:

$$\max_{\boldsymbol{x}^{(1:N)}} \text{UCB}_{t}^{(F)}(\boldsymbol{x}^{(1:N)}) - \max_{\boldsymbol{x}^{(1:N)}} \text{LCB}_{t}^{(F)}(\boldsymbol{x}^{(1:N)}) < \xi
\Rightarrow F(\boldsymbol{x}_{*}^{(1)}, \dots, \boldsymbol{x}_{*}^{(N)}) - F(\hat{\boldsymbol{x}}_{t}^{(1)}, \dots, \hat{\boldsymbol{x}}_{t}^{(N)}) < \xi.$$
(13)

Theorem 4.1 states that if the credible interval width for F is small, then regret r_t is also small. On the contrary, it does not guarantee whether the credible interval width becomes small or not. Theorem 4.2 shows that the interval width can be made arbitrarily small when (11) is used as the AF. Let $\gamma_t^{(n)}$ be a maximum information gain for $f^{(n)}$ at iteration t, and let $\gamma_t = \max_{n \in [N]} \gamma_t^{(n)}$. Here, the maximum information gain is a commonly used sample complexity measure in the context of the GP-based BO (Srinivas et al., 2010). The exact formulation is provided in Appendix A. The following theorem also holds.

Theorem 4.2. Assume that the same conditions as in Theorem 3.1 hold. Also assume that the Lipschitz continuity assumption (L2) holds. Let ξ be a positive number, and let $\eta_t = (1 + \log t)^{-1}$. Then, the following inequality holds after at most T iterations:

$$F(\boldsymbol{x}_*^{(1)}, \dots, \boldsymbol{x}_*^{(N)}) - F(\hat{\boldsymbol{x}}_T^{(1)}, \dots, \hat{\boldsymbol{x}}_T^{(N)}) < \xi,$$

where T is the smallest positive integer satisfying $T \in N\mathbb{Z}_{\geq 0} = \{0, N, 2N, \ldots\}$ and

$$\frac{8\beta C_4^2 N^3}{\log(1+\sigma^{-2})} \gamma_T \eta_T^{-2N-2} T^{-1} < \xi^2. \tag{14}$$

Here, each constant is given by $C_0 = L_{\sigma}\beta^{1/2} + L_f + 1$, $C_1 = \max\{1, L_f, L_f^{-1}\}$, $C_2 = 4N^2C_0^{2N-3}C_1^N$, $C_3 = NC_2^N$, $C_4 = (2\beta^{1/2} + 2)^NC_3^N$.

The inequality (14) still has the variable γ_T . Nevertheless, the order of γ_T for commonly used kernels such as the linear and Gaussian kernels is sub-linear under mild conditions (Srinivas et al., 2010). Hence, the integer T satisfying (14) exists in these cases. This indicates that a solution $\hat{x}_T^{(1)}, \ldots, \hat{x}_T^{(N)}$ that achieves an arbitrary accuracy ξ can be obtained in a finite number of observations.

In terms of the stopping criterion, if the accuracy parameter ξ is provided, we can use the condition (13) as the stopping criterion for EI- and CI-based AFs. Although EI-based AF is not necessarily terminated by this stopping criterion, Theorem 4.2 shows that CI-based AF terminates after at most T iteration that satisfies (14) when all assumptions hold.

5 Extensions

In this section, we consider an extension called *suspension* setting in which we are allowed to suspend the cascade process in the middle of the multistage decision-making process. Suspension is beneficial, especially when the output of a middle stage is significantly different from the prediction, and the output is not expected to be beneficial for the subsequent stages. For example, if a suspension occurs at stage n, the output $y^{(n-1)}$ of the previous stage remains unused, and this can be stored as a *stock*. If a stored stock turns out to be useful later, we can reuse the stock and resume the cascade process from the middle stage.

Formulation Let $\mathcal{S}_t^{(n)}$ be the set of stocks at stage $n \in \{0,...,N-1\}$ in iteration t ¹. Because the process can be resumed from the middle stage in the suspension setting, the user's task in each iteration t is to select the best pair $(y^{(n-1)}, \boldsymbol{x}^{(n)})$ from the set of candidates $\{\mathcal{S}_t^{(n)} \times \mathcal{X}^{(n)}\}_{n=0}^{N-1}$. Because of a user's choice, the used stock $y^{(n-1)}$ is removed from the set of stocks, and the newly obtained output $y^{(n)}$ is added to the set of stocks. The difference in the cost of each stage is important in the suspension setting because, for example, if the costs of the later stages are greater than those of former stages, then the suspension strategy can be more beneficial. Therefore, we introduce the cost of each stage $\lambda^{(n)} > 0$ for $n \in [N]$. Figure 2 shows a conceptual diagram of the suspension setting.

¹We set $S_{t}^{(0)} = \{0\}$ for all t.

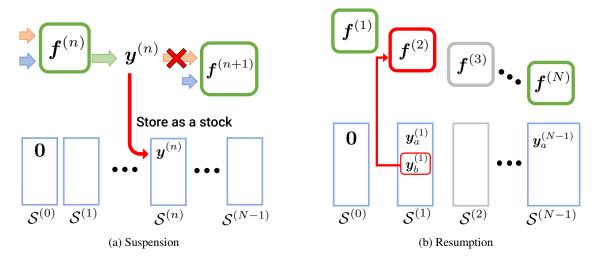


Figure 2: Conceptual diagram of the suspension setting. (a) shows the case where the output $y^{(n)}$ is stored as a stock in stage n, and the observation from the subsequent stage is suspended. (b) shows the case where the observation is reused from stage two using the stock $y_h^{(1)}$.

Acquisition function for suspension setting We propose the following AF for the suspension setting:

$$n_{t}, \boldsymbol{y}_{t}^{(n-1)}, \boldsymbol{x}_{t}^{(n)} = \underset{i \in [N], \\ \boldsymbol{y}^{(i-1)} \in \mathcal{S}_{t}^{(i-1)}, \\ \boldsymbol{x}^{(i)} \in \mathcal{X}^{(i)}}{\operatorname{arg max}} \widetilde{U}_{i}(\boldsymbol{y}^{(i-1)}, \boldsymbol{x}^{(i)}) / \sum_{j=i}^{N} \lambda^{(j)}.$$

$$(15)$$

There are two differences between the AF in (15) and the EI-based AF in (5c). First, in (15), based on the set of stocks $\{S_t^{(i-1)}\}_{i\in[N]}$, we determine which stage to resume from, which stock to use, and what input to use. Thus, (15) implicitly determines whether the sequential evaluation in cascade is suspended or not. Second, the utility is divided by the total cost from stages n to N, which suggests that a cost-effective choice is performed. Resuming from a later stage has advantages (considering cost) because the goal is to optimize the output of the final stage. The AF in (15) can be interpreted as an extension of the EI-based AF in (5c) because it handles the two cases of starting from the first stage and resuming from the middle stage using a stock. It is necessary to compute the utility function for many candidates when solving the optimization problem in (15). Nonetheless, this can be done efficiently by exploiting the fact that the evaluation of \widetilde{U}_n in stage n does not depend on the observations in the earlier stages.

Stock Reduction In the suspension setting, having a larger number of stocks provides us a wider choice. However, practically, it can be costly to store several stocks. In such a situation, it is necessary to be able to decide which stocks to retain and which ones to discard. A reasonable way is to discard the stocks that are not expected to contribute to the optimal solution. We implement this based on the credible interval.

For any stock
$$y^{(n)} \in \mathcal{S}^{(n)}$$
 in stage $0 \le n \le N-1$, let

$$F(y^{(n)}) = \max_{\boldsymbol{x}^{(n+1:N)}} F(\boldsymbol{x}^{(n+1:N)}|y^{(n)})$$

be the maximum function value when the observation is performed until the final stage using $y^{(n)}$. Therefore, the LCB

and UCB of $F(y^{(n)})$ are given as

$$\begin{split} & \operatorname{LCB}_{t}^{(F)}(y^{(n)}) = \max_{\boldsymbol{x}^{(n+1:N)}} \operatorname{LCB}_{t}^{(F)}(\boldsymbol{x}^{(n+1:N)}|y^{(n)}), \\ & \operatorname{UCB}_{t}^{(F)}(y^{(n)}) = \max_{\boldsymbol{x}^{(n+1:N)}} \operatorname{UCB}_{t}^{(F)}(\boldsymbol{x}^{(n+1:N)}|y^{(n)}). \end{split}$$

Then, the following theorem holds.

Theorem 5.1. For any $n \in [N-1]$ and $y^{(n)} \in \mathcal{S}^{(n)}$, under the same assumptions as in Theorem 3.1, assume that the following holds:

$$UCB_{t}^{(F)}(y^{(n)}) < \max_{\tilde{y} \in \bigcup_{s=0}^{N-1} S_{t}^{(s)}} LCB_{t}^{(F)}(\tilde{y}^{(s)}).$$
(16)

Then,
$$F(y^{(n)}) < F(\boldsymbol{x}_*^{(1)}, \dots, \boldsymbol{x}_*^{(N)})$$
 holds.

The proof of the theorem is presented in Appendix C. From Theorem 5.1, the condition (16) is used to decide which stocks to discard. Theorem 5.1 only guarantees that the stock will not become the optimal value. Suboptimal stocks may also be effectively used in the optimization process.

6 Experiments

We demonstrated the optimization performance of the proposed methods in both synthetic functions and a solar cell simulator. Details of the experimental settings are provided in Appendix F. First, we compared the methods in the sequential setting. We used CBO, EI-FN and random sampling (Random) as the comparison methods. In Random, each $\boldsymbol{x}^{(n)} \in \mathcal{X}^{(n)}$ is randomly and uniformly selected. Regarding CBO, its AF is optimized by considering the output of the previous stage as the controllable variable. Because the range of the previous output is unknown, we used a widely estimated range that was twice the actual range. Additionally, we set its hyperparameters κ_1, κ_2 to one. We also compared the proposed methods to a fully black-box BO that used EI and GP-UCB under a fully black-box model (FB-EI, FB-UCB). The proposed methods with EI- and CI-based AFs are labeled as EI-BASED and CI-BASED, respectively. We set the number of Monte Carlo sampling to S=1000, and we used $\eta_t=10^{-4}(1+\log t)^{-1}$ to calculate CI-BASED. In all the experiments, we employed a Gaussian kernel $k^{(n)}\left((w,x),(w',x')\right)=\sigma_f^{(n)}\exp\left(-\frac{(w-w')^2}{2\ell_w^2^{(n)}}-\sum_{d=1}^{D^{(n)}}\frac{(x_d-x'_d)^2}{2\ell_d^2^{(n)}}\right)$ and we set the noise variance of the GP model as $\sigma^2=10^{-4}$. The performance was evaluated by the simple regret $F(x_*^{(1)},\ldots,x_*^{(N)})-F(x_{\bar{t}}^{(1)},\ldots,x_{\bar{t}}^{(N)})$, where $\bar{t}=\arg\max_{1\leq t'\leq t}y_{t'}^{(N)}$. Additional results comparing EI-BASED and EI-FN are shown in Appendix G.

6.1 Synthetic Functions

We used sample paths from the GP priors, Rosenbrock function, Sphere function, and Matyas function as the synthetic functions. Regarding both functions, we constructed three- and five-stage cascade processes, and set $D^{(n)}=2$ for all n. We used $L_f=1, \beta^{1/2}=2$ for the calculation (7). In addition, 10 and 20 points for N=3 and N=5 were randomly selected and provided as the initial data.

Sample Paths from GP Priors: We employed the random Fourier feature (Rahimi and Recht, 2008) to sample $f^{(n)}$ from the GP prior and constructed F using them. Each $f^{(n)}$ was sampled ten times, and the experiments were conducted with two different random seeds for each. The hyperparameters were set to $\sigma_f^{(n)} = 15.02, \ell_d^{(n)} = 3, \ell_w^{(n)} = 3$. We also set the domain of the control parameter to $\mathcal{X}^{(n)} = [-10, 10]^{D^{(n)}}$.

For the following synthetic functions, we ran experiments with 20 different random seeds. Furthermore, we scaled $f^{(n)}$ such that the range of the function value is equal to the input domain for numerical stability. The GP hyperparameters were selected by maximizing the marginal likelihood at every iteration.

Rosenbrock Function: Each $f^{(n)}$ is Rosenbrock function, whose domain of the control parameters were set to $\mathcal{X}^{(n)} = [-2,2]^{D^{(n)}}$. We perform the experiments with the number of stages N=3 and 5. We set $\boldsymbol{x}^{(1)} \in \mathbb{R}^3$ and $\boldsymbol{x}^{(n)} \in \mathbb{R}^2$ for each $n=2,\ldots,N$, and output $y^{(n)} \in \mathbb{R}$ for $n \in [N]$.

Sphere function: Each $f^{(n)}$ is Sphere function, whose domain of the control parameters were set to $\mathcal{X}^{(n)} = [-5.12, 5.12]^{D^{(n)}}$. Each output $y^{(n)} \in \mathbb{R}$ for $n \in [N]$ and the number of stages is N = 3. We set $\boldsymbol{x}^{(1)} \in \mathbb{R}^3$ and $\boldsymbol{x}^{(2)}, \boldsymbol{x}^{(3)} \in \mathbb{R}^2$.

Matyas function: Each $f^{(n)}$ is Matyas function, whose domain of the control parameters were set to $\mathcal{X}^{(n)} = [-10, 10]^{D^{(n)}}$. Each output $y^{(n)} \in \mathbb{R}$ for $n \in [N]$ and the number of stages is N = 3. We set $\boldsymbol{x}^{(1)} \in \mathbb{R}^2$ and $x^{(2)}, x^{(3)} \in \mathbb{R}^1$.

Figure 3 shows the average value of the simple regret. We see that our proposed methods and EI-FN clearly outperform other baselines including CBO. Although EI-BASED, which can be roughly seen as the adaptive version of EI-FN, is comparable to EI-FN in most experiments, EI-BASED shows better performance than EI-FN in the Sphere function. This can be seen as a benefit of adaptive decision-making. Although CI-BASED has superior theoretical properties, CI-BASED is inferior to EI-BASED except for Rosenbrock (N=3) and Matyas functions. One of the reasons for these results is the setting of the hyperparameters, such as β and L_f .

6.2 Solar Cell Simulator

We applied the proposed methods to the solar cell simulator. This simulator consists of three-stage processes. Stages one and two are two-step annealing processes to diffuse phosphorus into the silicon substrate from the surface, forming a p-n junction near the surface. The controllable parameters of stage one are the phosphorus concentration at the surface, temperature, and time of the first-step annealing. In addition, the controllable parameters of stage two are the temperature and time of the second-step annealing. The outputs of stages one and two are the four parameters that indicate the distribution of phosphorus concentration in the depth direction. In stage three, the solar cell is constructed using controllable parameters composed of wafer thickness and boron concentration of the substrate, and the performance is evaluated under standard measurement conditions. The final output is the power generation efficiency of the solar cell, and our goal is to maximize this output. Regarding the real-world simulators, the simulators of stages one and two are based on the physical model (Bentzen, 2006). Moreover, the simulator of stage three was constructed using the data collected from PC1Dmod6.2 (Haug and Greulich, 2016). In stages one and two, the simulators produce vector outputs. However, CBO does not support vector outputs, so we calculated its AF by replacing the predictive mean and variance with the mean vector and covariance matrix, respectively. The domain of the controllable parameters are $\mathcal{X}^{(1)} = [700, 1050] \times [100, 5000] \times [19, 21.18], \mathcal{X}^{(2)} = [700, 1050] \times [100, 5000], \text{ and } \mathcal{X}^{(3)} = [50, 250] \times [14, 17].$ We randomly chose 20 points as the initial data. In addition, we set $L_f = 0.1, \beta^{1/2} = 2$ in this setting. Furthermore, we tuned the hyperparameters by maximizing the marginal likelihood and ran the experiment for 50 iterations using 20 different random seeds.

Figure 4 shows the average of the best observed value $\max_{1 \le t' \le t} y_{t'}^{(N)}$. This result shows that the proposed method outperforms the existing methods in the simulator experiments. It is also confirmed that the best value found in 50 iterations in the existing methods is achieved in less than half of the iterations in the proposed method. In a comparison between EI-BASED and EI-FN, the error bars are not overlapped after the 40 iteration. Thus, EI-BASED shows a slightly small but substantial improvement by adaptive decision-making.

6.3 Hydrogen Plasma Treatment Process

We applied the proposed method to the hydrogen plasma treatment (HPT) process, which is a part of the production process of solar cells. In the previous practical study, one of the authors (KK) optimized one-stage HPT process parameters through real experiments using simple BO (Miyagawa et al., 2021b,a). In this study, we extended this HPT process to the virtual two-stage cascade process. The first stage is the HPT process with 7 inputs, temperature, pressure, flow rate, process time, electrode distance, radio frequency power, and cycle time, and 2 outputs, saturation current density, and contact resistance. The second process is the solar cell production process in which surface electrode width is the controllable parameter. The final output is the power generation efficiency of the solar cell, and our goal is to maximize this output as in the case of the solar cell simulation. The domain of the controllable parameters are $\mathcal{X}^{(1)} = [50, 300] \times [0.25, 4] \times [100, 1000] \times [10, 100] \times [270, 420] \times [10, 40] \times [15, 60]$ and $\mathcal{X}^{(2)} = [0.01, 0.1]$. Since the real dataset is small with respect to the input domain, we used surrogate objectives, which are sample paths of GPs fitting to the real dataset for each stage. The details of these sample paths are shown in Appendix F. Other experimental settings are set as with the solar cell simulator experiment.

Figure 5 shows the average of the best observed value $\max_{1 \le t' \le t} y_{t'}^{(N)}$. Our proposed methods EI-BASED and CI-BASED are superior to other baselines including EI-FN and CBO. In particular, the difference between EI-BASED and EI-FN implies the improvement by adaptive decision-making.

6.4 Suspension Setting

We also conducted experiments in a suspension setting using the proposed method (15) (EI-BASED-SUS). In this setting, we used the sample path function with N=3 and 5. For the cost of each stage $\lambda:=(\lambda^{(1)},\lambda^{(2)},\lambda^{(3)})$, we consider two settings: $\lambda=(1,1,1)$, $\lambda=(1,1,10)$. Furthermore, we apply the stock reduction rule (16) to EI-BASED-SUS and executed it in both settings. We refer to this as EI-SUS-R. The results are shown in Figure 6(a) and 6(b). Comparing EI-BASED and EI-BASED-SUS, we can observe that the performance is improved by incorporating the suspension. Moreover, the performance did not deteriorate even when the stock reduction rule was applied. In addition, the stocks are not consumed in the simulator, and once a stock is acquired, it can be used a number of times. In this case, we can reduce the number of observations in the earlier stages by reusing the stock. We compared the situation in which stocks are available only once (EI-SUS (1)) and the situation in which stocks can be used a number of times (EI-SUS (∞)). From Figure 6(c), we confirm that EI-SUS (∞) performs a more efficient optimization.

Conclusion

We proposed a new BO framework for cascade-type multistage processes that often appear in science and engineering. Moreover, we have designed two AFs based on CIs and EI by handling intractable predictive distributions using different approaches. From both the theoretical analysis and numerical experiments, it is confirmed that the proposed

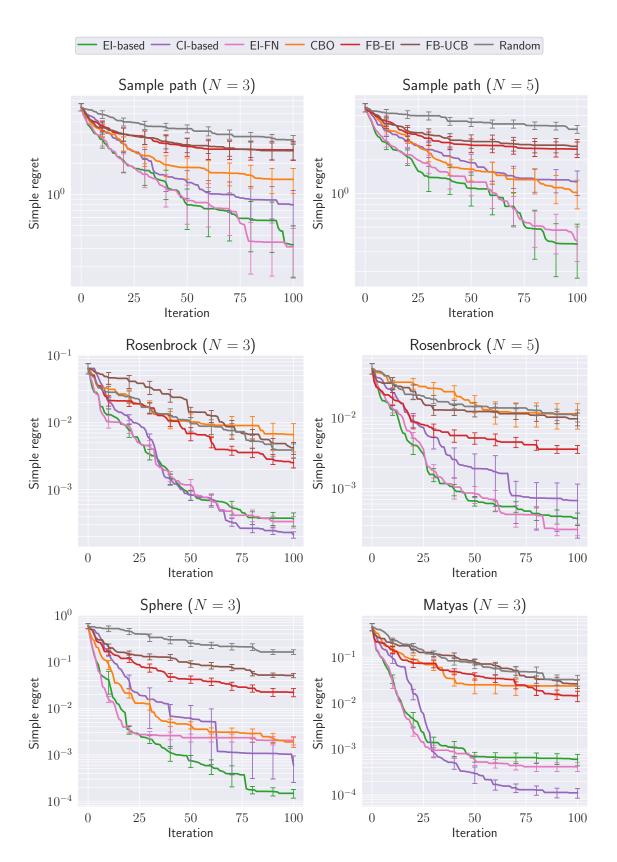


Figure 3: Experimental results of the synthetic functions. The solid line represents the average performance, and the error bar represents the standard error.

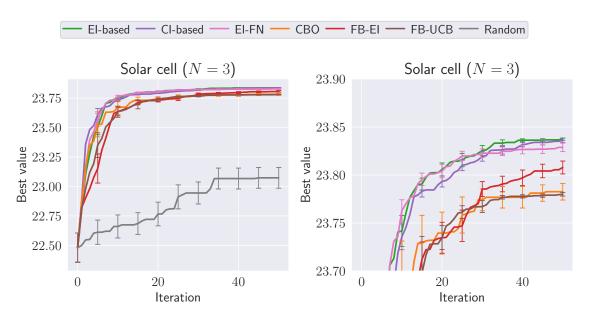


Figure 4: Results of the solar cell simulator. The right plot is an enlarged version of the left plot.

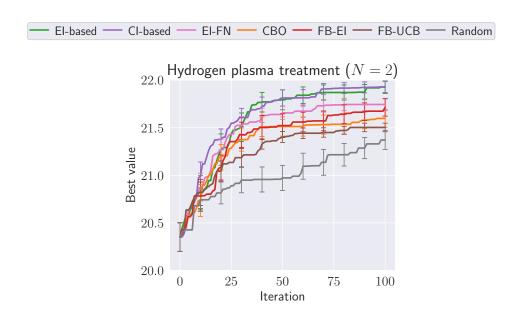


Figure 5: Results of the hydrogen plasma treatment.

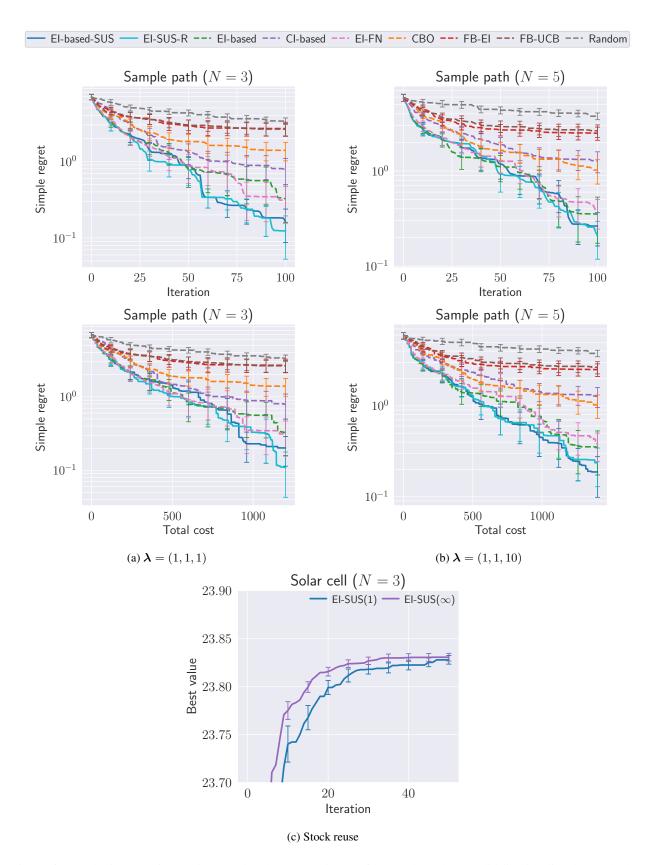


Figure 6: Results in extension setting. In the above experiments for sample paths, a solid line implies the methods with suspension and a dashed line represents a sequential method.

methods have a superior performance.

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Appendix

A Generalization of Problem Setting

Hereafter, we consider the generalized settings, including vector output and noisy observations. First, we generalize the problem setting in this section. In Appendix C, we consider the noiseless setting. We also consider the noisy observation setting in Appendix D and provide the optimization algorithm. Furthermore, we discuss the conditions of our theorems in Appendix E. Details of our experiments and additional experiments are described in Appendix F and G, respectively.

Let $\mathcal{Y}^{(n)} \subset \mathbb{R}^{M^{(n)}}$ be the $M^{(n)}$ -dimensional output space², and vector-output black-box function of stage n is denoted by $\boldsymbol{f}^{(n)}$, and $f_m^{(n)}$ denotes the m-th function of $\boldsymbol{f}^{(n)}$. Output $\boldsymbol{y}^{(n)}$ corresponding to an input $(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)})$ is observed with noise $\boldsymbol{\epsilon}^{(n)}$: $\boldsymbol{y}^{(n)} = \boldsymbol{f}^{(n)}(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)}) + \boldsymbol{\epsilon}^{(n)}$. The noiseless settings are the case of $\boldsymbol{\epsilon}^{(n)} = \boldsymbol{0}$. Furthermore, we consider that $\boldsymbol{\epsilon}^{(n)}$ is uniformly bounded and zero mean noise in Appendix D.

In order to construct a surrogate model of $f^{(n)}$, we set $\mathcal{GP}(0,k^{(n)})$ to the prior for each $f_m^{(n)}$, where $\mathcal{GP}(\mu,k^{(n)})$ represents the GP with mean function μ and kernel function $k^{(n)}$. Additionally, we assume that $k^{(n)}$ is a positive-definite kernel and $\forall (\boldsymbol{y}^{(n-1)},\boldsymbol{x}^{(n)}) \in \mathcal{Y}^{(n-1)} \times \mathcal{X}^{(n)}, \ k^{(n)}\left((\boldsymbol{y}^{(n-1)},\boldsymbol{x}^{(n)}),(\boldsymbol{y}^{(n-1)},\boldsymbol{x}^{(n)})\right) \leq 1.$ Let $\mathcal{D}_t^{(n)} = \left\{\left((\boldsymbol{y}_i^{(n-1)},\boldsymbol{x}_i^{(n)}),\boldsymbol{y}_i^{(n)}\right)\right\}_{i=1}^{L_t^{(n)}}$ be observed data of stage n at iteration t. As the noise model of GP, we use $\boldsymbol{\epsilon}^{(n)} \sim \mathcal{N}(\mathbf{0},\sigma^2\boldsymbol{I}_{M^{(n)}})$, where $\boldsymbol{I}_{M^{(n)}}$ denotes $M^{(n)} \times M^{(n)}$ identity matrix. Note that this noise model is different from the actual noise assumption. Given the observation $\mathcal{D}_t^{(n)}$, the posterior of $f_m^{(n)}$ is also GP, and the predictive distribution of $f_m^{(n)}(\boldsymbol{y}^{(n-1)},\boldsymbol{x}^{(n)})$ is given by:

$$\begin{split} f_m^{(n)}(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)}) &\sim \mathcal{N}\big(\mu_{m,t}^{(n)}(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)}), \ \sigma_{m,t}^{(n)\,2}(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)})\big), \\ \mu_{m,t}^{(n)}(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)}) &= \boldsymbol{k} \left(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)}\right)^{\top} (\boldsymbol{K}_t^{(n)} + \sigma^2 \boldsymbol{I}_{L_t^{(n)}})^{-1} \boldsymbol{y}_m^{(n)}, \\ \sigma_{m,t}^{(n)\,2}(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)}) &= k^{(n)} \left((\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)}), (\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)}) \right) \\ &- \boldsymbol{k} (\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)})^{\top} (\boldsymbol{K}_t^{(n)} + \sigma^2 \boldsymbol{I}_{L_t^{(n)}})^{-1} \boldsymbol{k} (\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)}). \end{split}$$

Here, $\boldsymbol{k}(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)}) = \left[k^{(n)}\left((\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)}), (\boldsymbol{y}_i^{(n-1)}, \boldsymbol{x}_i^{(n)})\right)\right]_{i=1}^{L_t^{(n)}}, \ \boldsymbol{y}_m^{(n)} = \left[y_{1m}^{(n)}, \dots, y_{Lm}^{(n)}\right]^{\top}, \ \text{and} \ \boldsymbol{K}_t^{(n)}$ is a kernel matrix which has $k^{(n)}\big((\boldsymbol{y}_i^{(n-1)}, \boldsymbol{x}_i^{(n)}), (\boldsymbol{y}_j^{(n-1)}, \boldsymbol{x}_j^{(n)})\big)$ in (i, j)-th element. In addition, we define $\boldsymbol{\mu}_t^{(n)}(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)}) = \left[\mu_{m,t}^{(n)}(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)})\right]_{m=1}^{M^{(n)}}.$

For a GP model of $f_m^{(n)}$, we give a definition of the maximum information gain. Let $A^{(n)} = \{\boldsymbol{a}_1^{(n)}, \dots, \boldsymbol{a}_T^{(n)}\} \subset \mathcal{Y}^{(n-1)} \times \mathcal{X}^{(n)}$ be a finite set of sampling points. We define $\boldsymbol{y}_{A,m}^{(n)} \in \mathbb{R}^T$ as observation vector w.r.t. $A^{(n)}$, whose i-th element is given by $\boldsymbol{y}_{\boldsymbol{a}_i,m}^{(n)} = f_m^{(n)}(\boldsymbol{a}_i) + \varepsilon_{\boldsymbol{a}_i,m}^{(n)}$. Then, the maximum information gain $\gamma_{m,T}^{(n)}$ is defined as:

$$\gamma_{m,T}^{(n)} = \max_{A^{(n)} \subset \mathcal{Y}^{(n-1)} \times \mathcal{X}^{(n)}, |A^{(n)}| = T} \mathbf{I}(\boldsymbol{y}_{A,m}^{(n)}; f_m^{(n)}),$$

where $I(\boldsymbol{y}_{A,m}^{(n)};f_m^{(n)})$ is the mutual information between $\boldsymbol{y}_{A,m}^{(n)}$ and $f_m^{(n)}$. Furthermore, it is known that this mutual information can be written in closed form as follows (Srinivas et al., 2010):

$$I(\boldsymbol{y}_{A,m}^{(n)}; f_m^{(n)}) = \frac{1}{2} \log \det \left(\boldsymbol{I}_{|A^{(n)}|} + \sigma^{-2} \boldsymbol{K}_{A^{(n)}}^{(n)} \right),$$

where
$$m{K}_{A^{(n)}}^{(n)} = \left[k^{(n)}(m{a}_i^{(n)}, m{a}_j^{(n)})
ight]_{m{a}_i^{(n)} \in A^{(n)}, \; m{a}_j^{(n)} \in A^{(n)}}.$$

Additionally, we define $S_t^{(n)}$ as the set of stocks in stage n at iteration t.

A.1 Proofs of Theorems

Theorem 3.1 is a special case of Theorem C.7 with $M^{(n)}=1$ for all n. Likewise, Theorems 4.1 and 4.2 are corresponding to Theorems C.6 and C.10 with $M^{(n)}=1$, respectively. The proofs of these theorems are given in the generalized problem setting. Moreover, we also provide the proof of Theorem 5.1 in Corollary C.8.

²Since we focus on single-objective optimization, the output of the final stage is assumed to be scalar (i.e., $M^{(N)} = 1$).

B Prediction of Cascade Processes using Bayesian Quadrature

In this section, we consider the cascade process as a Bayesian quadrature (O'Hagan, 1991) framework and introduce one of its problems. For black-box functions at each stage of the cascade process, we consider a predictive model using GP. The problem is that it is difficult to predict each stage from the first stage because each stage contains controllable variables and outputs from the previous stage that are not controllable. Nevertheless, the output from the previous stage can be predicted using the posterior distribution. Therefore, integrating the black-box function of each stage with respect to this posterior distribution, i.e., taking the expectation, allows prediction of each stage with respect to the average case of uncontrollable inputs. This approach is known as Bayesian quadrature, and furthermore, since each stage follows a GP, it is known that the integration of the black-box function is again a GP (see, e.g., (Papoulis and Pillai, 2002)). Therefore, the advantage of this approach is that it is easy to construct credible intervals based on the properties of GP. However, this modeling has the problem that it cannot always correctly predict the target it originally wants to predict.

Lemma B.1. Suppose that $f_1: \mathbb{R} \to \mathbb{R}$ follows $\mathcal{GP}(0, k_1(x, x'))$. Also suppose that $f_2: \mathbb{R}^2 \to \mathbb{R}$ follows $\mathcal{GP}(0, k_2((x_1, x_2), (x'_1, x'_2)))$. Assume that the first variable of f_2 is the output of f_1 . Then, the stochastic process $f_2(f_1(x_1), x_2)$ is not necessarily the same as

$$\mathbb{E}_{f_1(x_1) \sim \mathcal{GP}(0, k_1(x, x'))} [f_2(f_1(x_1), x_2)]. \tag{B.1}$$

Proof. Let $k_1(x,x') = \exp(-(x-x')^2)$ and $k_2(y,y') = y^\top y'$. Since the expectation of GP with respect to inputs is again a GP, (B.1) follows GP. Therefore, the probability distribution given by (B.1) at point $x_1 = x_2 = 0$ follows some normal distribution. On the other hand, since $f_1(x_1) \sim \mathcal{GP}(0, k_1(x,x'))$, from the definition of $k_1(x,x')$ we have $f_1(0) \sim N(0,1)$. Similarly, we get $f_2(f_1(0),0) \sim N(0,f_1^2(0)) \stackrel{\mathrm{d}}{=} N(0,\chi_1^2) \stackrel{\mathrm{d}}{=} \sqrt{\chi_1^2}N(0,1)$, where χ_1^2 is the chi-squared distribution with one degree of freedom. The mean and variance of $\sqrt{\chi_1^2}N(0,1)$ are zero and one, respectively. Furthermore, the fourth moment of $\sqrt{\chi_1^2}N(0,1)$ is given by

$$\mathbb{E}\left[\left(\sqrt{\chi_1^2}N(0,1)\right)^4\right] = \mathbb{E}[(\chi_1^2)^2]\mathbb{E}[N(0,1))^4] = (\mathbb{V}[\chi_1^2] + \mathbb{E}[\chi_1^2]^2)3 = 9.$$

Hence, $\sqrt{\chi_1^2}N(0,1)$ does not follow a normal distribution because the fourth moment of the normal distribution with mean zero and variance one, i.e., the standard normal distribution, is three. Thus, the stochastic process $f_2(f_1(x_1), x_2)$ is not the same as (B.1).

Although it is possible to construct a GP prediction model as an integral of GP, the final stage does not necessarily follow GP. Hence, it is not always easy to judge whether the composition of the credible interval or the design of AF based on the constructed GP prediction model is appropriate or not. Therefore, modeling the final stage of the cascade process based on the integration of GP is not the most natural approach.

C Cascade Process Optimization Using CI-based AFs under Noiseless Setting

In this section, we consider CI-based cascade process optimization methods without observation noise.

C.1 Credible Interval

We construct a valid CI for the objective function $F(\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)})$. First, we assume the following regularity assumption which is commonly assumed in many BO studies.

Assumption C.1 (Regularity assumption under noiseless setting). For each $n \in [N]$, let $\mathcal{Y}^{(n-1)} \times \mathcal{X}^{(n)}$ be a compact set, and let $\mathcal{H}_{k^{(n)}}$ be an RKHS corresponding to the kernel $k^{(n)}$. In addition, for each $n \in [N]$ and $m \in [M^{(n)}]$, assume that $f_m^{(n)} \in \mathcal{H}_{k^{(n)}}$ with $\|f_m^{(n)}\|_{k^{(n)}} \leq B$, where B > 0 is some constant, and $\|\cdot\|_{k^{(n)}}$ denotes the RKHS norm on $\mathcal{H}_{k^{(n)}}$. Furthermore, assume that the observation noise $\epsilon_m^{(n)}$ is zero.

Under this assumption, it is known that the following lemma holds.

Lemma C.2 (Abbasi-Yadkori 2012, Theorem 3.11). Assume that Assumption C.1 holds. Define $\beta = B^2$. Then, for any $n \in [N]$ and $m \in [M^{(n)}]$, the following inequality holds:

$$\left| f_m^{(n)}(\boldsymbol{w}, \boldsymbol{x}) - \mu_{m,t}^{(n)}(\boldsymbol{w}, \boldsymbol{x}) \right| \leq \beta^{1/2} \sigma_{m,t}^{(n)}(\boldsymbol{w}, \boldsymbol{x}), \ \forall \boldsymbol{w} \in \mathcal{Y}^{(n-1)}, \ \forall \boldsymbol{x} \in \mathcal{X}^{(n)}, \ \forall t \geq 1.$$

Based on Lemma C.2, we construct the valid CI. However, we cannot use Lemma C.2 to construct CIs directly because the input $w \in \mathcal{Y}^{(n-1)}$ is the output of the previous stage. In order to avoid this issue, we introduce additional assumptions for Lipschitz continuity.

Assumption C.3 (Lipschitz continuity for $f_m^{(n)}$). Assume that $f_m^{(n)}$ is L_f -Lipschitz continuous with respect to L_1 -distance for any $n \in \{2, ..., N\}$ and $m \in [M^{(n)}]$, where $L_f > 0$ is a Lipschitz constant.

Assumption C.4 (Lipschitz continuity for $\sigma_m^{(n)}$). Assume that $\sigma_{m,t}^{(n)}$ is L_{σ} -Lipschitz continuous with respect to L_1 -distance for any $n \in \{2, \ldots, N\}$, $m \in [M^{(n)}]$ and $t \ge 1$, where $L_{\sigma} > 0$ is a Lipschitz constant.

Then, the following theorem gives CIs for the N-stage cascade process.

Theorem C.5 (CIs for N-stage cascade process). Assume that Assumptions C.1 and C.3 hold. Define $\beta = B^2$ and

$$\begin{split} \boldsymbol{z}^{(n)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n)}) &= \begin{cases} \boldsymbol{f}^{(1)}(\boldsymbol{0}, \boldsymbol{x}^{(1)}) & (n = 1), \\ \boldsymbol{f}^{(n)}(\boldsymbol{z}^{(n-1)}(\boldsymbol{x}^{(1:n-1)}), \boldsymbol{x}^{(n)}) & (2 \leq n \leq N), \end{cases} \\ \tilde{\boldsymbol{\mu}}_t^{(n)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n)}) &= \begin{cases} \boldsymbol{\mu}_t^{(1)}(\boldsymbol{0}, \boldsymbol{x}^{(1)}) & (n = 1), \\ \boldsymbol{\mu}_t^{(n)}(\tilde{\boldsymbol{\mu}}^{(n-1)}(\boldsymbol{x}^{(1:n-1)}), \boldsymbol{x}^{(n)}) & (2 \leq n \leq N), \end{cases} \\ \tilde{\sigma}_{m,t}^{(n)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n)}) &= \begin{cases} \sigma_{m,t}^{(1)}(\boldsymbol{0}, \boldsymbol{x}^{(1)}) & (n = 1), \\ \sigma_{m,t}^{(n)}(\tilde{\boldsymbol{\mu}}_t^{(n-1)}(\boldsymbol{x}^{(1:n-1)}), \boldsymbol{x}^{(n)}) & (2 \leq n \leq N), \end{cases} \\ + L_f \sum_{s=1}^{M^{(n-1)}} \tilde{\sigma}_{s,t}^{(n-1)}(\boldsymbol{x}^{(1:n-1)}) & (2 \leq n \leq N). \end{cases}$$

Moreover, assume that $\tilde{\boldsymbol{\mu}}_t^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}) \in \mathcal{Y}^{(n)}$ for any $n \in [N]$, $t \ge 1$ and $(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}) \in \mathcal{X}^{(1)} \times \cdots \times \mathcal{X}^{(n)}$. Then, it follows that

$$|z_m^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}) - \tilde{\mu}_{m,t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)})| \le \beta^{1/2} \tilde{\sigma}_{m,t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}),$$

where $m \in [M^{(n)}]$, and $z_m^{(n)}(\cdot)$ and $\tilde{\mu}_{m,t}^{(n)}(\cdot)$ are the m-th element of $\mathbf{z}_m^{(n)}(\cdot)$ and $\tilde{\mu}_{m,t}^{(n)}(\cdot)$, respectively. In particular, when n=N, it follows that

$$|F(\boldsymbol{x}^{(1)},\dots,\boldsymbol{x}^{(N)}) - \tilde{\mu}_{1,t}^{(N)}(\boldsymbol{x}^{(1)},\dots,\boldsymbol{x}^{(N)})| \leq \quad \beta^{1/2}\tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}^{(1)},\dots,\boldsymbol{x}^{(N)}).$$

Proof. Fix $\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n)}$, $t \geq 1$ and $m \in [M^{(n)}]$. For simplicity, hereafter, we sometimes omit the notation $(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n)})$ such as $z_m^{(n)}$ and $\tilde{\mu}_{m,t}^{(n)}$. Then, for $i \in [M^{(2)}]$, it follows that

$$\begin{split} |z_{i}^{(2)} - \tilde{\mu}_{i,t}^{(2)}| &= |z_{i}^{(2)} - f_{i}^{(2)}(\tilde{\mu}_{t}^{(1)}, \boldsymbol{x}^{(2)}) + f_{i}^{(2)}(\tilde{\mu}_{t}^{(1)}, \boldsymbol{x}^{(2)}) - \tilde{\mu}_{i,t}^{(2)}| \\ &\leq |z_{i}^{(2)} - f_{i}^{(2)}(\tilde{\mu}_{t}^{(1)}, \boldsymbol{x}^{(2)})| + |f_{i}^{(2)}(\tilde{\mu}_{t}^{(1)}, \boldsymbol{x}^{(2)}) - \tilde{\mu}_{i,t}^{(2)}| \\ &= |z_{i}^{(2)}(\boldsymbol{z}^{(1)}, \boldsymbol{x}^{(2)}) - f_{i}^{(2)}(\tilde{\mu}_{t}^{(1)}, \boldsymbol{x}^{(2)})| + |f_{i}^{(2)}(\tilde{\mu}_{t}^{(1)}, \boldsymbol{x}^{(2)}) - \mu_{i,t}^{(2)}(\tilde{\mu}_{t}^{(1)}, \boldsymbol{x}^{(2)})| \\ &\leq L_{f} \|\boldsymbol{z}^{(1)} - \tilde{\mu}_{t}^{(1)}\|_{1} + \beta^{1/2} \sigma_{i,t}^{(2)}(\tilde{\mu}_{t}^{(1)}, \boldsymbol{x}^{(2)}) \\ &= \beta^{1/2} \sigma_{i,t}^{(2)}(\tilde{\mu}_{t}^{(1)}, \boldsymbol{x}^{(2)}) + L_{f} \sum_{m=1}^{M^{(1)}} |z_{m}^{(1)} - \tilde{\mu}_{m,t}^{(1)}| \\ &\leq \beta^{1/2} \sigma_{i,t}^{(2)}(\tilde{\mu}_{t}^{(1)}, \boldsymbol{x}^{(2)}) + L_{f} \sum_{m=1}^{M^{(1)}} \beta^{1/2} \sigma_{m,t}^{(1)}(\boldsymbol{0}, \boldsymbol{x}^{(1)}) \\ &= \beta^{1/2} \tilde{\sigma}_{i,t}^{(2)}(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}). \end{split} \tag{C.1}$$

Similarly, $z_j^{(3)}$ and $\tilde{\mu}_{j,t}^{(3)}$ satisfy that

$$|z_{j}^{(3)} - \tilde{\mu}_{j,t}^{(3)}| = |z_{j}^{(3)} - f_{j}^{(3)}(\tilde{\boldsymbol{\mu}}_{t}^{(2)}, \boldsymbol{x}^{(3)}) + f_{j}^{(3)}(\tilde{\boldsymbol{\mu}}_{t}^{(2)}, \boldsymbol{x}^{(3)}) - \tilde{\mu}_{j,t}^{(3)}|$$

$$\leq |z_{j}^{(3)} - f_{j}^{(3)}(\tilde{\boldsymbol{\mu}}_{t}^{(2)}, \boldsymbol{x}^{(3)})| + |f_{j}^{(3)}(\tilde{\boldsymbol{\mu}}_{t}^{(2)}, \boldsymbol{x}^{(3)}) - \tilde{\mu}_{j,t}^{(3)}|$$

$$\leq L_{f} \|\boldsymbol{z}^{(2)} - \tilde{\boldsymbol{\mu}}_{t}^{(2)}\|_{1} + \beta^{1/2} \sigma_{j,t}^{(3)}(\tilde{\boldsymbol{\mu}}_{t}^{(2)}, \boldsymbol{x}^{(3)})$$

$$= \beta^{1/2} \sigma_{j,t}^{(3)}(\tilde{\boldsymbol{\mu}}_{t}^{(2)}, \boldsymbol{x}^{(3)}) + L_{f} \sum_{i=1}^{M^{(2)}} |z_{i}^{(2)} - \tilde{\mu}_{i,t}^{(2)}|. \tag{C.2}$$

Hence, by substituting (C.1) into (C.2), we get

$$|z_{j}^{(3)} - \tilde{\mu}_{j,t}^{(3)}| \leq \beta^{1/2} \left(\sigma_{j,t}^{(3)}(\tilde{\boldsymbol{\mu}}_{t}^{(2)}, \boldsymbol{x}^{(3)}) + L_{f} \sum_{u=1}^{M^{(2)}} \tilde{\sigma}_{u,t}^{(2)}(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}) \right)$$
$$= \beta^{1/2} \tilde{\sigma}_{j,t}^{(3)}(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \boldsymbol{x}^{(3)}).$$

By repeating this process up to n, we have Theorem C.5.

From Theorem C.5, we can construct the valid CI $Q_t^{(F)}({m x}^{(1)},\dots,{m x}^{(N)})$ of $F({m x}^{(1)},\dots,{m x}^{(N)})$ as follows:

$$Q_{t}^{(F)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) = [\tilde{\mu}_{1,t}^{(N)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) \pm \beta^{1/2} \tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)})]$$

$$= [LCB_{t}^{(F)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}), UCB_{t}^{(F)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)})]. \tag{C.3}$$

Next, we consider the property of estimated solutions based on the proposed CI (C.3). For any $t \ge 1$, we define the estimated solution $(\hat{x}_t^{(1)}, \dots, \hat{x}_t^{(N)})$ as

$$(\hat{\boldsymbol{x}}_t^{(1)}, \dots, \hat{\boldsymbol{x}}_t^{(N)}) = \underset{(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) \in \mathcal{X}, 1 \leq \tilde{t} \leq t}{\operatorname{arg\,max}} \operatorname{LCB}_{\tilde{t}}^{(F)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}). \tag{C.4}$$

Then, the following theorem holds.

Theorem C.6. Let $(\hat{x}_t^{(1)}, \dots, \hat{x}_t^{(N)})$ be the estimated solution given by (C.4). Assume that the same assumption as in Theorem C.5 holds. Then, for any $t \geq 1$ and $\xi > 0$, it follows that

$$\max_{\boldsymbol{x}^{(1:N)} \in \mathcal{X}} \text{UCB}_{t}^{(F)}(\boldsymbol{x}^{(1:N)}) - \max_{\boldsymbol{x}^{(1:N)} \in \mathcal{X}} \text{LCB}_{t}^{(F)}(\boldsymbol{x}^{(1:N)}) < \xi$$
$$\Rightarrow F(\boldsymbol{x}_{*}^{(1)}, \dots, \boldsymbol{x}_{*}^{(N)}) - F(\hat{\boldsymbol{x}}_{t}^{(1)}, \dots, \hat{\boldsymbol{x}}_{t}^{(N)}) < \xi.$$

Proof. From the definition of CIs, using Theorem C.5 we have

$$F(\boldsymbol{x}_*^{(1)}, \dots, \boldsymbol{x}_*^{(N)}) \leq \text{UCB}_t^{(F)}(\boldsymbol{x}_*^{(1)}, \dots, \boldsymbol{x}_*^{(N)}),$$

$$\text{LCB}_t^{(F)}(\hat{\boldsymbol{x}}_t^{(1)}, \dots, \hat{\boldsymbol{x}}_t^{(N)}) \leq F(\hat{\boldsymbol{x}}_t^{(1)}, \dots, \hat{\boldsymbol{x}}_t^{(N)}),$$

where $\hat{t} = \arg\max_{(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) \in \mathcal{X}, 1 \leq \tilde{t} \leq t} LCB_{\tilde{t}}^{(F)}(\boldsymbol{x}^{(1:N)})$. Similarly, from the definition of $(\hat{\boldsymbol{x}}_t^{(1)}, \dots, \hat{\boldsymbol{x}}_t^{(N)})$, noting that

$$\max_{\boldsymbol{x}^{(1:N)} \in \mathcal{X}} \mathrm{LCB}_t^{(F)}(\boldsymbol{x}^{(1:N)}) \leq \mathrm{LCB}_{\hat{t}}^{(F)}(\hat{\boldsymbol{x}}_t^{(1:N)}, \dots, \hat{\boldsymbol{x}}_t^{(N)}),$$

we get

$$F(\boldsymbol{x}_*^{(1)}, \dots, \boldsymbol{x}_*^{(N)}) \leq \mathrm{UCB}_t^{(F)}(\boldsymbol{x}_*^{(1)}, \dots, \boldsymbol{x}_*^{(N)}) \leq \max_{\boldsymbol{x}^{(1:N)} \in \mathcal{X}} \mathrm{UCB}_t^{(F)}(\boldsymbol{x}^{(1:N)}),$$

$$\max_{\boldsymbol{x}^{(1:N)} \in \mathcal{X}} \mathrm{LCB}_t^{(F)}(\boldsymbol{x}^{(1:N)}) \leq \mathrm{LCB}_t^{(F)}(\hat{\boldsymbol{x}}_t^{(1)}, \dots, \hat{\boldsymbol{x}}_t^{(N)}) \leq F(\hat{\boldsymbol{x}}_t^{(1)}, \dots, \hat{\boldsymbol{x}}_t^{(N)}).$$

This implies that

$$F(\boldsymbol{x}_{*}^{(1)}, \dots, \boldsymbol{x}_{*}^{(N)}) - F(\hat{\boldsymbol{x}}_{t}^{(1)}, \dots, \hat{\boldsymbol{x}}_{t}^{(N)})$$

$$\leq \max_{\boldsymbol{x}^{(1:N)} \in \mathcal{X}} \text{UCB}_{t}^{(F)}(\boldsymbol{x}^{(1:N)}) - \max_{\boldsymbol{x}^{(1:N)} \in \mathcal{X}} \text{LCB}_{t}^{(F)}(\boldsymbol{x}^{(1:N)}). \tag{C.5}$$

Therefore, by combining (C.5) and

$$\max_{\boldsymbol{x}^{(1:N)} \in \mathcal{X}} \mathrm{UCB}_t^{(F)}(\boldsymbol{x}^{(1:N)}) - \max_{(\boldsymbol{x}^{(1:N)}) \in \mathcal{X}} \mathrm{LCB}_t^{(F)}(\boldsymbol{x}^{(1:N)}) < \xi,$$

we get Theorem C.6.

Finally, we consider the construction of CIs when the observations up to the s-th stage are given. Let s be an integer with $0 \le s \le N-1$, and let \boldsymbol{y} be an element of $\mathcal{Y}^{(s)}$. Then, for each $n \in \{s+1,\ldots,N\}, m \in [M^{(n)}], t \ge 1$ and $\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}$, we define $\boldsymbol{z}^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y}), \ \tilde{\boldsymbol{\mu}}_t^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y})$ and $\tilde{\sigma}_{m,t}^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y})$ as

$$\begin{split} \boldsymbol{z}^{(n)}(\boldsymbol{x}^{(s+1)}, \dots, \boldsymbol{x}^{(n)} | \boldsymbol{y}) &= \begin{cases} \boldsymbol{f}^{(s+1)}(\boldsymbol{y}, \boldsymbol{x}^{(s+1)}) & (n = s + 1), \\ \boldsymbol{f}^{(n)}(\boldsymbol{z}^{(n-1)}(\boldsymbol{x}^{(s+1:n-1)} | \boldsymbol{y}), \boldsymbol{x}^{(n)}) & (n \geq s + 2), \end{cases} \\ \tilde{\boldsymbol{\mu}}_t^{(n)}(\boldsymbol{x}^{(s+1)}, \dots, \boldsymbol{x}^{(n)} | \boldsymbol{y}) &= \begin{cases} \boldsymbol{\mu}_t^{(s+1)}(\boldsymbol{y}, \boldsymbol{x}^{(s+1)}) & (n = s + 1), \\ \boldsymbol{\mu}_t^{(n)}(\tilde{\boldsymbol{\mu}}^{(n-1)}(\boldsymbol{x}^{(s+1:n-1)} | \boldsymbol{y}), \boldsymbol{x}^{(n)}) & (n \geq s + 2), \end{cases} \\ \tilde{\sigma}_{m,t}^{(n)}(\boldsymbol{x}^{(s+1)}, \dots, \boldsymbol{x}^{(n)} | \boldsymbol{y}) &= \begin{cases} \boldsymbol{\sigma}_{m,t}^{(s+1)}(\boldsymbol{y}, \boldsymbol{x}^{(s+1)}) & (n = s + 1), \\ \boldsymbol{\sigma}_{m,t}^{(n)}(\tilde{\boldsymbol{\mu}}_t^{(n-1)}(\boldsymbol{x}^{(s+1:n-1)} | \boldsymbol{y}), \boldsymbol{x}^{(n)}) & \\ \boldsymbol{\sigma}_{m,t}^{(n)}(\tilde{\boldsymbol{\mu}}_t^{(n-1)}(\boldsymbol{x}^{(s+1:n-1)} | \boldsymbol{y}), \boldsymbol{x}^{(n)}) & \\ \boldsymbol{\tau}_{m,t}^{(n)}(\tilde{\boldsymbol{\mu}}_t^{(n-1)}(\boldsymbol{x}^{(s+1:n-1)} | \boldsymbol{y}), \boldsymbol{x}^{(n)}) & \\ \boldsymbol{\tau}_{m,t}^{(n)}(\tilde{\boldsymbol{\mu}}_t^{(n)}(\boldsymbol{x}^{(n)}, \boldsymbol{x}^{(n)}) & (n \geq s + 2), \end{cases} \end{split}$$

Moreover, we formally define $\boldsymbol{z}^{(s)}(\boldsymbol{x}^{(s+1)},\boldsymbol{x}^{(s)}|\boldsymbol{y}) = \tilde{\boldsymbol{\mu}}_t^{(s)}(\boldsymbol{x}^{(s+1)},\boldsymbol{x}^{(s)}|\boldsymbol{y}) = \boldsymbol{y}$ and $\tilde{\sigma}_{m,t}^{(s)}(\boldsymbol{x}^{(s+1)},\boldsymbol{x}^{(s)}|\boldsymbol{y}) = 0$. Then, the following theorem holds.

Theorem C.7 (CIs for N-stage cascade process under given observation). Assume that Assumptions C.1 and C.3 hold. Define $\beta = B^2$, and assume that $\tilde{\boldsymbol{\mu}}_t^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y}) \in \mathcal{Y}^{(n)}$ for any $s \in \{0,\ldots,N-1\}$, $n \in \{s+1,\ldots,N\}$, $\boldsymbol{y} \in \mathcal{Y}^{(s)}$, $t \geq 1$ and $(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}) \in \mathcal{X}^{(s+1)} \times \cdots \times \mathcal{X}^{(n)}$. Then, it follows that

$$|z_m^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y}) - \tilde{\mu}_{m,t}^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y})| \leq \beta^{1/2}\tilde{\sigma}_{m,t}^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y})$$

where $m \in [M^{(n)}]$, and $z_m^{(n)}(\cdot|\boldsymbol{y})$ and $\tilde{\mu}_{m,t}^{(n)}(\cdot|\boldsymbol{y})$ are the m-th element of $\boldsymbol{z}_m^{(n)}(\cdot|\boldsymbol{y})$ and $\tilde{\mu}_{m,t}^{(n)}(\cdot|\boldsymbol{y})$, respectively.

Proof. By using the same argument as in the proof of Theorem C.5, we get Theorem C.7.

Based on Theorem C.7, we give a stock reduction rule. For each $t \ge 1$ and $\mathbf{y} \in \mathcal{Y}^{(s)}$ with $0 \le s \le N-1$, we define $F(\mathbf{y})$, $\mathrm{LCB}_t^{(F)}(\mathbf{y})$ and $\mathrm{UCB}_t^{(F)}(\mathbf{y})$ as

$$\begin{split} F(\boldsymbol{y}) &= \max_{\boldsymbol{x}^{(s+1)}\cdots\boldsymbol{x}^{(N)}} \boldsymbol{z}^{(N)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N)}|\boldsymbol{y}), \\ \text{LCB}_t^{(F)}(\boldsymbol{y}) &= \max_{\boldsymbol{x}^{(s+1)}\cdots\boldsymbol{x}^{(N)}} (\tilde{\mu}_{1,t}^{(N)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N)}|\boldsymbol{y}) - \beta^{1/2}\tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N)}|\boldsymbol{y})), \\ \text{UCB}_t^{(F)}(\boldsymbol{y}) &= \max_{\boldsymbol{x}^{(s+1)}\cdots\boldsymbol{x}^{(N)}} (\tilde{\mu}_{1,t}^{(N)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N)}|\boldsymbol{y}) + \beta^{1/2}\tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N)}|\boldsymbol{y})), \end{split}$$

where $\tilde{\mu}_{1,t}^{(N)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N)}|\boldsymbol{y})$ is the first element of $\tilde{\boldsymbol{\mu}}_t^{(N)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N)}|\boldsymbol{y})$. Then, the following corollary holds.

Corollary C.8 (Stock reduction). Assume that the same assumption as in Theorem C.7 holds. Let $t \ge 1$, and let $S_t^{(u)}$ be a set of stocks at stage $u \in \{0, \dots, N-1\}$ in iteration t. Assume that an element y in $S_t^{(s)}$ satisfies

$$\mathrm{UCB}_t^{(F)}(\boldsymbol{y}) < \max_{\tilde{\boldsymbol{y}} \in \bigcup_{u=0}^{N-1} \mathcal{S}_t^{(u)}} \mathrm{LCB}_t^{(F)}(\tilde{\boldsymbol{y}}).$$

Then, it follows that $F(y) < F(x_*^{(1)}, \dots, x_*^{(N)})$.

Proof. From Theorems C.5 and C.7, noting that $y \in \mathcal{S}_t^{(u)}$ is the observed value corresponding to some input, it follows that

$$F(\boldsymbol{y}) \leq \text{UCB}_{t}^{(F)}(\boldsymbol{y})$$

$$< \max_{\tilde{\boldsymbol{y}} \in \bigcup_{u=0}^{N-1} \mathcal{S}_{t}^{(u)}} \text{LCB}_{t}^{(F)}(\tilde{\boldsymbol{y}})$$

$$\leq \max_{(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) \in \mathcal{X}} \boldsymbol{z}^{(N)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)} | \boldsymbol{0})$$

$$= F(\boldsymbol{x}_{*}^{(1)}, \dots, \boldsymbol{x}_{*}^{(N)}).$$

C.2 Cascade Process Upper Confidence Bound

Here, we consider a UCB-based optimization strategy, and give a cascade process upper confidence bound (cUCB) AF. For each iteration $t \ge 1$ and input $(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)})$, we define cUCB as

$$cUCB_t(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) = \tilde{\mu}_{1,t}^{(N)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) + \beta^{1/2}\tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}).$$

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Next, we consider the theoretical property of cUCB. Suppose that the next evaluation point is selected by

$$(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(N)}) = \underset{(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) \in \mathcal{X}}{\arg \max} \text{cUCB}_t(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}).$$
 (C.6)

Moreover, in order to evaluate the goodness of the optimization strategy, we introduce the regret r_t , cumulative regret R_T and simple regret $r_T^{(S)}$ as

$$r_t = F(\boldsymbol{x}_*^{(1)}, \dots, \boldsymbol{x}_*^{(N)}) - F(\boldsymbol{x}_t^{(1)}, \dots, \boldsymbol{x}_t^{(N)}),$$

$$R_T = \sum_{t=1}^{T} r_t, \quad r_T^{(S)} = \min_{1 \le t \le T} r_t.$$

Then, the following theorem gives regret bounds for R_T and $r_T^{(S)}$.

Theorem C.9. Assume that Assumptions C.1, C.3 and C.4 hold. Define $\beta = B^2$, and assume that $\tilde{\boldsymbol{\mu}}_t^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y}) \in \mathcal{Y}^{(n)}$ for any $s \in \{0,\ldots,N-1\}$, $n \in \{s+1,\ldots,N\}$, $\boldsymbol{y} \in \mathcal{Y}^{(s)}$, $t \geq 1$ and $(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}) \in \mathcal{X}^{(s+1)} \times \cdots \times \mathcal{X}^{(n)}$. Then, when the optimization is performed using cUCB, the following inequality holds for any $T \geq 1$:

$$R_T \leq \sqrt{\frac{8\beta C_0^{2(N-1)} M_{prod}^2 M_{sum}^2}{\log(1+\sigma^{-2})} T \gamma_T,}$$

$$r_T^{(S)} \leq T^{-1/2} \sqrt{\frac{8\beta C_0^{2(N-1)} M_{prod}^2 M_{sum}^2}{\log(1+\sigma^{-2})} \gamma_T,}$$

where $C_0 = L_\sigma \beta^{1/2} + L_f + 1$, $M_{prod} = \prod_{n=1}^N M^{(n)}$ and $M_{sum} = \sum_{n=1}^N M^{(n)}$.

Proof. From the definition of $\tilde{\sigma}_{m,t}^{(n)}(\cdot)$, using Lipschitz continuity of $\sigma_{m,t}^{(n)}(\cdot)$ we have

$$\begin{split} &\tilde{\sigma}_{m,t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}) \\ &= \sigma_{m,t}^{(n)}(\boldsymbol{z}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) + L_f \sum_{s=1}^{M^{(n-1)}} \tilde{\sigma}_{s,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}) \\ &+ \sigma_{m,t}^{(n)}(\tilde{\mu}_t^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) - \sigma_{m,t}^{(n)}(\boldsymbol{z}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) \\ &\leq \sigma_{m,t}^{(n)}(\boldsymbol{z}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) + L_f \sum_{s=1}^{M^{(n-1)}} \tilde{\sigma}_{s,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}) \\ &+ |\sigma_{m,t}^{(n)}(\boldsymbol{z}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) - \sigma_{m,t}^{(n)}(\tilde{\mu}_t^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)})| \\ &\leq \sigma_{m,t}^{(n)}(\boldsymbol{z}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) + L_f \sum_{s=1}^{M^{(n-1)}} \tilde{\sigma}_{s,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)})| \\ &+ L_\sigma \sum_{s=1}^{M^{(n-1)}} |z_s^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}) - \tilde{\mu}_{s,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)})| \\ &\leq \sigma_{m,t}^{(n)}(\boldsymbol{z}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) + L_f \sum_{s=1}^{M^{(n-1)}} \tilde{\sigma}_{s,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}) \\ &+ L_\sigma \beta^{1/2} \sum_{s=1}^{M^{(n-1)}} \tilde{\sigma}_{s,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}) \end{pmatrix}$$

$$= \sigma_{m,t}^{(n)}(\boldsymbol{z}^{(n-1)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n-1)}), \boldsymbol{x}^{(n)}) + (L_{\sigma}\beta^{1/2} + L_{f}) \sum_{s=1}^{M^{(n-1)}} \tilde{\sigma}_{s,t}^{(n-1)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n-1)})$$

$$\leq \sigma_{m,t}^{(n)}(\boldsymbol{z}^{(n-1)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n-1)}), \boldsymbol{x}^{(n)}) + C_{0} \sum_{s=1}^{M^{(n-1)}} \tilde{\sigma}_{s,t}^{(n-1)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n-1)}). \tag{C.7}$$

Thus, by repeating the same argument as (C.7) up to N, we get

$$\begin{split} &\tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N)}) \\ &\leq \sigma_{1,t}^{(N)}(\boldsymbol{z}^{(N-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N-1)}),\boldsymbol{x}^{(N)}) + C_0 \sum_{s=1}^{M^{(N-1)}} \tilde{\sigma}_{s,t}^{(N-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N-1)}) \\ &\leq \sigma_{1,t}^{(N)}(\boldsymbol{z}^{(N-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N-1)}),\boldsymbol{x}^{(N)}) \\ &+ C_0 \sum_{s=1}^{M^{(N-1)}} \sigma_{s,t}^{(N-1)}(\boldsymbol{z}^{(N-2)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N-2)}),\boldsymbol{x}^{(N-1)}) \\ &+ C_0^2 M^{(N-1)} \sum_{u=1}^{M^{(N-2)}} \tilde{\sigma}_{u,t}^{(N-2)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N-2)}) \\ &\leq \\ \vdots \\ &\leq \sigma_{1,t}^{(N)}(\boldsymbol{z}^{(N-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N-1)}),\boldsymbol{x}^{(N)}) \\ &+ \sum_{n=1}^{N-1} C_0^{N-n} \prod_{s=n+1}^{N} M^{(s)} \sum_{m=1}^{M^{(n)}} \left[\sigma_{m,t}^{(n)}(\boldsymbol{z}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) \right] \\ &\leq C_0^{N-1} M_{\mathrm{prod}} \sum_{n=1}^{N} \sum_{m=1}^{M^{(n)}} \sigma_{m,t}^{(n)}(\boldsymbol{z}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}). \end{split}$$

In addition, using the Cauchy-Schwarz inequality, it follows that

$$\tilde{\sigma}_{1,t}^{(N)2}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) \\
\leq C_0^{2(N-1)} M_{\text{prod}}^2 \left(\sum_{n=1}^N \sum_{m=1}^{M^{(n)}} 1 \right) \left(\sum_{n=1}^N \sum_{m=1}^{M^{(n)}} \sigma_{m,t}^{(n)2}(\boldsymbol{z}^{(n-1)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n-1)}), \boldsymbol{x}^{(n)}) \right) \\
= C_0^{2(N-1)} M_{\text{prod}}^2 M_{\text{sum}} \cdot \sum_{n=1}^N \sum_{m=1}^{M^{(n)}} \sigma_{m,t}^{(n)2}(\boldsymbol{z}^{(n-1)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n-1)}), \boldsymbol{x}^{(n)}). \tag{C.8}$$

Moreover, from Theorem C.5 and the selection rule (C.6), $F(\boldsymbol{x}_*^{(1)},\ldots,\boldsymbol{x}_*^{(N)})$ can be bounded as follows:

$$F(\boldsymbol{x}_{*}^{(1)}, \dots, \boldsymbol{x}_{*}^{(N)}) \leq \text{cUCB}_{t}(\boldsymbol{x}_{*}^{(1)}, \dots, \boldsymbol{x}_{*}^{(N)})$$

$$\leq \text{cUCB}_{t}(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(N)})$$

$$= \tilde{\mu}_{1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(N)}) + \beta^{1/2} \tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(N)}).$$

Similarly, since $F(\boldsymbol{x}_{t+1}^{(1)},\dots,\boldsymbol{x}_{t+1}^{(N)})$ can be bounded as

$$F(\boldsymbol{x}_{t+1}^{(1)},\ldots,\boldsymbol{x}_{t+1}^{(N)}) \geq \tilde{\mu}_{1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)},\ldots,\boldsymbol{x}_{t+1}^{(N)}) - \beta^{1/2}\tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)},\ldots,\boldsymbol{x}_{t+1}^{(N)}),$$

we get

$$r_{t} = F(\boldsymbol{x}_{*}^{(1)}, \dots, \boldsymbol{x}_{*}^{(N)}) - F(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(N)})$$

$$\leq 2\beta^{1/2} \tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(N)}). \tag{C.9}$$

Here, from the Cauchy–Schwarz inequality, R_T^2 can be evaluated as

$$R_T^2 = \left(\sum_{t=1}^T r_t\right)^2 \le T \sum_{t=1}^T r_t^2. \tag{C.10}$$

Hence, by combining (C.8) and (C.9) we have

$$\sum_{t=1}^{T} r_{t}^{2} \leq 4 \sum_{t=1}^{T} \left(\beta C_{0}^{2(N-1)} M_{\text{prod}}^{2} M_{\text{sum}} \sum_{n=1}^{N} \sum_{m=1}^{M^{(n)}} \sigma_{m,t}^{(n)2}(\boldsymbol{z}^{(n-1)}(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(n-1)}), \boldsymbol{x}_{t+1}^{(n)}) \right) \\
\leq 4 \beta C_{0}^{2(N-1)} M_{\text{prod}}^{2} M_{\text{sum}} sum_{n=1}^{N} \sum_{m=1}^{M^{(n)}} \sum_{t=1}^{T} \left[\sigma_{m,t}^{(n)2}(\boldsymbol{z}^{(n-1)}(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(n-1)}), \boldsymbol{x}_{t+1}^{(n)}) \right]. \tag{C.11}$$

Furthermore, by using the same argument as in Lemma 5.3 and 5.4 of (Srinivas et al., 2010), under the assumption $k^{(n)}(\cdot,\cdot) \leq 1$ we get

$$\sum_{t=1}^{T} \sigma_{m,t}^{(n)2}(\boldsymbol{z}^{(n-1)}(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(n-1)}), \boldsymbol{x}_{t+1}^{(n)}) \le \frac{2}{\log(1+\sigma^{-2})} \gamma_{m,T}^{(n)} \le \frac{2}{\log(1+\sigma^{-2})} \gamma_{T}. \tag{C.12}$$

Thus, from (C.11) and (C.12) we obtain

$$\sum_{t=1}^{T} r_t^2 \le \frac{8\beta C_0^{2(N-1)} M_{\text{prod}}^2 M_{\text{sum}}^2}{\log(1+\sigma^{-2})} \gamma_T. \tag{C.13}$$

Hence, by using (C.10) and (C.13), it follows that

$$R_t \le \sqrt{\frac{8\beta C_0^{2(N-1)} M_{\text{prod}}^2 M_{\text{sum}}^2}{\log(1+\sigma^{-2})} T\gamma_T}.$$

Finally, since $r_T^{(S)}$ satisfies

$$Tr_T^{(S)} \le \sum_{t=1}^{T} r_t = R_T \le \sqrt{\frac{8\beta C_0^{2(N-1)} M_{\text{prod}}^2 M_{\text{sum}}^2}{\log(1+\sigma^{-2})}} T\gamma_T,$$

the following inequality holds:

$$r_T^{(\mathrm{S})} \leq T^{-1/2} \sqrt{\frac{8\beta C_0^{2(N-1)} M_{\mathrm{prod}}^2 M_{\mathrm{sum}}^2}{\log(1+\sigma^{-2})} \gamma_T}.$$

C.3 Optimistic Improvement-based AF

In this subsection, we consider sequential observations of a cascade process from stage 1 to N. For each iteration $t \in \{0, N, 2N, \ldots\} \equiv N\mathbb{Z}_{\geq 0}$, users determine $\boldsymbol{x}_{t+1}^{(1)}$ and observe $\boldsymbol{y}_{t+1}^{(1)} = \boldsymbol{f}^{(1)}(\boldsymbol{0}, \boldsymbol{x}_{t+1}^{(1)})$. After that, users choose

 $m{x}_{t+2}^{(2)}$ and observe $m{y}_{t+2}^{(2)} = m{f}^{(2)}(m{y}_{t+1}^{(1)}, m{x}_{t+2}^{(2)})$. By repeating this operation, users obtain $m{y}_{t+N}^{(N)} = m{f}^{(N)}(m{y}_{t+N-1}^{(N-1)}, m{x}_{t+N}^{(N)})$ finally. We design the CI-based AF according to the following strategy: (1) given an observation $m{y}^{(n)}$, we seek the maximum of F if it is expected to be found; (2) if the maximum is not expected to be found, we collect the information by using another policy. We use the optimistic improvement for (1), and we adopt uncertainty sampling (US) policy for (2). First, we define the pessimistic maximum of $F(m{x}^{(1)}, \dots, m{x}^{(N)})$ as

$$Q_T = \max_{(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)})} \left(\tilde{\mu}_{1, T}^{(N)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) - \beta^{1/2} \tilde{\sigma}_{1, T}^{(N)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) \right).$$

In addition, given the observation $y^{(n-1)}$ in stage n-1, we define the pessimistic maximum of F obtained through $y^{(n-1)}$ as follows:

$$LCB_{t}^{(F)}(\boldsymbol{y}^{(n-1)}) = \max_{\boldsymbol{x}^{(n:N)}} \left(\tilde{\mu}_{1,t}^{(N)}(\boldsymbol{x}^{(n:N)}|\boldsymbol{y}^{(n-1)}) - \beta^{1/2}\tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}^{(n:N)}|\boldsymbol{y}^{(n-1)}) \right),$$

where the max operator is not necessary when n = N. Similarly, the optimistic maximum for given the input $(y^{(n-1)}, x^{(n)})$ is defined as follows:

$$\mathrm{UCB}_t^{(F)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) = \max_{\boldsymbol{x}^{(n+1:N)}} \left(\tilde{\mu}_{1,t}^{(N)}(\boldsymbol{x}^{(n:N)}|\boldsymbol{y}^{(n-1)}) + \beta^{1/2} \tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}^{(n:N)}|\boldsymbol{y}^{(n-1)}) \right).$$

Then, we define the optimistic improvement w.r.t. $(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)})$ as follows:

$$a_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) = \text{UCB}_t^{(F)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) - \max\{\text{LCB}_t^{(F)}(\boldsymbol{y}^{(n-1)}), Q_{t+n-1}\}.$$
(C.14)

Furthermore, we define the maximum uncertainty

$$b_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) = \max_{(\boldsymbol{x}^{(n+1)},\dots,\boldsymbol{x}^{(N)})} \tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}^{(n)},\dots,\boldsymbol{x}^{(N)}|\boldsymbol{y}^{(n-1)}). \tag{C.15}$$

Using (C.14) and (C.15), optimistic improvement-based AF (presented as CI-based AF in section 3.2) $c_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)})$ is defined as

$$c_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) = \max \left\{ a_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}), \eta_t b_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) \right\},$$

where η_t is some learning rate tends to zero. Therefore, given the observation $y^{(n-1)}$ at iteration t, the next observation point is given by

$$\boldsymbol{x}_{t+n}^{(n)} = \underset{\boldsymbol{x}^{(n)} \in \mathcal{X}^{(n)}}{\arg \max} c_t^{(n)} (\boldsymbol{x}^{(n)} | \boldsymbol{y}_{t+n-1}^{(n-1)}), \tag{C.16}$$

where $y^{(0)} = 0$.

Theorem C.10. Assume that Assumptions C.1, C.3 and C.4 hold. Also assume that $\tilde{\boldsymbol{\mu}}_t^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y})\in\mathcal{Y}^{(n)}$ for any $s\in\{0,\ldots,N-1\}$, $n\in\{s+1,\ldots,N\}$, $\boldsymbol{y}\in\mathcal{Y}^{(s)}$, $t\geq 1$ and $(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)})\in\mathcal{X}^{(s+1)}\times\cdots\times\mathcal{X}^{(n)}$. Let ξ be a positive number, and define $\beta=B^2$ and $\eta_t=(1+\log t)^{-1}$. Then, when the optimization is performed using (C.16), the estimated solution $(\hat{\boldsymbol{x}}_T^{(1)},\ldots,\hat{\boldsymbol{x}}_T^{(N)})$ satisfies that

$$F(\boldsymbol{x}_*^{(1)}, \dots, \boldsymbol{x}_*^{(N)}) - F(\hat{\boldsymbol{x}}_T^{(1)}, \dots, \hat{\boldsymbol{x}}_T^{(N)}) < \xi,$$

where T is the smallest positive integer satisfying $T \in N\mathbb{Z}_{>0}$ and

$$\frac{8\beta C_4^2 M_{sum}^2 N}{\log(1+\sigma^{-2})} \gamma_T \eta_T^{-2N-2} T^{-1} < \xi^2.$$

Here, C_4 is the positive constant given by

$$C_1 = \max\{1, L_f, L_f^{-1}\}, C_2 = 4NM_{\textit{prod}}^2 M_{\textit{sum}} C_0^{2N-3} C_1^N, C_3 = NC_2^N, C_4 = (2\beta^{1/2} + 2)^N C_3^N.$$

In order to prove Theorem C.10, we give four lemmas.

Lemma C.11. Assume that the same condition as in Theorem C.10 holds. Let $s \in \{1, ..., N-1\}$ and $n \in \{s+1, ..., N\}$. Then, for any iteration $t \geq 1$, element $m \in [M^{(n)}]$ and input $\mathbf{x}^{(1)}, ..., \mathbf{x}^{(N)}$, the following inequality holds:

$$\begin{split} &|\sigma_{m,t}^{(n)}(\tilde{\boldsymbol{\mu}}_t^{(n-1)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(n-1)}|\boldsymbol{z}^{(s-1)}),\boldsymbol{x}^{(n)}) - \sigma_{m,t}^{(n)}(\tilde{\boldsymbol{\mu}}_t^{(n-1)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n-1)}|\boldsymbol{z}^{(s)}),\boldsymbol{x}^{(n)})| \\ &\leq 2M_{prod}C_0^{N-1}\sum_{p=0}^{n-s-1}\sum_{i=1}^{M^{(n-1-p)}} \left[\sigma_{i,t}^{(n-1-p)}(\tilde{\boldsymbol{\mu}}_t^{(n-2-p)}(\boldsymbol{x}^{(s:n-2-p)}|\boldsymbol{z}^{(s-1)}),\boldsymbol{x}^{(n-1-p)})\right]. \end{split}$$

Proof. From Lipschitz continuity of $\sigma_{m,t}^{(n)}(\cdot)$, the following holds:

$$\begin{split} &|\sigma_{m,t}^{(n)}(\tilde{\boldsymbol{\mu}}_{t}^{(n-1)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(n-1)}|\boldsymbol{z}^{(s-1)}),\boldsymbol{x}^{(n)}) - \sigma_{m,t}^{(n)}(\tilde{\boldsymbol{\mu}}_{t}^{(n-1)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n-1)}|\boldsymbol{z}^{(s)}),\boldsymbol{x}^{(n)})| \\ &\leq L_{\sigma} \|\tilde{\boldsymbol{\mu}}_{t}^{(n-1)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(n-1)}|\boldsymbol{z}^{(s-1)}) - \tilde{\boldsymbol{\mu}}_{t}^{(n-1)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n-1)}|\boldsymbol{z}^{(s)})\|_{1} \\ &= L_{\sigma} \sum_{j=1}^{M^{(n-1)}} |\tilde{\boldsymbol{\mu}}_{j,t}^{(n-1)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(n-1)}|\boldsymbol{z}^{(s-1)}) - \tilde{\boldsymbol{\mu}}_{j,t}^{(n-1)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n-1)}|\boldsymbol{z}^{(s)})| \\ &= L_{\sigma} \sum_{j=1}^{M^{(n-1)}} |\boldsymbol{\mu}_{j,t}^{(n-1)}(\tilde{\boldsymbol{\mu}}_{t}^{(n-2)}(\boldsymbol{x}^{(s:n-2)}|\boldsymbol{z}^{(s-1)}),\boldsymbol{x}^{(n-1)}) - \boldsymbol{\mu}_{j,t}^{(n-1)}(\tilde{\boldsymbol{\mu}}_{t}^{(n-2)}(\boldsymbol{x}^{(s+1:n-2)}|\boldsymbol{z}^{(s)}),\boldsymbol{x}^{(n-1)})|. \end{aligned} \tag{C.17}$$

Here, noting that

$$f_m^{(k)}(\boldsymbol{y}, \boldsymbol{x}) - \beta^{1/2} \sigma_{m,t}^{(k)}(\boldsymbol{y}, \boldsymbol{x}) \le \mu_{m,t}^{(k)}(\boldsymbol{y}, \boldsymbol{x})$$

$$\le f_m^{(k)}(\boldsymbol{y}, \boldsymbol{x}) + \beta^{1/2} \sigma_{m,t}^{(k)}(\boldsymbol{y}, \boldsymbol{x}),$$

we have

$$|\mu_{m,t}^{(k)}(\boldsymbol{y},\boldsymbol{x}) - \mu_{m,t}^{(k)}(\boldsymbol{y}',\boldsymbol{x})|$$

$$\leq |f_{m}^{(k)}(\boldsymbol{y},\boldsymbol{x}) - f_{m}^{(k)}(\boldsymbol{y}',\boldsymbol{x})| + \beta^{1/2}\sigma_{m,t}^{(k)}(\boldsymbol{y},\boldsymbol{x}) + \beta^{1/2}\sigma_{m,t}^{(k)}(\boldsymbol{y}',\boldsymbol{x})$$

$$\leq |f_{m}^{(k)}(\boldsymbol{y},\boldsymbol{x}) - f_{m}^{(k)}(\boldsymbol{y}',\boldsymbol{x})| + \beta^{1/2}|\sigma_{m,t}^{(k)}(\boldsymbol{y},\boldsymbol{x}) - \sigma_{m,t}^{(k)}(\boldsymbol{y}',\boldsymbol{x})| + 2\beta^{1/2}\sigma_{m,t}^{(k)}(\boldsymbol{y}',\boldsymbol{x})$$

$$\leq (L_{f} + \beta_{t}^{1/2}L_{\sigma})||\boldsymbol{y} - \boldsymbol{y}'||_{1} + 2\beta^{1/2}\sigma_{m,t}^{(k)}(\boldsymbol{y}',\boldsymbol{x}). \tag{C.18}$$

Therefore, by substituting (C.18) into (C.17), it follows that

$$\begin{split} &|\sigma_{m,t}^{(n)}(\tilde{\boldsymbol{\mu}}_{t}^{(n-1)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(n-1)}|\boldsymbol{z}^{(s-1)}),\boldsymbol{x}^{(n)}) - \sigma_{m,t}^{(n)}(\tilde{\boldsymbol{\mu}}_{t}^{(n-1)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n-1)}|\boldsymbol{z}^{(s)}),\boldsymbol{x}^{(n)})| \\ &\leq 2\beta^{1/2}L_{\sigma}\sum_{j=1}^{M^{(n-1)}}\sigma_{j,t}^{(n-1)}(\tilde{\boldsymbol{\mu}}_{t}^{(n-2)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n-2)}|\boldsymbol{z}^{(s)}),\boldsymbol{x}^{(n-1)}) + L_{\sigma}M^{(n-1)}(L_{f} + \beta^{1/2}L_{\sigma}) \\ &\cdot \|\tilde{\boldsymbol{\mu}}_{t}^{(n-2)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(n-2)}|\boldsymbol{z}^{(s-1)}) - \tilde{\boldsymbol{\mu}}_{t}^{(n-2)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n-2)}|\boldsymbol{z}^{(s)})\|_{1} \\ &\leq 2\beta^{1/2}L_{\sigma}\sum_{j=1}^{M^{(n-1)}}\sigma_{j,t}^{(n-1)}(\tilde{\boldsymbol{\mu}}_{t}^{(n-2)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n-2)}|\boldsymbol{z}^{(s)}),\boldsymbol{x}^{(n-1)}) \\ &+ L_{\sigma}M^{(n-1)}(L_{f} + \beta^{1/2}L_{\sigma})\sum_{i=1}^{M^{(n-2)}}|\tilde{\boldsymbol{\mu}}_{i,t}^{(n-2)}(\boldsymbol{x}^{(s:n-2)}|\boldsymbol{z}^{(s-1)}) - \tilde{\boldsymbol{\mu}}_{i,t}^{(n-2)}(\boldsymbol{x}^{(s+1:n-2)}|\boldsymbol{z}^{(s)})| \\ &\leq 2\beta^{1/2}L_{\sigma}\sum_{j=1}^{M^{(n-1)}}\sigma_{j,t}^{(n-1)}(\tilde{\boldsymbol{\mu}}_{t}^{(n-2)}(\boldsymbol{x}^{(s:n-2)}|\boldsymbol{z}^{(s-1)}),\boldsymbol{x}^{(n-1)}) \end{split}$$

$$\begin{split} &+2\beta^{1/2}L_{\sigma}M^{(n-1)}(L_{f}+\beta^{1/2}L_{\sigma})\cdot\sum_{i=1}^{M^{(n-2)}}\sigma_{i,t}^{(n-2)}(\tilde{\mu}_{t}^{(n-3)}(x^{(s)},\ldots,x^{(n-3)}|z^{(s-1)}),x^{(n-2)})\\ &+L_{\sigma}M^{(n-1)}M^{(n-2)}(L_{f}+\beta^{1/2}L_{\sigma})^{2}\sum_{q=1}^{M^{(n-3)}}\left[|\tilde{\mu}_{q,t}^{(n-3)}(x^{(s:n-3)}|z^{(s-1)})-\tilde{\mu}_{q,t}^{(n-3)}(x^{(s+1:n-3)}|z^{(s)})|\right]\\ &\leq\\ &\vdots\\ &\leq2\beta^{1/2}L_{\sigma}M_{\mathrm{prod}}(L_{f}+\beta^{1/2}L_{\sigma}+1)^{N-2}\\ &\cdot\sum_{p=0}^{n-s-2}\sum_{i=1}^{M^{(n-1-p)}}\left[\sigma_{i,t}^{(n-1-p)}\left(\tilde{\mu}_{t}^{(n-2-p)}(x^{(s:n-2-p)}|z^{(s-1)}),x^{(n-1-p)}\right)\right]\\ &+2M_{\mathrm{prod}}\beta^{1/2}L_{\sigma}(L_{f}+\beta^{1/2}L_{\sigma}+1)^{N-2}\sum_{q=1}^{M^{(s)}}\sigma_{q,t}^{(s)}(z^{(s-1)},x^{(s)})\\ &\leq2M_{\mathrm{prod}}(L_{f}+\beta^{1/2}L_{\sigma}+1)^{N-1}\sum_{p=0}^{n-s-1}\sum_{i=1}^{M^{(n-1-p)}}\left[\sigma_{i,t}^{(n-1-p)}(\tilde{\mu}_{t}^{(n-2-p)}(x^{(s:n-2-p)}|z^{(s-1)}),x^{(n-1-p)})\right]\\ &\leq2M_{\mathrm{prod}}C_{0}^{N-1}\sum_{p=0}^{n-s-1}\sum_{i=1}^{M^{(n-1-p)}}\left[\sigma_{i,t}^{(n-1-p)}(\tilde{\mu}_{t}^{(n-2-p)}(x^{(s)},\ldots,x^{(n-2-p)}|z^{(s-1)}),x^{(n-1-p)})\right]. \end{split}$$

Lemma C.12. Assume that the same condition as in Theorem C.10 holds. Let $s \in \{1, ..., N-1\}$, and let $j \ge 0$ be an integer with $s+j \le N$. Then, for any iteration $t \ge 1$, element $m \in [M^{(n)}]$ and input $\mathbf{x}^{(1)}, ..., \mathbf{x}^{(N)}$, the following inequality holds:

$$\begin{split} \tilde{\sigma}_t^{(N-j)}(\boldsymbol{x}^{(s)}, \dots, \boldsymbol{x}^{(N-j)} | \boldsymbol{z}^{(s-1)}) &\leq \tilde{C}_2 \tilde{\sigma}_t^{(N-j)}(\boldsymbol{x}^{(s+1)}, \dots, \boldsymbol{x}^{(N-j)} | \boldsymbol{z}^{(s)}) + \tilde{C}_2 \sum_{i=1}^{M^{(s)}} \sigma_{i,t}^{(s)}(\boldsymbol{z}^{(s-1)}, \boldsymbol{x}^{(s)}) \\ &+ \tilde{C}_2 \tilde{\sigma}_t^{(N-j-1)}(\boldsymbol{x}^{(s)}, \dots, \boldsymbol{x}^{(N-j-1)} | \boldsymbol{z}^{(s-1)}), \end{split}$$

where

$$\begin{split} & \tilde{\sigma}_t^{(N-j)}(\boldsymbol{x}^{(s)}, \dots, \boldsymbol{x}^{(N-j)} | \boldsymbol{z}^{(s-1)}) \\ & = \sum_{p=j}^{N-s} \prod_{q=1}^p M^{(N-q+1)} L_f^p \sum_{i=1}^{M^{(N-p)}} \left[\sigma_{i,t}^{(N-p)}(\tilde{\boldsymbol{\mu}}_t^{(N-p-1)}(\boldsymbol{x}^{(s)}, \dots, \boldsymbol{x}^{(N-p-1)} | \boldsymbol{z}^{(s-1)}), \boldsymbol{x}^{(N-p)}) \right] \end{split}$$

and $\tilde{C}_2 = 4NM_{prod}^2 M_{sum} C_0^{2N-2} C_1^N$.

Proof. From the definition of $\tilde{\sigma}_t^{(N-j)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(N-j)}|\boldsymbol{z}^{(s-1)})$, the following inequality holds:

$$\begin{split} &\tilde{\sigma}_{t}^{(N-j)}(\boldsymbol{x}^{(s)}, \dots, \boldsymbol{x}^{(N-j)} | \boldsymbol{z}^{(s-1)}) \\ &= \sum_{p=j}^{N-s} \prod_{q=1}^{p} M^{(N-q+1)} L_{f}^{p} \sum_{i=1}^{M^{(N-p)}} \left[\sigma_{i,t}^{(N-p)}(\tilde{\boldsymbol{\mu}}_{t}^{(N-p-1)}(\boldsymbol{x}^{(s)}, \dots, \boldsymbol{x}^{(N-p-1)} | \boldsymbol{z}^{(s-1)}), \boldsymbol{x}^{(N-p)}) \right] \\ &\leq M_{\text{prod}} C_{0}^{N-1} \sum_{p=j}^{N-s} \sum_{i=1}^{M^{(N-p)}} \left[\sigma_{i,t}^{(N-p)}(\tilde{\boldsymbol{\mu}}_{t}^{(N-p-1)}(\boldsymbol{x}^{(s)}, \dots, \boldsymbol{x}^{(N-p-1)} | \boldsymbol{z}^{(s-1)}), \boldsymbol{x}^{(N-p)}) \right] \end{split}$$

$$\begin{split} &= M_{\text{prod}}C_0^{N-1} \sum_{p=j}^{N-s-1} \sum_{i=1}^{M^{(N-p)}} \left[\sigma_{i,t}^{(N-p)} \big(\tilde{\boldsymbol{\mu}}_t^{(N-p-1)} (\boldsymbol{x}^{(s+1)}, \dots, \boldsymbol{x}^{(N-p-1)} | \boldsymbol{z}^{(s)}), \boldsymbol{x}^{(N-p)} \big) \right] \\ &+ M_{\text{prod}}C_0^{N-1} \sum_{p=j}^{N-s-1} \sum_{i=1}^{M^{(N-p)}} \left(\sigma_{i,t}^{(N-p)} \big(\tilde{\boldsymbol{\mu}}_t^{(N-p-1)} (\boldsymbol{x}^{(s)}, \dots, \boldsymbol{x}^{(N-p-1)} | \boldsymbol{z}^{(s-1)}), \boldsymbol{x}^{(N-p)} \right) \\ &- \sigma_{i,t}^{(N-p)} \big(\tilde{\boldsymbol{\mu}}_t^{(N-p-1)} (\boldsymbol{x}^{(s+1)}, \dots, \boldsymbol{x}^{(N-p-1)} | \boldsymbol{z}^{(s)}), \boldsymbol{x}^{(N-p)} \big) \right) + M_{\text{prod}}C_0^{N-1} \sum_{i=1}^{M^{(s)}} \sigma_{i,t}^{(s)} (\boldsymbol{z}^{(s-1)}, \boldsymbol{x}^{(s)}). \end{split}$$

Thus, from Lemma C.11 we get

$$\begin{split} &|\sigma_{i,t}^{(N-p)}(\tilde{\boldsymbol{\mu}}_t^{(N-p-1)}(\boldsymbol{x}^{(s)},\dots,\boldsymbol{x}^{(N-p-1)}|\boldsymbol{z}^{(s-1)}),\boldsymbol{x}^{(N-p)})\\ &-\sigma_{i,t}^{(N-p)}(\tilde{\boldsymbol{\mu}}_t^{(N-p-1)}(\boldsymbol{x}^{(s+1)},\dots,\boldsymbol{x}^{(N-p-1)}|\boldsymbol{z}^{(s)}),\boldsymbol{x}^{(N-p)})|\\ &\leq 2M_{\mathrm{prod}}C_0^{N-1}\sum_{r=0}^{N-p-s-1}\\ &\cdot\sum_{j=1}^{M^{(N-p-1-r)}}\left[\sigma_{j,t}^{(N-p-1-r)}\left(\tilde{\boldsymbol{\mu}}_t^{(N-p-2-r)}(\boldsymbol{x}^{(s)},\dots,\boldsymbol{x}^{(N-p-2-r)}|\boldsymbol{z}^{(s-1)}),\boldsymbol{x}^{(N-p-1-r)}\right)\right]. \end{split}$$

By using this, $\tilde{\sigma}_t^{(N-j)}({m x}^{(s)},\dots,{m x}^{(N-j)}|{m z}^{(s-1)})$ can be written as

$$\begin{split} &\tilde{\sigma}_{t}^{(N-j)}(\boldsymbol{x}^{(s)}, \dots, \boldsymbol{x}^{(N-j)} | \boldsymbol{z}^{(s-1)}) \\ &\leq M_{\text{prod}} C_{0}^{N-2} \sum_{p=j}^{N-s-1} \sum_{i=1}^{M^{(N-p)}} \sigma_{i,t}^{(N-p)} \left(\tilde{\boldsymbol{\mu}}_{t}^{(N-p-1)}(\boldsymbol{x}^{(s+1)}, \dots, \boldsymbol{x}^{(N-p-1)} | \boldsymbol{z}^{(s)}), \boldsymbol{x}^{(N-p)} \right) \\ &+ M_{\text{prod}} C_{0}^{N-2} \sum_{i=1}^{M^{(s)}} \sigma_{i,t}^{(s)}(\boldsymbol{z}^{(s-1)}, \boldsymbol{x}^{(s)}) + 2 M_{\text{prod}}^{2} C_{0}^{2N-2} M_{\text{sum}} \\ &\cdot \sum_{p=j}^{N-s-1} \sum_{r=0}^{N-p-s-1} \sum_{j=1}^{M^{(N-p-1-r)}} \left[\sigma_{j,t}^{(N-p-1-r)} \left(\tilde{\boldsymbol{\mu}}_{t}^{(N-p-2-r)}(\boldsymbol{x}^{(s:N-p-2-r)} | \boldsymbol{z}^{(s-1)}), \boldsymbol{x}^{(N-p-1-r)} \right) \right]. \end{split}$$

Here, we set v = p + r. Then, noting that $|\{(p, r) \mid p + r = a\}| \le 2a$, we obtain

$$\begin{split} &\tilde{\sigma}_{t}^{(N-j)}(\boldsymbol{x}^{(s)},\dots,\boldsymbol{x}^{(N-j)}|\boldsymbol{z}^{(s-1)}) \\ &\leq M_{\text{prod}}C_{0}^{N-2} \sum_{p=j}^{N-s-1} \sum_{i=1}^{M^{(N-p)}} \sigma_{i,t}^{(N-p)} \left(\tilde{\boldsymbol{\mu}}_{t}^{(N-p-1)}(\boldsymbol{x}^{(s+1)},\dots,\boldsymbol{x}^{(N-p-1)}|\boldsymbol{z}^{(s)}),\boldsymbol{x}^{(N-p)} \right) \\ &+ 2M_{\text{prod}}^{2}C_{0}^{2N-2} M_{\text{sum}} \sum_{v=j}^{N-s-1} 2N \sum_{j=1}^{M^{(N-v-1)}} \sigma_{j,t}^{(N-v-1)} \left(\tilde{\boldsymbol{\mu}}_{t}^{(N-v-2)}(\boldsymbol{x}^{(s)},\dots,\boldsymbol{x}^{(N-v-2)}|\boldsymbol{z}^{(s-1)}),\boldsymbol{x}^{(N-v-1)} \right) \\ &+ M_{\text{prod}}C_{0}^{N-2} \sum_{i=1}^{M^{(s)}} \sigma_{i,t}^{(s)}(\boldsymbol{z}^{(s-1)},\boldsymbol{x}^{(s)}) \\ &\leq 4NM_{\text{prod}}^{2}C_{0}^{2N-2} M_{\text{sum}} \sum_{p=j}^{N-s-1} \sum_{i=1}^{M^{(N-p)}} \sigma_{i,t}^{(N-p)} \left(\tilde{\boldsymbol{\mu}}_{t}^{(N-p-1)}(\boldsymbol{x}^{(s+1)},\dots,\boldsymbol{x}^{(N-p-1)}|\boldsymbol{z}^{(s)}),\boldsymbol{x}^{(N-p)} \right) \\ &+ 4NM_{\text{prod}}^{2}C_{0}^{2N-2} M_{\text{sum}} \sum_{v=j}^{N-s-1} \sum_{j=1}^{M^{(N-v-1)}} \sigma_{j,t}^{(N-v-1)} \left(\tilde{\boldsymbol{\mu}}_{t}^{(N-v-2)}(\boldsymbol{x}^{(s)},\dots,\boldsymbol{x}^{(N-v-2)}|\boldsymbol{z}^{(s-1)}),\boldsymbol{x}^{(N-v-1)} \right) \end{split}$$

$$\begin{split} &+4NM_{\mathrm{prod}}^{2}C_{0}^{2N-2}M_{\mathrm{sum}}C_{1}^{N}\sum_{i=1}^{M^{(s)}}\sigma_{i,t}^{(s)}(\boldsymbol{z}^{(s-1)},\boldsymbol{x}^{(s)})\\ &\leq \tilde{C}_{2}\tilde{\sigma}_{t}^{(N-j)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N-j)}|\boldsymbol{z}^{(s)})+\tilde{C}_{2}\tilde{\sigma}_{t}^{(N-j-1)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(N-j-1)}|\boldsymbol{z}^{(s-1)})\\ &+\tilde{C}_{2}\sum_{i=1}^{M^{(s)}}\sigma_{i,t}^{(s)}(\boldsymbol{z}^{(s-1)},\boldsymbol{x}^{(s)}). \end{split}$$

Lemma C.13. Assume that the same condition as in Theorem C.10 holds. Let $s \in \{1, ..., N-1\}$ and $n \in \{s+1, ..., N\}$. Then, for any iteration $t \geq 1$, element $m \in [M^{(n)}]$ and input $\mathbf{x}^{(1)}, ..., \mathbf{x}^{(N)}$, the following inequality holds:

$$\tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}^{(s:N)}|\boldsymbol{z}^{(s-1)}) \leq C_3 \tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}^{(s+1:N)}|\boldsymbol{z}^{(s)}) + C_3 \sum_{i=1}^{M^{(s)}} \sigma_{i,t}^{(s)}(\boldsymbol{z}^{(s-1)},\boldsymbol{x}^{(s)}).$$

Proof. By repeatedly using Lemma C.12, we obtain

$$\begin{split} &\tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(N)}|\boldsymbol{z}^{(s-1)}) \\ &= \tilde{\sigma}_{t}^{(N-0)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(N-0)}|\boldsymbol{z}^{(s-1)}) \\ &\leq \tilde{C}_{2}\tilde{\sigma}_{t}^{(N-0)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N-0)}|\boldsymbol{z}^{(s)}) + \tilde{C}_{2}\sum_{i=1}^{M^{(s)}}\sigma_{i,t}^{(s)}(\boldsymbol{z}^{(s-1)},\boldsymbol{x}^{(s)}) + \tilde{C}_{2}\tilde{\sigma}_{t}^{(N-1)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(N-1)}|\boldsymbol{z}^{(s-1)}) \\ &\leq \tilde{C}_{2}\tilde{\sigma}_{t}^{(N-0)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N-0)}|\boldsymbol{z}^{(s)}) + \tilde{C}_{2}\sum_{i=1}^{M^{(s)}}\sigma_{i,t}^{(s)}(\boldsymbol{z}^{(s-1)},\boldsymbol{x}^{(s)}) + \tilde{C}_{2}^{2}\sum_{i=1}^{M^{(s)}}\sigma_{i,t}^{(s)}(\boldsymbol{z}^{(s-1)},\boldsymbol{x}^{(s)}) \\ &+ \tilde{C}_{2}^{2}\tilde{\sigma}_{t}^{(N-1)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N-1)}|\boldsymbol{z}^{(s)}) + \tilde{C}_{2}^{2}\tilde{\sigma}_{t}^{(N-2)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(N-2)}|\boldsymbol{z}^{(s-1)}) \\ &\leq \\ \vdots \\ &\leq (\tilde{C}_{2} + \tilde{C}_{2}^{2} + \cdots + \tilde{C}_{2}^{N-1})\tilde{\sigma}_{t}^{(N-0)}(\boldsymbol{x}^{(s+1:N-0)}|\boldsymbol{z}^{(s)}) + (\tilde{C}_{2} + \tilde{C}_{2}^{2} + \cdots + \tilde{C}_{2}^{N-1})\sum_{i=1}^{M^{(s)}}\sigma_{i,t}^{(s)}(\boldsymbol{z}^{(s-1)},\boldsymbol{x}^{(s)}) \\ &\leq (N-1)\tilde{C}_{2}^{N-1}\tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N)}|\boldsymbol{z}^{(s)}) + (N-1)\tilde{C}_{2}^{N-1}\sum_{i=1}^{M^{(s)}}\sigma_{i,t}^{(s)}(\boldsymbol{z}^{(s-1)},\boldsymbol{x}^{(s)}). \end{split}$$

In addition, $(N-1)\tilde{C}_2^{N-1}$ can be bounded by

$$\begin{split} (N-1)\tilde{C}_2^{N-1} &\leq N\tilde{C}_2^{N-1} \\ &= N(4NM_{\mathrm{prod}}^2 M_{\mathrm{sum}} C_0^{2N-2} C_1^N)^{N-1} \\ &\leq N(4NM_{\mathrm{prod}}^2 M_{\mathrm{sum}} C_1^N)^N C_0^{2N^2-4N+2} \\ &\leq N(4NM_{\mathrm{prod}}^2 M_{\mathrm{sum}} C_1^N)^N C_0^{2N^2-4N+N} \\ &= N(4NM_{\mathrm{prod}}^2 M_{\mathrm{sum}} C_0^{2N-3} C_1^N)^N \\ &= NC_2^N = C_3, \end{split}$$

we get Lemma C.13.

Lemma C.14. Assume that the same condition as in Theorem C.10 holds. Let $n \in [N]$ and $\mathbf{y}^{(n-1)} \in \mathcal{Y}^{(n-1)}$. Then, for any iteration $t \ge 1$ and input $\mathbf{x}^{(n)} \in \mathcal{X}^{(n)}$, the following inequality holds:

$$\eta_t b_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) \le c_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)})
\le (2\beta^{1/2} + \eta_t) b_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}).$$

Proof. From the definition of $c_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)})$, it is clear that $\eta_t b_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) \leq c_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)})$. On the other hand, from the definition of $\mathrm{UCB}_t^{(F)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)})$, letting

$$(\tilde{\boldsymbol{x}}^{(n+1)}, \dots, \tilde{\boldsymbol{x}}^{(N)}) = \underset{(\boldsymbol{x}^{(n+1)}, \dots, \boldsymbol{x}^{(N)})}{\arg\max} \left(\tilde{\mu}_{1,t}^{(N)}(\boldsymbol{x}^{(n:N)}|\boldsymbol{y}^{(n-1)}) + \beta^{1/2} \tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}^{(n:N)}|\boldsymbol{y}^{(n-1)}) \right)$$

we obtain

$$UCB_{t}^{(F)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) = \tilde{\mu}_{1.t}^{(N)}(\boldsymbol{x}^{(n)}, \tilde{\boldsymbol{x}}^{(n+1)}..., \tilde{\boldsymbol{x}}^{(N)}|\boldsymbol{y}^{(n-1)}) + \beta^{1/2}\tilde{\sigma}_{1.t}^{(N)}(\boldsymbol{x}^{(n)}, \tilde{\boldsymbol{x}}^{(n+1)},..., \tilde{\boldsymbol{x}}^{(N)}|\boldsymbol{y}^{(n-1)}).$$

Similarly, $LCB_t^{(F)}(\boldsymbol{y}^{(n-1)})$ can be bounded as follows:

$$LCB_{t}^{(F)}(\boldsymbol{y}^{(n-1)}) \geq \tilde{\mu}_{1,t}^{(N)}(\boldsymbol{x}^{(n)}, \tilde{\boldsymbol{x}}^{(n+1)}\dots, \tilde{\boldsymbol{x}}^{(N)}|\boldsymbol{y}^{(n-1)}) - \beta^{1/2}\tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}^{(n)}, \tilde{\boldsymbol{x}}^{(n+1)}, \dots, \tilde{\boldsymbol{x}}^{(N)}|\boldsymbol{y}^{(n-1)}).$$

Hence, from the definition of $a_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)})$ and $b_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)})$, we get

$$\begin{split} a_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) &\leq \mathrm{UCB}_t^{(F)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) - \mathrm{LCB}_t^{(F)}(\boldsymbol{y}^{(n-1)}) \\ &\leq 2\beta^{1/2}\tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}^{(n)},\tilde{\boldsymbol{x}}^{(n+1)},\dots,\tilde{\boldsymbol{x}}^{(N)}|\boldsymbol{y}^{(n-1)}) \\ &\leq 2\beta^{1/2}b_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}). \end{split}$$

Therefore, $c_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)})$ can be written as

$$\begin{split} c_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) &= \max\{a_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}), \eta_t b_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)})\} \\ &\leq \max\{2\beta^{1/2}b_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}), \eta_t b_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)})\} \\ &\leq (2\beta^{1/2} + \eta_t)b_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}). \end{split}$$

By using these lemmas, we prove Theorem C.10.

Proof. Let $t \in N\mathbb{Z}_{\geq 0}$. Then, from Lemma C.14, $\boldsymbol{x}_{t+1}^{(1)}$ satisfies that

$$c_t^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0}) \le (2\beta^{1/2} + \eta_t)b_t^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0})$$

$$= (2\beta^{1/2} + \eta_t)\tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \tilde{\boldsymbol{x}}^{(2)}, \dots, \tilde{\boldsymbol{x}}^{(N)}|\boldsymbol{0}). \tag{C.19}$$

Thus, by combining (C.19) and Lemma C.13, $c_t^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0})$ can be bounded as follows:

$$\begin{split} c_{t}^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0}) \\ &\leq (2\beta^{1/2} + \eta_{t})C_{3} \sum_{i=1}^{M^{(1)}} \sigma_{i,t}^{(1)}(\boldsymbol{0}, \boldsymbol{x}_{t+1}^{(1)}) + (2\beta^{1/2} + \eta_{t})C_{3}\tilde{\sigma}_{1,t}^{(N)}(\tilde{\boldsymbol{x}}^{(2)}, \dots, \tilde{\boldsymbol{x}}^{(N)}|\boldsymbol{y}^{(1)}) \\ &\leq (2\beta^{1/2} + \eta_{t})C_{3} \sum_{i=1}^{M^{(1)}} \sigma_{i,t}^{(1)}(\boldsymbol{0}, \boldsymbol{x}_{t+1}^{(1)}) + (2\beta^{1/2} + \eta_{t})C_{3}b_{t}^{(2)}(\tilde{\boldsymbol{x}}^{(2)}|\boldsymbol{y}^{(1)}) \\ &\leq (2\beta^{1/2} + \eta_{t})C_{3} \sum_{i=1}^{M^{(1)}} \sigma_{i,t}^{(1)}(\boldsymbol{0}, \boldsymbol{x}_{t+1}^{(1)}) + (2\beta^{1/2} + \eta_{t})C_{3}\eta_{t}^{-1}c_{t}^{(2)}(\tilde{\boldsymbol{x}}^{(2)}|\boldsymbol{y}^{(1)}) \\ &\leq (2\beta^{1/2} + \eta_{t})C_{3} \sum_{i=1}^{M^{(1)}} \sigma_{i,t}^{(1)}(\boldsymbol{0}, \boldsymbol{x}_{t+1}^{(1)}) + (2\beta^{1/2} + \eta_{t})C_{3}\eta_{t}^{-1}c_{t}^{(2)}(\boldsymbol{x}_{t+2}^{(2)}|\boldsymbol{y}^{(1)}) \\ &\leq (2\beta^{1/2} + \eta_{t})C_{3} \sum_{i=1}^{M^{(1)}} \sigma_{i,t}^{(1)}(\boldsymbol{0}, \boldsymbol{x}_{t+1}^{(1)}) + (2\beta^{1/2} + \eta_{t})^{2}C_{3}\eta_{t}^{-1}b_{t}^{(2)}(\boldsymbol{x}_{t+2}^{(2)}|\boldsymbol{y}^{(1)}) \\ &\leq (2\beta^{1/2} + \eta_{t})C_{3} \sum_{i=1}^{M^{(1)}} \sigma_{i,t}^{(1)}(\boldsymbol{0}, \boldsymbol{x}_{t+1}^{(1)}) + (2\beta^{1/2} + \eta_{t})^{2}C_{3}\eta_{t}^{-1} \cdot \tilde{\sigma}_{1,t}^{(N)}(\boldsymbol{x}_{t+2}^{(2)}, \tilde{\boldsymbol{x}}^{(3)}, \dots, \tilde{\boldsymbol{x}}^{(N)}|\boldsymbol{y}^{(1)}). \end{split}$$

Hence, by using Lemma C.13 again, we have

$$c_{t}^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0}) \leq (2\beta^{1/2} + \eta_{t} + 1)^{N} C_{3}^{N} \eta_{t}^{-N} \sum_{n=1}^{N} \sum_{i=1}^{M^{(n)}} \sigma_{i,t}^{(n)}(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}_{t+n}^{(n)})$$

$$\leq (2\beta^{1/2} + 1 + 1)^{N} C_{3}^{N} \eta_{t}^{-N} \sum_{n=1}^{N} \sum_{i=1}^{M^{(n)}} \sigma_{i,t}^{(n)}(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}_{t+n}^{(n)})$$

$$= C_{4} \eta_{t}^{-N} \sum_{n=1}^{N} \sum_{i=1}^{M^{(n)}} \sigma_{i,t}^{(n)}(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}_{t+n}^{(n)}).$$

This implies that

$$c_t^{(1)2}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0}) \leq C_4^2 M_{\text{sum}} \eta_t^{-2N} \sum_{n=1}^N \sum_{i=1}^{M^{(n)}} \sigma_{i,t}^{(n)2}(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}_{t+n}^{(n)}),$$

where the inequality is given by the Cauchy–Schwarz inequality. Next, let $T \in N\mathbb{Z}_{\geq 0}$ and K = T/N. Then, the following inequality holds:

$$\begin{split} \sum_{t \in N\mathbb{Z}_{\geq 0}}^{KN} c_t^{(1)2}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0}) &\leq C_4^2 M_{\text{sum}} \eta_T^{-2N} \sum_{n=1}^N \sum_{i=1}^{M^{(n)}} \sum_{t \in N\mathbb{Z}_{\geq 0}}^T \sigma_{i,t}^{(n)2}(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}_{t+n}^{(n)}) \\ &\leq \frac{2}{\log(1+\sigma^{-2})} C_4^2 M_{\text{sum}} \eta_T^{-2N} \sum_{n=1}^N \sum_{i=1}^{M^{(n)}} \gamma_T \\ &= \frac{2C_4^2 M_{\text{sum}}^2}{\log(1+\sigma^{-2})} \gamma_T \eta_T^{-2N}. \end{split}$$

Similarly, let $T^* = \arg\min_{t \in N\mathbb{Z}_{>0}, t \leq T} c_t^{(1)2}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0})$. Then, we obtain

$$Kc_{T^*}^{(1)2}(\boldsymbol{x}_{T^*+1}^{(1)}|\boldsymbol{0}) \le \sum_{t \in N\mathbb{Z}_{\ge 0}}^{KN} c_t^{(1)2}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0})$$

 $\le \frac{2C_4^2 M_{ ext{sum}}^2}{\log(1+\sigma^{-2})} \gamma_T \eta_T^{-2N}.$

This implies that

$$c_{T^*}^{(1)}(\boldsymbol{x}_{T^*+1}^{(1)}|\boldsymbol{0}) \le \sqrt{\frac{2C_4^2 M_{\text{sum}}^2}{\log(1+\sigma^{-2})} \gamma_T \eta_T^{-2N} K^{-1}}.$$
(C.20)

Furthermore, from the property of CIs and the definition of the estimated solution, the following inequalities hold:

$$\begin{split} F(\boldsymbol{x}_{*}^{(1)}, \dots, \boldsymbol{x}_{*}^{(N)}) &\leq \min_{t \in N\mathbb{Z}_{\geq 0}, t \leq T} \mathrm{UCB}_{t}^{(F)}(\boldsymbol{x}_{*}^{(1)}, \dots, \boldsymbol{x}_{*}^{(N)}) \leq \mathrm{UCB}_{T^{*}}^{(F)}(\boldsymbol{x}_{*}^{(1)}, \dots, \boldsymbol{x}_{*}^{(N)}) \\ F(\hat{\boldsymbol{x}}_{T}^{(1)}, \dots, \hat{\boldsymbol{x}}_{T}^{(N)}) &\geq \max_{t \in N\mathbb{Z}_{\geq 0}, t \leq T} \mathrm{LCB}_{t}^{(F)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) \geq \mathrm{LCB}_{T^{*}}^{(F)}(\boldsymbol{x}_{*}^{(1)}, \dots, \boldsymbol{x}_{*}^{(N)}). \end{split}$$

This implies that

$$F(\boldsymbol{x}_{*}^{(1)}, \dots, \boldsymbol{x}_{*}^{(N)}) - F(\hat{\boldsymbol{x}}_{T}^{(1)}, \dots, \hat{\boldsymbol{x}}_{T}^{(N)}) \leq 2\beta^{1/2} \tilde{\sigma}_{1, T^{*}}^{(N)}(\boldsymbol{x}_{*}^{(1)}, \dots, \boldsymbol{x}_{*}^{(N)})$$

$$\leq 2\beta^{1/2} b_{T^{*}}^{(1)}(\boldsymbol{x}_{*}^{(1)}|\boldsymbol{0})$$

$$< 2\beta^{1/2} \eta_{T^{*}}^{-1} c_{T^{*}}^{(1)}(\boldsymbol{x}_{*}^{(1)}|\boldsymbol{0}) < 2\beta^{1/2} \eta_{T}^{-1} c_{T^{*}}^{(1)}(\boldsymbol{x}_{T^{*}+1}^{(1)}|\boldsymbol{0}).$$

Finally, noting that K = T/N, from (C.20) we obtain

$$\begin{split} F(\boldsymbol{x}_*^{(1)}, \dots, \boldsymbol{x}_*^{(N)}) - F(\hat{\boldsymbol{x}}_T^{(1)}, \dots, \hat{\boldsymbol{x}}_T^{(N)}) &\leq 2\beta^{1/2} \eta_T^{-1} \sqrt{\frac{2C_4^2 M_{\text{sum}}^2}{\log(1 + \sigma^{-2})} \gamma_T \eta_T^{-2N} K^{-1}} \\ &= \sqrt{\frac{8\beta C_4^2 M_{\text{sum}}^2 N}{\log(1 + \sigma^{-2})} \gamma_T \eta_T^{-2N - 2} T^{-1}} \\ &< \sqrt{\xi^2} = \xi. \end{split}$$

D Cascade Process Optimization Using CI-based AFs under Noisy Setting

In this section, we consider CI-based cascade process optimization methods with observation noise. Hereafter, we assume that the observation noise $\epsilon_m^{(n)}$ is a random variable with $\mathbb{E}[\epsilon_m^{(n)}] = 0$ and $-A \leq \epsilon_m^{(n)} \leq A$, where A is some positive constant. In addition, we assume that $\epsilon_1^{(1)}, \dots, \epsilon_{M^{(N)}}^{(N)}$ are mutually independent, and the distribution of the noise vector $\boldsymbol{\epsilon} = (\epsilon_1^{(1)}, \dots, \epsilon_{M^{(N)}}^{(N)})^{\top}$ is known. Finally, we also assume that noise vectors with respect to iteration t, $\epsilon_1, \dots, \epsilon_t$, are independent and identically distributed random variables having the same distribution of $\boldsymbol{\epsilon}$.

Next, we define several notations. For each $n \in [N]$, let $\tilde{\mathcal{Y}}^{(n)}(\supset \mathcal{Y}^{(n)})$ be a set satisfying

$$\forall \boldsymbol{w} \in \tilde{\mathcal{Y}}^{(n-1)}, \forall \boldsymbol{x} \in \mathcal{X}^{(n)}, f^{(n)}(\boldsymbol{w}, \boldsymbol{x}) + \boldsymbol{\epsilon}^{(n)} \in \tilde{\mathcal{Y}}^{(n)},$$

where $\tilde{\mathcal{Y}}^{(0)} = \{\mathbf{0}\}$ and $\boldsymbol{\epsilon}^{(n)} = (\epsilon_1^{(n)}, \dots, \epsilon_{M^{(n)}}^{(n)})^{\top}$. Note that $\boldsymbol{z}^{(n)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n)}) \in \mathcal{Y}^{(n)} \subset \tilde{\mathcal{Y}}^{(n)}$. In addition, for any realization $\boldsymbol{\epsilon}$ and input $\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n)}$, we define $\boldsymbol{z}^{(n)}_{\boldsymbol{\epsilon}}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n)})$ as

$$m{z}_{m{\epsilon}}^{(n)}(m{x}^{(1)},\ldots,m{x}^{(n)}) = egin{cases} m{f}^{(1)}(m{0},m{x}^{(1)}) + m{\epsilon}^{(1)} & (n=1), \ m{f}^{(n)}(m{z}_{m{\epsilon}}^{(n-1)}(m{x}^{(1)},\ldots,m{x}^{(n-1)}),m{x}^{(n)}) + m{\epsilon}^{(n)} & (n \geq 2). \end{cases}$$

Furthermore, we define the function $G(\boldsymbol{x}^{(1)},\dots,\boldsymbol{x}^{(N)})$ as

$$G(x^{(1)},...,x^{(N)}) = \mathbb{E}_{\epsilon}[z_{\epsilon}^{(N)}(x^{(1)},...,x^{(n)})].$$

The function $G(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N)})$ is the expected value of the final-stage output with respect to $\boldsymbol{\epsilon}$ when $(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N)})$ is used. We emphasize that $F(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N)}) \neq G(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N)})$ in general. Similarly, we define the optimal solution of each function as

$$egin{aligned} & (m{x}_{F,*}^{(1)}, \dots, m{x}_{F,*}^{(N)}) = \mathop{rg\max}_{(m{x}^{(1)}, \dots, m{x}^{(N)}) \in \mathcal{X}} F(m{x}^{(1)}, \dots, m{x}^{(N)}), \ & (m{x}_{G,*}^{(1)}, \dots, m{x}_{G,*}^{(N)}) = \mathop{rg\max}_{(m{x}^{(1)}, \dots, m{x}^{(N)}) \in \mathcal{X}} G(m{x}^{(1)}, \dots, m{x}^{(N)}). \end{aligned}$$

By using these, for the selected input $x_t^{(1)}, \dots, x_t^{(N)}$ at iteration t, we define the expected regret $r_{G,t}$, cumulative expected regret $R_{G,T}$ and simple expected regret $r_{G,T}^{(S)}$ as

$$r_{G,t} = G(\boldsymbol{x}_{G,*}^{(1)}, \dots, \boldsymbol{x}_{G,*}^{(N)}) - G(\boldsymbol{x}_{t}^{(1)}, \dots, \boldsymbol{x}_{t}^{(N)}),$$

$$R_{G,t} = \sum_{t=1}^{T} r_{G_{t}}, \quad r_{G,T}^{(S)} = \min_{1 \le t \le T} r_{G,t}.$$

We also define the regret $r_{F,t}$, cumulative regret $R_{F,T}$ and simple regret $r_{F,T}^{(S)}$ as

$$r_{F,t} = F(oldsymbol{x}_{F,*}^{(1)}, \dots, oldsymbol{x}_{F,*}^{(N)}) - F(oldsymbol{x}_{t}^{(1)}, \dots, oldsymbol{x}_{t}^{(N)}),$$
 $R_{F,t} = \sum_{t=1}^{T} r_{F_t}, \quad r_{F,T}^{(S)} = \min_{1 \le t \le T} r_{F,t}.$

Finally, let $(\hat{\boldsymbol{x}}_{F,t}^{(1)},\ldots,\hat{\boldsymbol{x}}_{F,t}^{(N)})$ and $(\hat{\boldsymbol{x}}_{G,t}^{(1)},\ldots,\hat{\boldsymbol{x}}_{G,t}^{(N)})$ be respectively estimated solutions of $(\boldsymbol{x}_{F,*}^{(1)},\ldots,\boldsymbol{x}_{F,*}^{(N)})$ and $(\boldsymbol{x}_{G,*}^{(1)},\ldots,\boldsymbol{x}_{G,*}^{(N)})$ at iteration t. Then, we define the regrets for estimated solutions, $\hat{r}_{F,t}$ and $\hat{r}_{G,t}$, as

$$\hat{r}_{F,t} = F(\boldsymbol{x}_{F,*}^{(1)}, \dots, \boldsymbol{x}_{F,*}^{(N)}) - F(\hat{\boldsymbol{x}}_{F,t}^{(1)}, \dots, \hat{\boldsymbol{x}}_{F,t}^{(N)}),$$

$$\hat{r}_{G,t} = G(\boldsymbol{x}_{G,*}^{(1)}, \dots, \boldsymbol{x}_{G,*}^{(N)}) - G(\hat{\boldsymbol{x}}_{G,t}^{(1)}, \dots, \hat{\boldsymbol{x}}_{G,t}^{(N)}).$$

D.1 Credible Interval

In this section, we construct a valid CI under the noisy setting. First, we introduce the following regularity assumption instead of Assumption C.1.

Assumption D.1 (Regularity assumption under noisy setting). For each $n \in [N]$, let $\tilde{\mathcal{Y}}^{(n-1)} \times \mathcal{X}^{(n)}$ be a compact set, and let $\mathcal{H}_{k^{(n)}}$ be an RKHS corresponding to the kernel $k^{(n)}$. In addition, for each $n \in [N]$ and $m \in [M^{(n)}]$, assume that $f_m^{(n)} \in \mathcal{H}_{k^{(n)}}$ with $\|f_m^{(n)}\|_{k^{(n)}} \leq B$, where B > 0 is some constant. Furthermore, assume that the observation noise $\epsilon_m^{(n)}$ is a random variable with $\mathbb{E}[\epsilon_m^{(n)}] = 0$ and $-A \leq \epsilon_m^{(n)} \leq A$, where A is some positive constant. All elements of $\epsilon = (\epsilon_1^{(1)}, \dots, \epsilon_{M^{(N)}}^{(N)})$ are mutually independent, and $\epsilon_1, \epsilon_2, \dots$ are i.i.d. random variables having the same distribution of ϵ .

Then, the following lemma holds under the noisy setting.

Lemma D.2 (Abbasi-Yadkori 2012, Theorem 3.11). Assume that Assumption D.1 holds. Let $\delta \in (0,1)$, and define

$$\beta_t^{(n)} = \Big(B + \frac{A}{\sigma}\sqrt{\log\det\left(\boldsymbol{I}_{L_t^{(n)}} + \sigma^{-2}\boldsymbol{K}_t^{(n)}\right) + 2\log(1/\delta)}\Big)^2.$$

Then, for any $n \in [N]$ and $m \in [M^{(n)}]$, the following inequality holds with probability at least $1 - \delta$:

$$\left| f_m^{(n)}(\boldsymbol{w}, \boldsymbol{x}) - \mu_{m,t}^{(n)}(\boldsymbol{w}, \boldsymbol{x}) \right| \leq (\beta_t^{(n)})^{1/2} \sigma_{m,t}^{(n)}(\boldsymbol{w}, \boldsymbol{x}), \ \forall \boldsymbol{w} \in \tilde{\mathcal{Y}}^{(n-1)}, \ \forall \boldsymbol{x} \in \mathcal{X}^{(n)}, \ \forall t \geq 1.$$

Proof. From Theorem 3.11 of (Abbasi-Yadkori, 2012), it is sufficient to show that $\epsilon_m^{(n)}$ has A-sub-Gaussian property, i.e.,

$$\mathbb{E}[\exp(\lambda \epsilon_m^{(n)})] \le \exp(\lambda^2 A^2 / 2) \quad \forall \lambda \in \mathbb{R}. \tag{D.1}$$

Noting that $\epsilon_m^{(n)}$ is a zero mean and bounded random variable, using Hoeffding's lemma (Massart, 2007) we have

$$\mathbb{E}[\exp(\lambda \epsilon_m^{(n)})] \le \exp(\lambda^2 (A - (-A))^2 / 8)$$
$$= \exp(\lambda^2 A^2 / 2) \quad \forall \lambda \in \mathbb{R}.$$

Thus, $\epsilon_m^{(n)}$ has A-sub-Gaussian property (D.1).

From Lemma D.2, we have the following uniform bound.

Corollary D.3. Assume that Assumption D.1 holds. Let $\delta \in (0,1)$, and define

$$\beta_t^{(n)} = \left(B + \frac{A}{\sigma} \sqrt{\log \det \left(\boldsymbol{I}_{L_t^{(n)}} + \sigma^{-2} \boldsymbol{K}_t^{(n)}\right) + 2\log(M_{sum}/\delta)}\right)^2,$$

$$\beta_t = \max_{1 \le n \le N, 1 \le \tilde{t} \le t} \beta_{\tilde{t}}^{(n)}.$$
(D.2)

Then, for any $n \in [N]$ and $m \in [M^{(n)}]$, the following inequality holds with probability at least $1 - \delta$:

$$\left| f_m^{(n)}(\boldsymbol{w}, \boldsymbol{x}) - \mu_{m,t}^{(n)}(\boldsymbol{w}, \boldsymbol{x}) \right| \leq \beta_t^{1/2} \sigma_{m,t}^{(n)}(\boldsymbol{w}, \boldsymbol{x}), \ \forall \boldsymbol{w} \in \tilde{\mathcal{Y}}^{(n-1)}, \ \forall \boldsymbol{x} \in \mathcal{X}^{(n)}, \ \forall t \geq 1.$$

From Corollary D.3, we can also construct a valid CI for the N-stage cascade process under the noisy setting. First, we construct CIs for $\boldsymbol{z}_{\epsilon}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)})$ and $G(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N)})$. For any iteration $t\geq 1$, realization ϵ and input $(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)})$, we define $\tilde{\boldsymbol{z}}_{\epsilon,t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)})$ as

$$\tilde{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}) = \begin{cases} \boldsymbol{\epsilon}^{(1)} + \boldsymbol{\mu}_t^{(1)}(\boldsymbol{0},\boldsymbol{x}^{(1)}) & (n=1), \\ \boldsymbol{\epsilon}^{(n)} + \boldsymbol{\mu}_t^{(n)}(\tilde{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) & (n \geq 2). \end{cases}$$

Similarly, we define $\tilde{\sigma}^{(n)}_{{\boldsymbol{\epsilon}},m,t}({\boldsymbol{x}}^{(1)},\dots,{\boldsymbol{x}}^{(n)})$ as

$$\tilde{\sigma}_{\epsilon,m,t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}) = \sigma_{m,t}^{(n)}(\tilde{\boldsymbol{z}}_{\epsilon,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) \\
+ L_f \sum_{s=1}^{M^{(n-1)}} \tilde{\sigma}_{\epsilon,s,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),$$

where $m \in [M^{(n)}]$ and $\tilde{\sigma}^{(1)}_{\epsilon,s,t}(\boldsymbol{x}^{(1)}) = \sigma^{(1)}_{s,t}(\boldsymbol{0},\boldsymbol{x}^{(1)})$. Then, the following holds.

Theorem D.4. Assume that Assumptions C.3 and D.1 hold. Also assume that $\tilde{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}) \in \tilde{\mathcal{Y}}^{(n)}$ for any $n \in [N]$, iteration $t \geq 1$, realization $\boldsymbol{\epsilon}$ and input $(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)})$. Let $\delta \in (0,1)$, and define β_t by D.2. Then, the following inequality holds with probability at least $1 - \delta$:

$$|z_{\epsilon,m}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}) - \tilde{z}_{\epsilon,m,t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)})| \leq \beta_t^{1/2} \tilde{\sigma}_{\epsilon,m,t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}),$$

$$\forall n \in [N], m \in [M^{(n)}], t \geq 1, \epsilon, (\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}),$$

where $z_{\epsilon,m}^{(n)}$ and $\tilde{z}_{\epsilon,m,t}^{(n)}$ are the m-th element of $z_{\epsilon}^{(n)}$ and $\tilde{z}_{\epsilon,t}^{(n)}$, respectively.

Proof. By using the same argument as in the proof of Theorem C.5, we get Theorem D.4.

From Theorem D.4, taking expectation with respect to ϵ , we get the following corollary.

Corollary D.5. Assume that the same condition as in Theorem D.4 holds. Let $\delta \in (0,1)$, and define β_t by (D.2). Then, with probability at least $1 - \delta$, the following inequality holds for any $n \in [N]$, $m \in [M^{(n)}]$, iteration $t \ge 1$ and input $x^{(1)}, \ldots, x^{(n)}$:

$$\mathbb{E}_{\boldsymbol{\epsilon}} [\tilde{z}_{\boldsymbol{\epsilon},m,t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}) - \beta_t^{1/2} \tilde{\sigma}_{\boldsymbol{\epsilon},m,t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)})] \\
\leq \mathbb{E}_{\boldsymbol{\epsilon}} [z_{\boldsymbol{\epsilon},m}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)})] \\
\leq \mathbb{E}_{\boldsymbol{\epsilon}} [\tilde{z}_{\boldsymbol{\epsilon},m,t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}) + \beta_t^{1/2} \tilde{\sigma}_{\boldsymbol{\epsilon},m,t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)})].$$

In particular, when n = N and m = 1, it follows that

$$\mathbb{E}_{\epsilon}[\tilde{z}_{\epsilon,1,t}^{(N)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N)}) - \beta_{t}^{1/2}\tilde{\sigma}_{\epsilon,1,t}^{(N)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N)})] \\
\leq G(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N)}) \\
\leq \mathbb{E}_{\epsilon}[\tilde{z}_{\epsilon,1,t}^{(N)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N)}) + \beta_{t}^{1/2}\tilde{\sigma}_{\epsilon,1,t}^{(N)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N)})].$$

D.2 UCB-based Optimization Strategy for Expected Regrets

Here, we give a UCB-based AF and regret bounds for $R_{G,T}$ and $r_{G,T}^{(S)}$. We define an expected cascade process upper confidence bound (EcUCB) as

$$EcUCB_{t}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) = \mathbb{E}_{\epsilon}[\tilde{z}_{\epsilon, 1, t}^{(N)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) + \beta_{t}^{1/2}\tilde{\sigma}_{\epsilon, 1, t}^{(N)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)})].$$

By using this AF, we select the next evaluation point $(m{x}_{t+1}^{(1)},\dots,m{x}_{t+1}^{(N)})$ by

$$(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(N)}) = \underset{(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) \in \mathcal{X}}{\operatorname{arg \, max}} \operatorname{EcUCB}_{t}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}). \tag{D.3}$$

Moreover, let $\tilde{A} = \{\tilde{a}_1, \dots, \tilde{a}_T\}$ be a subset of $\tilde{\mathcal{Y}}^{(n-1)} \times \mathcal{X}^{(n)}$, and let $\boldsymbol{y}_{m,\tilde{A}}^{(n)}$ be a random vector, where the i-th element of $\boldsymbol{y}_{m,\tilde{A}}^{(n)}$ is given by $y_{m,\tilde{a}_i}^{(n)} = f_m^{(n)}(\tilde{a}_i) + \varepsilon_{\tilde{a}_i}^{(n)}$. Then, the maximum information gain $\tilde{\gamma}_{m,T}^{(n)}$ at iteration T is given by

$$\tilde{\gamma}_{m,T}^{(n)} = \max_{\tilde{A} \subset \tilde{\mathcal{Y}}^{(n-1)} \times \mathcal{X}^{(n)}, |\tilde{A}| = T} \mathbf{I}(\boldsymbol{y}_{m,\tilde{A}}^{(n)}; f_m^{(n)}).$$

Furthermore, we define $\tilde{\gamma}_T = \max_{1 \leq n \leq N, 1 \leq m \leq M^{(n)}} \tilde{\gamma}_{m,T}^{(n)}$. Then, the following theorem gives regret bounds for $R_{G,T}$ and $r_{G,T}^{(S)}$.

Theorem D.6. Assume that Assumptions C.3, C.4 and D.1 hold. Also assume that $\tilde{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}) \in \tilde{\mathcal{Y}}^{(n)}$ for any $n \in [N]$, iteration $t \geq 1$, realization $\boldsymbol{\epsilon}$ and input $(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)})$. Let $\delta \in (0,1)$, and define β_t by (D.2). Then, when the optimization is performed using D.3, the following holds:

$$\begin{split} & \mathbb{P}\left(R_{G,T} \leq \sqrt{32M_{prod}^2M_{sum}^2TC_{0,T}^{2N}\left(\log(5M_{sum}/\delta) + \frac{\tilde{\gamma}_T}{2\log(1+\sigma^{-2})}\right)} \quad \forall T \geq 1\right) \geq 1 - 2\delta, \\ & \mathbb{P}\left(r_{G,T}^{(S)} \leq T^{-1/2}\sqrt{32M_{prod}^2M_{sum}^2C_{0,T}^{2N}\left(\log(5M_{sum}/\delta) + \frac{\tilde{\gamma}_T}{2\log(1+\sigma^{-2})}\right)} \quad \forall T \geq 1\right) \geq 1 - 2\delta, \end{split}$$

where $C_{0,t} = (1 + L_{\sigma})\beta_t^{1/2} + L_f + 1$.

Proof. From Theorem D.4 and the definition of $\tilde{\sigma}_{\epsilon,m,t}^{(n)}(\cdot)$, noting that $\sigma_{m,t}^{(n)}(\cdot)$ is Lipschitz continuity, the following inequality holds with probability at least $1 - \delta$:

$$\begin{split} &\tilde{\sigma}_{\epsilon,m,t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}) \\ &= \sigma_{m,t}^{(n)}(\boldsymbol{z}_{\epsilon}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) + L_f \sum_{s=1}^{M^{(n-1)}} \tilde{\sigma}_{\epsilon,s,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}) \\ &+ \sigma_{m,t}^{(n)}(\tilde{\boldsymbol{z}}_{\epsilon,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) - \sigma_{m,t}^{(n)}(\boldsymbol{z}_{\epsilon}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) \\ &\leq \sigma_{m,t}^{(n)}(\boldsymbol{z}_{\epsilon}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) + L_f \sum_{s=1}^{M^{(n-1)}} \tilde{\sigma}_{\epsilon,s,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}) \\ &+ |\sigma_{m,t}^{(n)}(\boldsymbol{z}_{\epsilon}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) - \sigma_{m,t}^{(n)}(\tilde{\boldsymbol{z}}_{\epsilon,s,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) \\ &+ |\sigma_{m,t}^{(n)}(\boldsymbol{z}_{\epsilon}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) - \tilde{\sigma}_{m,t}^{(n)}(\tilde{\boldsymbol{z}}_{\epsilon,s,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) \\ &\leq \sigma_{m,t}^{(n)}(\boldsymbol{z}_{\epsilon}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) + L_f \sum_{s=1}^{M^{(n-1)}} \tilde{\sigma}_{\epsilon,s,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}) \\ &\leq \sigma_{m,t}^{(n)}(\boldsymbol{z}_{\epsilon}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) + L_f \sum_{s=1}^{M^{(n-1)}} \tilde{\sigma}_{\epsilon,s,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}) \\ &= \sigma_{m,t}^{(n)}(\boldsymbol{z}_{\epsilon}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) + (L_{\sigma}\beta_t^{1/2} + L_f) \sum_{s=1}^{M^{(n-1)}} \tilde{\sigma}_{\epsilon,s,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}) \\ &\leq \sigma_{m,t}^{(n)}(\boldsymbol{z}_{\epsilon}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) + (L_{\sigma}\beta_t^{1/2} + L_f) \sum_{s=1}^{M^{(n-1)}} \tilde{\sigma}_{\epsilon,s,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}) \\ &\leq \sigma_{m,t}^{(n)}(\boldsymbol{z}_{\epsilon}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) + (L_{\sigma}\beta_t^{1/2} + L_f) \sum_{s=1}^{M^{(n-1)}} \tilde{\sigma}_{\epsilon,s,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}) \\ &\leq \sigma_{m,t}^{(n)}(\boldsymbol{z}_{\epsilon}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) + C_{0,t} \sum_{s=1}^{M^{(n-1)}} \tilde{\sigma}_{\epsilon,s,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}). \end{split}$$

Therefore, by repeating (D.4) we get

$$\begin{split} &\tilde{\sigma}_{\epsilon,1,t}^{(N)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N)}) \\ &\leq \sigma_{1,t}^{(N)}(\boldsymbol{z}_{\epsilon}^{(N-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N-1)}),\boldsymbol{x}^{(N)}) + C_{0,t} \sum_{s=1}^{M^{(N-1)}} \tilde{\sigma}_{\epsilon,s,t}^{(N-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N-1)}) \\ &\leq \sigma_{1,t}^{(N)}(\boldsymbol{z}_{\epsilon}^{(N-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N-1)}),\boldsymbol{x}^{(N)}) + C_{0,t} \sum_{s=1}^{M^{(N-1)}} \sigma_{s,t}^{(N-1)}(\boldsymbol{z}_{\epsilon}^{(N-2)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N-2)}),\boldsymbol{x}^{(N-1)}) \\ &\quad + C_{0,t}^2 M^{(N-1)} \sum_{u=1}^{M^{(N-2)}} \tilde{\sigma}_{\epsilon,u,t}^{(N-2)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N-2)}) \\ \vdots \\ &\leq C_{0,t}^{N-1} M_{\text{prod}} \sum_{n=1}^{N} \sum_{m=1}^{M^{(n)}} \sigma_{m,t}^{(n)}(\boldsymbol{z}_{\epsilon}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}), \end{split}$$

where $m{z}_{\epsilon}^{(0)}(m{x}^{(1)},m{x}^{(0)}) = m{0}$. Hence, from the Cauchy–Schwarz inequality, it follows that

$$\tilde{\sigma}_{\boldsymbol{\epsilon},1,t}^{(N)2}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(N)})$$

$$\leq C_{0,t}^{2(N-1)} M_{\text{prod}}^2 \left(\sum_{n=1}^N \sum_{m=1}^{M^{(n)}} 1 \right) \sum_{n=1}^N \sum_{m=1}^{M^{(n)}} \left[\sigma_{m,t}^{(n)2} (\boldsymbol{z}_{\epsilon}^{(n-1)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n-1)}), \boldsymbol{x}^{(n)}) \right] \\
= C_{0,t}^{2(N-1)} M_{\text{prod}}^2 M_{\text{sum}} \sum_{n=1}^N \sum_{m=1}^{M^{(n)}} \left[\sigma_{m,t}^{(n)2} (\boldsymbol{z}_{\epsilon}^{(n-1)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n-1)}), \boldsymbol{x}^{(n)}) \right]. \tag{D.5}$$

Next, from Corollary D.5 and the selection rule (D.3), the following holds:

$$G(\boldsymbol{x}_{G,*}^{(1)}, \dots, \boldsymbol{x}_{G,*}^{(N)}) \leq \text{EcUCB}_{t}(\boldsymbol{x}_{G,*}^{(1)}, \dots, \boldsymbol{x}_{G,*}^{(N)})$$

$$\leq \text{EcUCB}_{t}(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(N)})$$

$$= \mathbb{E}_{\epsilon}[\tilde{z}_{\epsilon,1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(N)}) + \beta_{t}^{1/2}\tilde{\sigma}_{\epsilon,1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(N)})].$$

Similarly, since $G(\boldsymbol{x}_{t+1}^{(1)},\dots,\boldsymbol{x}_{t+1}^{(N)})$ satisfies that

$$G(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(N)}) \geq \mathbb{E}_{\boldsymbol{\epsilon}}[\tilde{z}_{\boldsymbol{\epsilon}, 1, t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(N)}) \beta_{t}^{1/2} \tilde{\sigma}_{\boldsymbol{\epsilon}, 1, t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(N)})],$$

the regret $r_{G,t}$ can be bounded as follows:

$$r_{G,t} = G(\boldsymbol{x}_{G,*}^{(1)}, \dots, \boldsymbol{x}_{G,*}^{(N)}) - G(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(N)})$$

$$\leq 2\beta_t^{1/2} \mathbb{E}_{\epsilon} [\tilde{\sigma}_{\epsilon,1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(N)})]. \tag{D.6}$$

Therefore, by using (D.6), $R_{G,T}^2$ can be written as

$$R_{G,T}^{2} = \left(\sum_{t=1}^{T} r_{G,t}\right)^{2}$$

$$\leq T \sum_{t=1}^{T} r_{G,t}^{2}$$

$$\leq T \sum_{t=1}^{T} 4\beta_{t} \left(\mathbb{E}_{\epsilon} \left[\tilde{\sigma}_{\epsilon,1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(N)})\right]\right)^{2}$$

$$\leq T \sum_{t=1}^{T} 4\beta_{t} \mathbb{E}_{\epsilon} \left[\tilde{\sigma}_{\epsilon,1,t}^{(N)2}(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(N)})\right], \tag{D.7}$$

where the first inequality is given by the Cauchy–Schwarz inequality, and the last inequality is given by Jensen's inequality. Thus, by substituting (D.5) into (D.7), we obtain

$$R_{G,T}^2 \le 4T\beta_T \tilde{C}_T^{2(N-1)} M_{\text{prod}}^2 M_{\text{sum}} \sum_{t=1}^T \mathbb{E}_{\epsilon}[S_{\epsilon,t}], \tag{D.8}$$

where $S_{\epsilon,t}$ is given by

$$S_{m{\epsilon},t} = \sum_{n=1}^{N} \sum_{m=1}^{M^{(n)}} \sigma_{m,t}^{(n)2}(m{z}_{m{\epsilon}}^{(n-1)}(m{x}_{t+1}^{(1)},\ldots,m{x}_{t+1}^{(n-1)}),m{x}_{t+1}^{(n)}).$$

Here, since $k^{(n)}(\cdot,\cdot) \leq 1$, the random variable $S_{\epsilon,t}$ satisfies $0 \leq S_{\epsilon,t} \leq M_{\text{sum}}$. Hence, from Lemma 3

of (Kirschner and Krause, 2018), the following holds with probability at least $1 - \delta$:

$$\begin{split} \sum_{t=1}^{T} \mathbb{E}_{\epsilon}[S_{\epsilon,t}] &\leq 2 \sum_{t=1}^{T} S_{\epsilon_{t+1},t} + 4M_{\text{sum}} \log(1/\delta) + 8M_{\text{sum}} \log(4M_{\text{sum}}) + 1 \\ &\leq 2 \sum_{t=1}^{T} S_{\epsilon_{t+1},t} + 8M_{\text{sum}} \log(1/\delta) + 8M_{\text{sum}} \log(4M_{\text{sum}}) + 8M_{\text{sum}} \log 1.25 \\ &= 2 \sum_{t=1}^{T} S_{\epsilon_{t+1},t} + 8M_{\text{sum}} \log(5M_{\text{sum}}/\delta). \end{split} \tag{D.9}$$

Therefore, by combining (D.8) and (D.9), we have

$$R_{G,T}^{2} \leq 32T\beta_{T}C_{T,0}^{2(N-1)}M_{\text{prod}}^{2}M_{\text{sum}}^{2}\log(5M_{\text{sum}}/\delta)$$

$$+8T\beta_{T}C_{0,T}^{2(N-1)}M_{\text{prod}}^{2}M_{\text{sum}}\sum_{t=1}^{T}\sum_{t=1}^{N}\sum_{t=1}^{M^{(n)}}\left[\sigma_{m,t}^{(n)2}(\boldsymbol{z}_{\epsilon_{t+1}}^{(n-1)}(\boldsymbol{x}_{t+1}^{(1)},\ldots,\boldsymbol{x}_{t+1}^{(n-1)}),\boldsymbol{x}_{t+1}^{(n)})\right]. \tag{D.10}$$

Furthermore, by using the same argument as in Lemma 5.3 and 5.4 of (Srinivas et al., 2010), we get

$$\sum_{t=1}^{T} \sigma_{m,t}^{(n)2}(\boldsymbol{z}_{\boldsymbol{\epsilon}_{t+1}}^{(n-1)}(\boldsymbol{x}_{t+1}^{(1)}, \dots, \boldsymbol{x}_{t+1}^{(n-1)}), \boldsymbol{x}_{t+1}^{(n)}) \leq \frac{2}{\log(1+\sigma^{-2})} \tilde{\gamma}_{m,T}^{(n)} \\
\leq \frac{2}{\log(1+\sigma^{-2})} \tilde{\gamma}_{T}.$$
(D.11)

Hence, from (D.10) and (D.11), noting that $\beta_T \leq C_{0,T}^2$ we obtain

$$\begin{split} R_{G,T}^2 & \leq 32T\beta_T C_{0,T}^{2(N-1)} M_{\text{prod}}^2 M_{\text{sum}}^2 \log(5M_{\text{sum}}/\delta) + \frac{16}{\log(1+\sigma^{-2})} T\beta_T C_{0,T}^{2(N-1)} M_{\text{prod}}^2 M_{\text{sum}}^2 \tilde{\gamma}_T \\ & = 32T\beta_T C_{0,T}^{2(N-1)} M_{\text{prod}}^2 M_{\text{sum}}^2 \left(\log(5M_{\text{sum}}/\delta) + \frac{\tilde{\gamma}_T}{2\log(1+\sigma^{-2})} \right) \\ & \leq 32T C_{0,T}^{2N} M_{\text{prod}}^2 M_{\text{sum}}^2 \left(\log(5M_{\text{sum}}/\delta) + \frac{\tilde{\gamma}_T}{2\log(1+\sigma^{-2})} \right). \end{split}$$

Therefore, with probability at least $1 - 2\delta$, $R_{G,T}$ can be bounded as follows:

$$R_{G,T} \leq \sqrt{32M_{\text{prod}}^2 M_{\text{sum}}^2 T C_{0,T}^{2N} \left(\log(5M_{\text{sum}}/\delta) + \frac{\tilde{\gamma}_T}{2\log(1+\sigma^{-2})} \right)}.$$

Similarly, from the definition of $r_{G,T}^{(S)}$, it follows that

$$\begin{split} Tr_{G,T}^{(\mathrm{S})} & \leq \sum_{t=1}^{T} r_{G,t} = R_{G,T} \\ & \leq \sqrt{32 M_{\mathrm{prod}}^2 M_{\mathrm{sum}}^2 T C_{0,T}^{2N} \left(\log(5 M_{\mathrm{sum}}/\delta) + \frac{\tilde{\gamma}_T}{2 \log(1 + \sigma^{-2})} \right)}. \end{split}$$

D.3 Optimistic Improvement-based AF for the Expectation of the Final Stage Output

We give an optimistic improvement-based AF for G under the noisy setting. Let $s \in \{0, \dots, N-1\}$ and $\boldsymbol{y} \in \tilde{\mathcal{Y}}^{(s)}$. Then, we define $\boldsymbol{z}_{\boldsymbol{\epsilon}}^{(n)}(\cdot|\boldsymbol{y})$, $\tilde{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n)}(\cdot|\boldsymbol{y})$ and $\tilde{\sigma}_{\boldsymbol{\epsilon},m,t}^{(n)}(\cdot|\boldsymbol{y})$ as

$$\begin{split} \boldsymbol{z}_{\boldsymbol{\epsilon}}^{(n)}(\boldsymbol{x}^{(s+1)}, \dots, \boldsymbol{x}^{(n)}|\boldsymbol{y}) &= \begin{cases} \boldsymbol{\epsilon}^{(s+1)} + \boldsymbol{f}^{(s+1)}(\boldsymbol{y}, \boldsymbol{x}^{(s+1)}) & (n = s + 1), \\ \boldsymbol{\epsilon}^{(n)} + \boldsymbol{f}^{(n)}(\boldsymbol{z}_{\boldsymbol{\epsilon}}^{(n-1)}(\boldsymbol{x}^{(s+1:n-1)}|\boldsymbol{y}), \boldsymbol{x}^{(n)}) & (n \geq s + 2), \end{cases} \\ \tilde{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n)}(\boldsymbol{x}^{(s+1)}, \dots, \boldsymbol{x}^{(n)}|\boldsymbol{y}) &= \begin{cases} \boldsymbol{\epsilon}^{(s+1)} + \boldsymbol{\mu}_t^{(s+1)}(\boldsymbol{y}, \boldsymbol{x}^{(s+1)}) & (n = s + 1), \\ \boldsymbol{\epsilon}^{(n)} + \boldsymbol{\mu}_t^{(n)}(\tilde{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n-1)}(\boldsymbol{x}^{(s+1:n-1)}|\boldsymbol{y}), \boldsymbol{x}^{(n)}) & (n \geq s + 2), \end{cases} \\ \tilde{\boldsymbol{\sigma}}_{\boldsymbol{\epsilon},m,t}^{(n)}(\boldsymbol{x}^{(s+1)}, \dots, \boldsymbol{x}^{(n)}|\boldsymbol{y}) &= \boldsymbol{\sigma}_{m,t}^{(n)}(\tilde{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n-1)}(\boldsymbol{x}^{(s+1)}, \dots, \boldsymbol{x}^{(n-1)}|\boldsymbol{y}), \boldsymbol{x}^{(n)}) \\ &+ L_f \sum_{s=1}^{M^{(n-1)}} \tilde{\boldsymbol{\sigma}}_{\boldsymbol{\epsilon},s,t}^{(n-1)}(\boldsymbol{x}^{(s+1)}, \dots, \boldsymbol{x}^{(n-1)}|\boldsymbol{y}), \end{split}$$

where $\tilde{\sigma}^{(s)}_{\epsilon,m,t}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(s)}|\boldsymbol{y})=0$ and $\boldsymbol{z}^{(s)}_{\epsilon}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(s)}|\boldsymbol{y})=\tilde{\boldsymbol{z}}^{(s)}_{\epsilon,t}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(s)}|\boldsymbol{y})=\boldsymbol{y}$. Then, the following theorem holds.

Theorem D.7. Assume that Assumptions C.3 and D.1 hold. Also assume that $\tilde{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y})\in \tilde{\mathcal{Y}}^{(n)}$ for any $s\in\{0,\ldots,N-1\},\ n\in\{s+1,\ldots,N\}$, iteration $t\geq 1$, realization $\boldsymbol{\epsilon}$, given $\boldsymbol{y}\in\tilde{\mathcal{Y}}^{(s)}$ and input $(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)})$. Let $\delta\in(0,1)$, and define β_t by (D.2). Then, the following inequality holds with probability at least $1-\delta$:

$$|z_{\epsilon,m}^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y}) - \tilde{z}_{\epsilon,m,t}^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y})| \leq \beta_t^{1/2} \tilde{\sigma}_{\epsilon,m,t}^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y}),$$

where $m \in [M^{(n)}]$, and $z_{\boldsymbol{\epsilon},m}^{(n)}(\cdot|\boldsymbol{y})$ and $\tilde{z}_{\boldsymbol{\epsilon},m,t}^{(n)}(\cdot|\boldsymbol{y})$ are the m-th element of $z_{\boldsymbol{\epsilon}}^{(n)}(\cdot|\boldsymbol{y})$ and $\tilde{z}_{\boldsymbol{\epsilon},t}^{(n)}(\cdot|\boldsymbol{y})$, respectively.

Proof. By using the same argument as in the proof of Theorem C.5, we have Theorem D.7.

From Theorem D.7, taking expectation with respect to ϵ , we get the following corollary.

Corollary D.8. Assume that the same condition as in Theorem D.7 holds. Let $\delta \in (0,1)$, and define β_t by (D.2). Then, the following inequality holds with probability at least $1 - \delta$:

$$\begin{split} & \mathbb{E}_{\boldsymbol{\epsilon}|\boldsymbol{y}}[\tilde{\boldsymbol{z}}_{\boldsymbol{\epsilon},m,t}^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y}) - \beta_t^{1/2}\tilde{\sigma}_{\boldsymbol{\epsilon},m,t}^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y})] \\ & \leq \mathbb{E}_{\boldsymbol{\epsilon}|\boldsymbol{y}}[\boldsymbol{z}_{\boldsymbol{\epsilon},m}^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y})] \\ & \leq \mathbb{E}_{\boldsymbol{\epsilon}|\boldsymbol{y}}[\tilde{\boldsymbol{z}}_{\boldsymbol{\epsilon},m,t}^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y}) + \beta_t^{1/2}\tilde{\sigma}_{\boldsymbol{\epsilon},m,t}^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y})], \end{split}$$

where $\mathbb{E}_{\epsilon|y}[\cdot]$ is the conditional expectation of (\cdot) given y.

Based on this lemma, we give valid AFs. Let $n \in [N]$ and $\boldsymbol{y}^{(n-1)} \in \tilde{\mathcal{Y}}^{(n-1)}$. Then, for any $\boldsymbol{x}^{(n)} \in \mathcal{X}^{(n)}$ and iteration $t \geq 1$, we define the optimistic maximum value at the final stage under given $\boldsymbol{y}^{(n-1)}$, $\mathrm{UCB}_t^{(G)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)})$, as

$$\begin{split} & \text{UCB}_t^{(G)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) = \\ & \max_{(\boldsymbol{x}^{(n+1)}, \dots, \boldsymbol{x}^{(N)})} \mathbb{E}_{\boldsymbol{\epsilon}|\boldsymbol{y}^{(n-1)}} \Big[(\tilde{z}_{\boldsymbol{\epsilon}, 1, t}^{(N)}(\boldsymbol{x}^{(n)}, \dots, \boldsymbol{x}^{(N)}|\boldsymbol{y}^{(n-1)}) + \beta_t^{1/2} \tilde{\sigma}_{\boldsymbol{\epsilon}, 1, t}^{(N)}(\boldsymbol{x}^{(n)}, \dots, \boldsymbol{x}^{(N)}|\boldsymbol{y}^{(n-1)})) \Big], \end{split}$$

where the max operator is ignored when n = N. Similarly, we define the pessimistic maximum value at the final stage under given $\mathbf{y}^{(n-1)}$, $LCB_t^{(G)}(\mathbf{x}^{(n)}|\mathbf{y}^{(n-1)})$, as

$$\begin{split} & \text{LCB}_{t}^{(G)}(\boldsymbol{y}^{(n-1)}) \\ &= \max_{(\boldsymbol{x}^{(n)}, \dots, \boldsymbol{x}^{(N)})} \mathbb{E}_{\boldsymbol{\epsilon}|\boldsymbol{y}^{(n-1)}} \Big[(\tilde{z}_{\boldsymbol{\epsilon}, 1, t}^{(N)}(\boldsymbol{x}^{(n)}, \dots, \boldsymbol{x}^{(N)}|\boldsymbol{y}^{(n-1)}) - \beta_{t}^{1/2} \tilde{\sigma}_{\boldsymbol{\epsilon}, 1, t}^{(N)}(\boldsymbol{x}^{(n)}, \dots, \boldsymbol{x}^{(N)}|\boldsymbol{y}^{(n-1)})) \Big]. \end{split}$$

Moreover, for each $T \ge 1$, we define the pessimistic maximum value at the final stage as

$$Q_T = \max_{(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)})} \mathbb{E}_{\boldsymbol{\epsilon}} \Big[(\tilde{z}_{\boldsymbol{\epsilon}, 1, T}^{(N)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) - \beta_T^{1/2} \tilde{\sigma}_{\boldsymbol{\epsilon}, 1, T}^{(N)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)})) \Big].$$

Then, we define the pessimistic improvement for the final stage with respect to $x^{(n)}$ by

$$\tilde{a}_{t}^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) = \text{UCB}_{t}^{(G)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) - \max\{\text{LCB}_{t}^{(G)}(\boldsymbol{y}^{(n-1)}), Q_{t+n-1}\}$$

We also define the maximum uncertainty for the final stage with respect to $oldsymbol{x}^{(n)}$ as

$$\tilde{b}_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) = \max_{(\boldsymbol{x}^{(n+1)},....,\boldsymbol{x}^{(N)})} \mathbb{E}_{\boldsymbol{\epsilon}|\boldsymbol{y}^{(n-1)}}[\tilde{\sigma}_{\boldsymbol{\epsilon},1,t}^{(N)}(\boldsymbol{x}^{(n)},...,\boldsymbol{x}^{(N)}|\boldsymbol{y}^{(n-1)})].$$

Then, we give the AF $\tilde{c}_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)})$ by

$$\tilde{c}_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) = \max \Bigl\{ \tilde{a}_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}), \eta_t \tilde{b}_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) \Bigr\},$$

where η_t is a given learning rate. Furthermore, we select the next point $x_{t+n}^{(n)}$ by

$$\mathbf{x}_{t+n}^{(n)} = \underset{\mathbf{x}^{(n)} \in \mathcal{X}^{(n)}}{\arg \max} \tilde{c}_{t}^{(n)}(\mathbf{x}^{(n)}|\mathbf{y}_{t+n-1}^{(n-1)}),$$

$$\mathbf{y}_{t+n}^{(n)} = \mathbf{f}^{(n)}(\mathbf{y}_{t+n-1}^{(n-1)}, \mathbf{x}_{t+n}^{(n)}) + \epsilon_{t+n}^{(n)},$$
(D.12)

where $\boldsymbol{y}_t^{(0)} = \boldsymbol{0}$. Finally, we define the estimated solution $(\hat{\boldsymbol{x}}_{G,T}^{(1)}, \dots, \hat{\boldsymbol{x}}_{G,T}^{(N)})$ by using the pessimistic maximum value as follows:

$$(\hat{\boldsymbol{x}}_{G,T}^{(1)}, \dots, \hat{\boldsymbol{x}}_{G,T}^{(N)}) = \\ \underset{(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) \in \mathcal{X}, 1 \leq t \leq T}{\arg \max} \mathbb{E}_{\boldsymbol{\epsilon}} \Big[(\tilde{z}_{\boldsymbol{\epsilon}, 1, t}^{(N)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) - \beta_t^{1/2} \tilde{\sigma}_{\boldsymbol{\epsilon}, 1, t}^{(N)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)})) \Big].$$

Then, the following theorem holds.

Theorem D.9. Assume that Assumptions C.3, C.4 and D.1 hold. Also assume that $\tilde{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y})\in \tilde{\mathcal{Y}}^{(n)}$ for any $s\in\{0,\ldots,N-1\}$, $n\in\{s+1,\ldots,N\}$, iteration $t\geq 1$, realization $\boldsymbol{\epsilon}$, given $\boldsymbol{y}\in\tilde{\mathcal{Y}}^{(s)}$ and input $(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)})$. Let $\delta\in(0,1)$ and $\xi>0$, and define β_t by (D.2) and $\eta_t=(1+\log t)^{-1}$. Then, when the optimization is performed using (D.12), the following inequality holds with probability at least $1-(N+1)\delta$:

$$G(\boldsymbol{x}_{G,*}^{(1)}, \dots, \boldsymbol{x}_{G,*}^{(N)}) - G(\hat{\boldsymbol{x}}_{G,T}^{(1)}, \dots, \hat{\boldsymbol{x}}_{G,T}^{(N)}) < \xi,$$

where T is the smallest positive integer satisfying $T \in N\mathbb{Z}_{>0}$ and

$$\frac{N}{T}\sqrt{C_{6,T}^{2(N+2)}(C_7 + C_8T\tilde{\gamma}_T)} < \xi.$$

Here, $C_{6,t}$, C_7 and C_8 are given by $C_{2,t} = 4NM_{prod}^2M_{sum}C_{0,t}^{2N-2}C_1^N$, $C_{3,t} = NC_{2,t}^N$, $C_{6,t} = 2C_{3,t}\eta_t^{-1}(2\beta_t^{1/2} + 2)$, $C_5 = (1+L_f)^NM_{prod}M_{sum}$, $C_7 = 2\left(8C_5\log\frac{5C_5}{\delta}N\right)^2$, $C_8 = \frac{4M_{sum}^2}{\log(1+\sigma^{-2})}$.

In order to prove Theorem D.9, we give two lemmas.

Lemma D.10. Assume that the same condition as in Theorem D.4 holds. Then, the following holds with probability at least $1 - \delta$:

$$\tilde{\sigma}_{\boldsymbol{\epsilon},1,t}^{(N)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(N)}|\boldsymbol{z}_{\boldsymbol{\epsilon}}^{(s-1)}) \leq C_{3,t}\tilde{\sigma}_{\boldsymbol{\epsilon},1,t}^{(N)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N)}|\boldsymbol{z}_{\boldsymbol{\epsilon}}^{(s)}) + C_{3,t}\sum_{i=1}^{M^{(s)}} \sigma_{\boldsymbol{\epsilon},i,t}^{(s)}(\boldsymbol{z}_{\boldsymbol{\epsilon}}^{(s-1)},\boldsymbol{x}^{(s)}).$$

Proof. By using the same argument as in Lemma C.13, we have Lemma D.10.

Lemma D.11. Assume that the same condition as in Theorem D.4 holds. Then, the following inequality holds:

$$\eta_t \tilde{b}_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) \leq \tilde{c}_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) \leq (2\beta_t^{1/2} + \eta_t)\tilde{b}_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}).$$

Proof. By using the same argument as in Lemma C.14, we get Lemma D.11.

By using these lemmas, we prove Theorem D.9.

Proof. From Lemma D.11, the following holds:

$$\tilde{c}_{t}^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0}) \leq (2\beta_{t}^{1/2} + \eta_{t})\tilde{b}_{t}^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0})
= (2\beta_{t}^{1/2} + \eta_{t})\mathbb{E}_{\boldsymbol{\epsilon}}[\tilde{\sigma}_{\boldsymbol{\epsilon},1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)},\hat{\boldsymbol{x}}_{t+1}^{(2)},\dots,\hat{\boldsymbol{x}}_{t+1}^{(N)}|\boldsymbol{0})]$$

In addition, for the positive integer $NK \equiv T \in N\mathbb{Z}_{\geq 0}$ satisfying the theorem's inequality, $\tilde{c}_t^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0})$ satisfies that

$$\begin{split} \sum_{t \in N\mathbb{Z}_{\geq 0}}^{T} \tilde{c}_{t}^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0}) &\leq (2\beta_{T}^{1/2} + 2) \sum_{t \in N\mathbb{Z}_{\geq 0}}^{T} \mathbb{E}_{\boldsymbol{\epsilon}}[\tilde{\sigma}_{\boldsymbol{\epsilon},1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \hat{\boldsymbol{x}}_{t+1}^{(2)}, \dots, \hat{\boldsymbol{x}}_{t+1}^{(N)}|\boldsymbol{0})] \\ &= (2\beta_{T}^{1/2} + 2) \sum_{t \in N\mathbb{Z}_{> 0}}^{T} \mathbb{E}_{\boldsymbol{\epsilon}^{(1)}}[\mathbb{E}_{\boldsymbol{\epsilon}|\boldsymbol{\epsilon}^{(1)}} \left[\tilde{\sigma}_{\boldsymbol{\epsilon},1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \hat{\boldsymbol{x}}_{t+1}^{(2)}, \dots, \hat{\boldsymbol{x}}_{t+1}^{(N)}|\boldsymbol{0})|\boldsymbol{\epsilon}^{(1)}]\right]. \end{split}$$

Here, the conditional expectation $\mathbb{E}_{\epsilon|\epsilon^{(1)}}[\tilde{\sigma}^{(N)}_{\epsilon,1,t}(\boldsymbol{x}^{(1)}_{t+1},\hat{\boldsymbol{x}}^{(2)}_{t+1},\ldots,\hat{\boldsymbol{x}}^{(N)}_{t+1}|\mathbf{0})|\epsilon^{(1)}]$ is a non-negative random variable with respect to $\epsilon^{(1)}$, and satisfies that

$$\mathbb{E}_{\boldsymbol{\epsilon}|\boldsymbol{\epsilon}^{(1)}}[\tilde{\sigma}_{\boldsymbol{\epsilon},1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)},\hat{\boldsymbol{x}}_{t+1}^{(2)},\ldots,\hat{\boldsymbol{x}}_{t+1}^{(N)}|\boldsymbol{0})|\boldsymbol{\epsilon}^{(1)}] \leq (1+L_f)^N M_{\text{prod}} M_{\text{sum}} = C_5,$$

where the inequality is given by $k^{(n)}(\cdot,\cdot) \le 1$. Hence, from Lemma 3 of (Kirschner and Krause, 2018), the following holds with probability at least $1 - \delta$:

$$\begin{split} & \sum_{t \in N\mathbb{Z}_{\geq 0}}^{T} \mathbb{E}_{\boldsymbol{\epsilon}^{(1)}} \big[\mathbb{E}_{\boldsymbol{\epsilon}|\boldsymbol{\epsilon}^{(1)}} \big[\tilde{\sigma}_{\boldsymbol{\epsilon},1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \hat{\boldsymbol{x}}_{t+1}^{(2)}, \dots, \hat{\boldsymbol{x}}_{t+1}^{(N)}|\boldsymbol{0}) | \boldsymbol{\epsilon}^{(1)} \big] \big] \\ & \leq 4C_5 \log \frac{1}{\delta} + 8C_5 \log(4C_5) + 1 + 2 \sum_{t \in N\mathbb{Z}_{\geq 0}}^{T} \mathbb{E}_{\boldsymbol{\epsilon}|\boldsymbol{\epsilon}_{t}^{(1)}} \big[\tilde{\sigma}_{\boldsymbol{\epsilon},1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \hat{\boldsymbol{x}}_{t+1}^{(2)}, \dots, \hat{\boldsymbol{x}}_{t+1}^{(N)}|\boldsymbol{0}) | \boldsymbol{\epsilon}_{t}^{(1)} \big] \\ & \leq 8C_5 \log \frac{5C_5}{\delta} + 2 \sum_{t \in N\mathbb{Z}_{\geq 0}}^{T} \mathbb{E}_{\boldsymbol{\epsilon}|\boldsymbol{\epsilon}_{t}^{(1)}} \big[\tilde{\sigma}_{\boldsymbol{\epsilon},1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \hat{\boldsymbol{x}}_{t+1}^{(2)}, \dots, \hat{\boldsymbol{x}}_{t+1}^{(N)}|\boldsymbol{0}) | \boldsymbol{\epsilon}_{t}^{(1)} \big]. \end{split}$$

Moreover, from Lemma D.10, with probability at least $1 - \delta$ the following inequality holds uniformly:

$$\begin{split} & \mathbb{E}_{\boldsymbol{\epsilon}|\boldsymbol{\epsilon}_{t}^{(1)}}[\tilde{\sigma}_{\boldsymbol{\epsilon},1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)},\hat{\boldsymbol{x}}_{t+1}^{(2)},\ldots,\hat{\boldsymbol{x}}_{t+1}^{(N)}|\boldsymbol{0})|\boldsymbol{\epsilon}_{t}^{(1)}] \\ & \leq \mathbb{E}_{\boldsymbol{\epsilon}|\boldsymbol{\epsilon}_{t}^{(1)}}[C_{3,T}\tilde{\sigma}_{\boldsymbol{\epsilon},1,t}^{(N)}(\hat{\boldsymbol{x}}_{t+1}^{(2)},\ldots,\hat{\boldsymbol{x}}_{t+1}^{(N)}|\boldsymbol{y}_{t+1}^{(1)})] + C_{3,T}\sum_{i=1}^{M^{(1)}}\sigma_{\boldsymbol{\epsilon},1,t}^{(1)}(\boldsymbol{0},\boldsymbol{x}_{t+1}^{(1)}). \end{split}$$

Therefore, it follows that

$$\begin{split} &\sum_{t \in N \mathbb{Z}_{\geq 0}}^{T} \mathbb{E}_{\epsilon^{(1)}} \big[\mathbb{E}_{\epsilon | \epsilon^{(1)}} \big[\hat{\sigma}_{\epsilon, 1, t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \hat{\boldsymbol{x}}_{t+1}^{(2)}, \dots, \hat{\boldsymbol{x}}_{t+1}^{(N)} | \boldsymbol{0}) | \epsilon^{(1)} \big] \big] \\ &\leq 8C_5 \log \frac{5C_5}{\delta} + 2 \sum_{t \in N \mathbb{Z}_{\geq 0}}^{T} \mathbb{E}_{\epsilon | \epsilon_{t}^{(1)}} \big[\hat{\sigma}_{\epsilon, 1, t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \hat{\boldsymbol{x}}_{t+1}^{(2)}, \dots, \hat{\boldsymbol{x}}_{t+1}^{(N)} | \boldsymbol{0}) | \epsilon_{t}^{(1)} \big] \\ &\leq 8C_5 \log \frac{5C_5}{\delta} + 2C_{3,T} \sum_{t \in N \mathbb{Z}_{\geq 0}}^{T} \sum_{i=1}^{M} \sigma_{\epsilon, 1, t}^{(1)}(\boldsymbol{0}, \boldsymbol{x}_{t+1}^{(1)}) + 2C_{3,T} \sum_{t \in N \mathbb{Z}_{\geq 0}}^{T} \mathbb{E}_{\epsilon | \epsilon_{t}^{(1)}} \big[\hat{\sigma}_{\epsilon, 1, t}^{(N)}(\hat{\boldsymbol{x}}_{t+1}^{(1)}, \dots, \hat{\boldsymbol{x}}_{t+1}^{(N)} | \boldsymbol{y}_{t+1}^{(1)} \big] \\ &\leq 8C_5 \log \frac{5C_5}{\delta} + 2C_{3,T} \sum_{t \in N \mathbb{Z}_{\geq 0}}^{T} \sum_{i=1}^{M} \sigma_{\epsilon, 1, t}^{(1)}(\boldsymbol{0}, \boldsymbol{x}_{t+1}^{(1)}) + 2C_{3,T} \eta_T^{-1} \sum_{t \in N \mathbb{Z}_{\geq 0}}^{T} \eta_t \hat{b}_t^{(2)}(\hat{\boldsymbol{x}}_{t+1}^{(2)} | \boldsymbol{y}_{t+1}^{(1)}) \\ &\leq 8C_5 \log \frac{5C_5}{\delta} + 2C_{3,T} \sum_{t \in N \mathbb{Z}_{\geq 0}}^{T} \sum_{i=1}^{M} \sigma_{\epsilon, 1, t}^{(1)}(\boldsymbol{0}, \boldsymbol{x}_{t+1}^{(1)}) + 2C_{3,T} \eta_T^{-1} \sum_{t \in N \mathbb{Z}_{\geq 0}}^{T} \hat{c}_t^{(2)}(\hat{\boldsymbol{x}}_{t+1}^{(2)} | \boldsymbol{y}_{t+1}^{(1)}) \\ &\leq 8C_5 \log \frac{5C_5}{\delta} + 2C_{3,T} \sum_{t \in N \mathbb{Z}_{\geq 0}}^{T} \sum_{i=1}^{M} \sigma_{\epsilon, 1, t}^{(1)}(\boldsymbol{0}, \boldsymbol{x}_{t+1}^{(1)}) + 2C_{3,T} \eta_T^{-1} \sum_{t \in N \mathbb{Z}_{\geq 0}}^{T} \hat{c}_t^{(2)}(\hat{\boldsymbol{x}}_{t+2}^{(2)} | \boldsymbol{y}_{t+1}^{(1)}) \\ &\leq 8C_5 \log \frac{5C_5}{\delta} + 2C_{3,T} \sum_{t \in N \mathbb{Z}_{\geq 0}}^{T} \sum_{i=1}^{M} \sigma_{\epsilon, 1, t}^{(1)}(\boldsymbol{0}, \boldsymbol{x}_{t+1}^{(1)}) + 2C_{3,T} \eta_T^{-1}(2\beta_t^{1/2} + 2) \sum_{t \in N \mathbb{Z}_{\geq 0}}^{T} \hat{b}_t^{(2)}(\boldsymbol{x}_{t+2}^{(2)} | \boldsymbol{y}_{t+1}^{(1)}) \\ &\leq 8C_5 \log \frac{5C_5}{\delta} + 2C_{3,T} \sum_{t \in N \mathbb{Z}_{\geq 0}}^{T} \sum_{i=1}^{M} \sigma_{\epsilon, 1, t}^{(1)}(\boldsymbol{0}, \boldsymbol{x}_{t+1}^{(1)}) + 2C_{3,T} \eta_T^{-1}(2\beta_t^{1/2} + 2) \sum_{t \in N \mathbb{Z}_{\geq 0}}^{T} \hat{b}_t^{(2)}(\boldsymbol{x}_{t+2}^{(2)} | \boldsymbol{y}_{t+1}^{(1)}) \\ &\qquad \cdot \sum_{t \in N \mathbb{Z}_{\geq 0}^{T}} \mathbb{E}_{\epsilon^{(2)}} \Big[\mathbb{E}_{\epsilon | \boldsymbol{y}_{t+1}^{(1)}, \epsilon^{(2)}} \Big[\hat{\sigma}_{\epsilon, 1, t}^{(N)}(\boldsymbol{x}_{t+2}^{(2)}, \hat{\boldsymbol{x}}_{t+2}^{(3)}, \dots, \hat{\boldsymbol{x}}_{t+2}^{(N)} | \boldsymbol{y}_{t+1}^{(N)}) | \epsilon^{(2)} \Big] \Big] \\ &\leq 8C_5 \log \frac{5C_5}{\delta} + C_6 T \sum_{t \in N \mathbb{Z}_{\geq 0}^{T}} \mathbb{E}_{\epsilon^{(2)}} \Big[\hat{\sigma}_{\epsilon, 1, t}^{(N)}(\boldsymbol{x}_{t+2}^{(2)}, \hat{\boldsymbol{x}}_{t+2}^$$

By repeating this process, with probability at least $1 - (N+1)\delta$, the following holds:

$$\begin{split} & \sum_{t \in N\mathbb{Z}_{\geq 0}}^{T} \mathbb{E}_{\boldsymbol{\epsilon}^{(1)}} \big[\mathbb{E}_{\boldsymbol{\epsilon}|\boldsymbol{\epsilon}^{(1)}} \big[\tilde{\sigma}_{\boldsymbol{\epsilon},1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \hat{\boldsymbol{x}}_{t+1}^{(2)}, \dots, \hat{\boldsymbol{x}}_{t+1}^{(N)} | \boldsymbol{0}) | \boldsymbol{\epsilon}^{(1)} \big] \big] \\ & \leq 8C_5 \log \frac{5C_5}{\delta} N C_{6,T}^N + C_{6,T}^N \sum_{t \in N\mathbb{Z}_{\geq 0}}^{T} \sum_{n=1}^{N} \sum_{i=1}^{M^{(n)}} \sigma_{\boldsymbol{\epsilon},i,t}^{(n)}(\boldsymbol{y}_{t+n-1}^{(n-1)}, \boldsymbol{x}_{t+n}^{(n)}). \end{split}$$

By combining this and

$$\begin{split} \sum_{t \in N\mathbb{Z}_{\geq 0}}^{T} \tilde{c}_{t}^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0}) &\leq (2\beta_{T}^{1/2} + 2) \sum_{t \in N\mathbb{Z}_{\geq 0}}^{T} \mathbb{E}_{\boldsymbol{\epsilon}^{(1)}} \big[\mathbb{E}_{\boldsymbol{\epsilon}|\boldsymbol{\epsilon}^{(1)}} \Big[\tilde{\sigma}_{\boldsymbol{\epsilon},1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \hat{\boldsymbol{x}}_{t+1}^{(2)}, \dots, \hat{\boldsymbol{x}}_{t+1}^{(N)}|\boldsymbol{0}) | \boldsymbol{\epsilon}^{(1)} \big] \Big] \\ &\leq C_{6,T} \sum_{t \in N\mathbb{Z}_{\geq 0}}^{T} \mathbb{E}_{\boldsymbol{\epsilon}^{(1)}} \big[\mathbb{E}_{\boldsymbol{\epsilon}|\boldsymbol{\epsilon}^{(1)}} \Big[\tilde{\sigma}_{\boldsymbol{\epsilon},1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \hat{\boldsymbol{x}}_{t+1}^{(2)}, \dots, \hat{\boldsymbol{x}}_{t+1}^{(N)}|\boldsymbol{0}) | \boldsymbol{\epsilon}^{(1)} \big] \Big], \end{split}$$

we get

$$\sum_{t \in N\mathbb{Z}_{\geq 0}}^{T} \tilde{c}_{t}^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0}) \leq 8C_{5}\log \frac{5C_{5}}{\delta}NC_{6,T}^{N+1} + C_{6,T}^{N+1} \sum_{t \in N\mathbb{Z}_{\geq 0}}^{T} \sum_{n=1}^{N} \sum_{i=1}^{M^{(n)}} \sigma_{\boldsymbol{\epsilon},i,t}^{(n)}(\boldsymbol{y}_{t+n-1}^{(n-1)}, \boldsymbol{x}_{t+n}^{(n)}).$$

Thus, noting that $(a+b)^2 \leq 2a^2 + 2b^2$, using the Cauchy–Schwarz inequality and $\tilde{\gamma}_T$ we have

$$\left(\sum_{t \in N\mathbb{Z}_{\geq 0}}^{T} \tilde{c}_{t}^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0})\right)^{2} \leq 2\left(8C_{5}\log\frac{5C_{5}}{\delta}NC_{6,T}^{N+1}\right)^{2} + 2C_{6,T}^{2(N+1)}TM_{\text{sum}}\sum_{n=1}^{N}\sum_{i=1}^{M^{(n)}} \sigma_{\boldsymbol{\epsilon},i,t}^{(n)2}(\boldsymbol{y}_{t+n-1}^{(n-1)},\boldsymbol{x}_{t+n}^{(n)}) \\
\leq 2\left(8C_{5}\log\frac{5C_{5}}{\delta}NC_{6,T}^{N+1}\right)^{2} + 2C_{6,T}^{2(N+1)}TM_{\text{sum}}\frac{2M_{\text{sum}}\tilde{\gamma}_{T}}{\log(1+\sigma^{-2})} \\
= C_{6,T}^{2(N+1)}(C_{7} + C_{8}T\tilde{\gamma}_{T}).$$

This implies that

$$\sum_{t \in N\mathbb{Z}_{>0}}^{T} \tilde{c}_{t}^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0}) \leq \sqrt{C_{6,T}^{2(N+1)}(C_{7} + C_{8}T\tilde{\gamma}_{T})}.$$

Furthermore, letting $\tilde{t} = \arg\max_{t \in N\mathbb{Z}_{\geq 0}, t \leq T} \tilde{c}_t^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0})$ we get

$$K ilde{c}_{ ilde{t}}^{(1)}(oldsymbol{x}_{ ilde{t}+1}^{(1)}|oldsymbol{0}) \leq \sum_{t \in N\mathbb{Z}_{\geq 0}}^{T} ilde{c}_{t}^{(1)}(oldsymbol{x}_{t+1}^{(1)}|oldsymbol{0}) \\ \leq \sqrt{C_{6,T}^{2(N+1)}(C_{7} + C_{8}T ilde{\gamma}_{T})}.$$

By dividing both sides by K, we obtain

$$\tilde{c}_{\tilde{t}}^{(1)}(\boldsymbol{x}_{\tilde{t}+1}^{(1)}|\mathbf{0}) \leq K^{-1}\sqrt{C_{6,T}^{2(N+1)}(C_7 + C_8T\tilde{\gamma}_T)}
= \frac{N}{T}\sqrt{C_{6,T}^{2(N+1)}(C_7 + C_8T\tilde{\gamma}_T)}.$$
(D.13)

Finally, from the definition of the estimated solution and CIs, we get

$$\begin{split} G(\boldsymbol{x}_{G,*}^{(1)}, \dots, \boldsymbol{x}_{G,*}^{(N)}) &\leq \min_{t \in N\mathbb{Z}_{\geq 0}, t \leq T} \mathrm{UCB}_{t}^{(G)}(\boldsymbol{x}_{G,*}^{(1)}, \dots, \boldsymbol{x}_{G,*}^{(N)}) \leq \mathrm{UCB}_{\tilde{t}}^{(G)}(\boldsymbol{x}_{G,*}^{(1)}, \dots, \boldsymbol{x}_{G,*}^{(N)}) \\ G(\hat{\boldsymbol{x}}_{G,T}^{(1)}, \dots, \hat{\boldsymbol{x}}_{G,T}^{(N)}) &\geq \max_{t \in N\mathbb{Z}_{\geq 0}, t \leq T} \mathrm{LCB}_{t}^{(G)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) \\ &\geq \mathrm{LCB}_{\tilde{t}}^{(G)}(\boldsymbol{x}_{G,*}^{(1)}, \dots, \boldsymbol{x}_{G,*}^{(N)}). \end{split}$$

Thus, it follows that

$$\begin{split} G(\boldsymbol{x}_{G,*}^{(1)},\dots,\boldsymbol{x}_{G,*}^{(N)}) - G(\hat{\boldsymbol{x}}_{G,T}^{(1)},\dots,\hat{\boldsymbol{x}}_{G,T}^{(N)}) &\leq 2\beta_T^{1/2} \mathbb{E}_{\boldsymbol{\epsilon}}[\tilde{\sigma}_{\boldsymbol{\epsilon},1,\tilde{t}}^{(N)}(\boldsymbol{x}_{G,*}^{(1)},\dots,\boldsymbol{x}_{G,*}^{(N)})] \\ &\leq 2\beta_T^{1/2} \tilde{b}_{\tilde{t}}^{(1)}(\boldsymbol{x}_{G,*}^{(1)}|\boldsymbol{0}) \\ &\leq 2\beta_T^{1/2} \eta_{\tilde{t}}^{-1} \tilde{c}_{\tilde{t}}^{(1)}(\boldsymbol{x}_{G,*}^{(1)}|\boldsymbol{0}) \leq 2\beta_T^{1/2} \eta_T^{-1} \tilde{c}_{\tilde{t}}^{(1)}(\boldsymbol{x}_{\tilde{t}+1}^{(1)}|\boldsymbol{0}). \end{split}$$

Hence, by combining this and (D.13), we have

$$G(\boldsymbol{x}_{G,*}^{(1)}, \dots, \boldsymbol{x}_{G,*}^{(N)}) - G(\hat{\boldsymbol{x}}_{G,T}^{(1)}, \dots, \hat{\boldsymbol{x}}_{G,T}^{(N)}) \le 2\beta_T^{1/2} \eta_T^{-1} \frac{N}{T} \sqrt{C_{6,T}^{2(N+1)}(C_7 + C_8 T \tilde{\gamma}_T)}$$

$$\le C_{6,T} \frac{N}{T} \sqrt{C_{6,T}^{2(N+1)}(C_7 + C_8 T \tilde{\gamma}_T)}$$

$$= \frac{N}{T} \sqrt{C_{6,T}^{2(N+2)}(C_7 + C_8 T \tilde{\gamma}_T)} < \xi.$$

D.4 Optimistic Improvement-based AF for the Final Stage Output

We give an optimistic improvement-based AF for F under the noisy setting. First, we define the sum of the squares of the observation noise ϵ_{sum} as

$$\epsilon_{\text{sum}} = \sum_{n=1}^{N} \sum_{m=1}^{M^{(n)}} \epsilon_m^{(n)2}.$$

Note that ϵ_{sum} is bounded by $M_{\text{sum}}A^2$ under Assumption D.1. Moreover, we assume the following assumption for ϵ_{sum} .

Assumption D.12. Under Assumption D.1, there exists a positive constant C such that $\mathbb{P}(\epsilon_{sum} < V) > CV$ for any V with $0 < V \le M_{sum}A^2$.

For example, if ϵ_{sum} is a discrete random variable with $\mathbb{P}(\epsilon_{\text{sum}}=0)>0$, then Assumption D.12 holds. Similarly, if ϵ_{sum} is a continuous random variable whose probability density function $p_{\epsilon_{\text{sum}}}(x)$ satisfies $p_{\epsilon_{\text{sum}}}(x)>K>0$, where x is an arbitrary element of some interval [0,U]. Then, Assumption D.12 also holds. Thus, Assumption D.12 guarantees that ϵ_{sum} can take values within an arbitrary neighborhood of zero. Next, we define the variable $C_{9,t}$ as

$$C_{9,t} = 2\beta_t^{1/2} \eta_t^{-1} (2\beta_t^{1/2} + 2)^N C_{3,t}^N \eta_t^{-N},$$

where $\eta_t = (1 + \log t)^{-1}$. Then, we assume the following assumption.

Assumption D.13. For any $T \ge 1$, $C_{9,t}$ satisfies that

$$\sum_{t=T}^{t'} C_{9,t}^{-2} \to \infty \quad (as \ t' \to \infty).$$

Note that $C_{9,t}$ is a polynomial function on β_t . Furthermore, by considering the definition of β_t , the closed form of the mutual information, and $\tilde{\gamma}_t$, we can show that the order of $C_{9,t}$ is expressed as the polynomial function of $\tilde{\gamma}_t$. Here, under certain conditions, it is known that the order of $\tilde{\gamma}_t$ for commonly used kernels such as Gaussian kernels and linear kernels is a logarithmic order (Srinivas et al., 2010). Then, Assumption D.13 holds if we use such kernels. Under this setting, we propose an algorithm to the regret $r_{F,T}^{(S)}$.

First, for each $t \geq 1$, we define the estimated solution $\hat{x}_{F,t}^{(1)}, \ldots, \hat{x}_{F,t}^{(N)}$ as follows:

$$\hat{\boldsymbol{x}}_{F,t}^{(1)}, \dots, \hat{\boldsymbol{x}}_{F,t}^{(N)} = \underset{\substack{1 \leq t' \leq t \\ (\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) \in \mathcal{X}}}{\arg \max} (\tilde{z}_{\mathbf{0}, 1, t'}^{(N)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) - \beta_t^{1/2} \tilde{\sigma}_{\mathbf{0}, 1, t'}^{(N)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)})).$$

Then, we give the optimistic improvement-based AF. For any $n \in [N]$, given an observation $\boldsymbol{y}^{(n-1)}$ of stage n-1, optimistic maximum estimator $\widehat{\mathrm{UCB}}_t^{(F)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)})$ w.r.t. $\boldsymbol{x}^{(n)}$ is defined as:

$$\begin{split} \widehat{\text{UCB}}_t^{(F)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) \\ &= \max_{(\boldsymbol{x}^{(n+1)}, \dots, \boldsymbol{x}^{(N)})} \Big(\widehat{z}_{\mathbf{0}, 1, t}^{(N)}(\boldsymbol{x}^{(n)}, \dots, \boldsymbol{x}^{(N)}|\boldsymbol{y}^{(n-1)}) + \beta_t^{1/2} \widetilde{\sigma}_{\mathbf{0}, 1, t}^{(N)}(\boldsymbol{x}^{(n)}, \dots, \boldsymbol{x}^{(N)}|\boldsymbol{y}^{(n-1)}) \Big), \end{split}$$

where the max operator is not needed when n = N. Similarly, pessimistic maximum estimator $\widehat{LCB}_t^{(F)}(\boldsymbol{y}^{(n-1)})$ under given an observation $\boldsymbol{y}^{(n-1)}$ is defined as follows:

$$\widehat{LCB}_{t}^{(F)}(\boldsymbol{y}^{(n-1)}) = \max_{(\boldsymbol{x}^{(n)}, \dots, \boldsymbol{x}^{(N)})} \left(\widetilde{z}_{\mathbf{0}, 1, t}^{(N)}(\boldsymbol{x}^{(n)}, \dots, \boldsymbol{x}^{(N)} | \boldsymbol{y}^{(n-1)}) - \beta_{t}^{1/2} \widetilde{\sigma}_{\mathbf{0}, 1, t}^{(N)}(\boldsymbol{x}^{(n)}, \dots, \boldsymbol{x}^{(N)} | \boldsymbol{y}^{(n-1)}) \right).$$

Moreover, pessimistic maximum estimator of F is given by:

$$\hat{Q}_T = \max_{(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)})} \left(\tilde{z}_{\boldsymbol{0}, 1, T}^{(N)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) - \beta_t^{1/2} \tilde{\sigma}_{\boldsymbol{0}, 1, T}^{(N)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) \right).$$

Then, we define the optimistic improvement with w.r.t. $x^{(n)}$ as:

$$\hat{a}_{t}^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) = \widehat{\text{UCB}}_{t}^{(F)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) - \max\{\widehat{\text{LCB}}_{t}^{(F)}(\boldsymbol{y}^{(n-1)}), \hat{Q}_{t+n-1}\}.$$
(D.14)

Furthermore, we define the maximum uncertainty w.r.t. $(y^{(n-1)}, x^{(n)})$ as:

$$\hat{b}_{t}^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) = \max_{(\boldsymbol{x}^{(n+1)},\dots,\boldsymbol{x}^{(N)})} \tilde{\sigma}_{\mathbf{0},1,t}^{(N)}(\boldsymbol{x}^{(n)},\dots,\boldsymbol{x}^{(N)}|\boldsymbol{y}^{(n-1)}). \tag{D.15}$$

From (D.14) and (D.15), the AF $\hat{c}_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)})$ for this setting is given by:

$$\hat{c}_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) = \max\{\hat{a}_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}), \eta_t \hat{b}_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)})\},$$

where η_t is some learning rate tends to zero. Using this AF $\hat{c}_t^{(n)}$, we propose the following selection rule:

$$\mathbf{x}_{t+n}^{(n)} = \underset{\mathbf{x}^{(n)} \in \mathcal{X}^{(n)}}{\arg \max} \hat{c}_{t}^{(n)}(\mathbf{x}^{(n)}|\mathbf{y}_{t+n-1}^{(n-1)}),$$

$$\mathbf{y}_{t+n}^{(n)} = \mathbf{f}^{(n)}(\mathbf{y}_{t+n-1}^{(n-1)}, \mathbf{x}_{t+n}^{(n)}) + \boldsymbol{\epsilon}_{t+n}^{(n)},$$
(D.16)

where $y_t^{(0)} = \mathbf{0}$. Then, the following theorem holds.

Theorem D.14. Assume that Assumptions C.3, C.4, D.1, D.12 and D.13 hold. Also assume that $\tilde{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)}|\boldsymbol{y})\in \tilde{\mathcal{Y}}^{(n)}$ for any $s\in\{0,\ldots,N-1\}$, $n\in\{s+1,\ldots,N\}$, iteration $t\geq 1$, realization $\boldsymbol{\epsilon}$, given $\boldsymbol{y}\in\tilde{\mathcal{Y}}^{(s)}$ and input $(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n)})$. Let $\delta\in(0,1)$ and $\xi>0$, and define β_t by (D.2) and $\eta_t=(1+\log t)^{-1}$. Then, there exists a sequence $0=T_0< T_1< T_2<\cdots$ such that $T_k\in N\mathbb{Z}_{\geq 0}$ and

$$\mathbb{P}(\exists t \in N\mathbb{Z}_{\geq 0} \text{ s.t. } T_{k-1} \leq t \leq T_k, \ 2C_{9,t}^2 M_{sum} \epsilon_{sum,t} < \xi^2/2) > 1 - \frac{6\delta}{\pi^2 k^2}. \tag{D.17}$$

Moreover, when the optimization is performed using (D.16), the following inequality holds with probability at least $1-2\delta$:

$$F(\boldsymbol{x}_{F,*}^{(1)},\dots,\boldsymbol{x}_{F,*}^{(N)}) - F(\hat{\boldsymbol{x}}_{F,T_K}^{(1)},\dots,\hat{\boldsymbol{x}}_{F,T_K}^{(N)}) < \xi,$$

where T_K is an element of the sequence $\{T_k\}_{k=0}^{\infty}$ satisfying

$$\frac{4C_{9,T_K}^2M_{sum}^2}{\log(1+\sigma^{-2})}\tilde{\gamma}_{T_K}K^{-1}<\xi^2/2.$$

In order to prove Theorem D.14, we first give four lemmas.

Lemma D.15. Assume that the same condition as in Theorem D.14 holds. Then, for any $s \in \{1, ..., N-1\}$, $n \in \{s+1, ..., N\}$, $m \in [M^{(n)}]$, iteration $t \geq 1$, realization ϵ and input $\mathbf{x}^{(1)}, ..., \mathbf{x}^{(N)}$, the following holds with probability at least $1 - \delta$:

$$\begin{split} &|\sigma_{m,t}^{(n)}(\tilde{\boldsymbol{z}}_{\mathbf{0},t}^{(n-1)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(n-1)}|\boldsymbol{z}_{\boldsymbol{\epsilon}}^{(s-1)}),\boldsymbol{x}^{(n)}) - \sigma_{m,t}^{(n)}(\tilde{\boldsymbol{z}}_{\mathbf{0},t}^{(n-1)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(n-1)}|\boldsymbol{z}_{\boldsymbol{\epsilon}}^{(s)}),\boldsymbol{x}^{(n)})|\\ &\leq 2M_{prod}C_{0,t}^{N-1}\sum_{p=0}^{n-s-1}\sum_{i=1}^{M^{(n-1-p)}}\sigma_{i,t}^{(n-1-p)}\Big(\tilde{\boldsymbol{z}}_{\mathbf{0},t}^{(n-2-p)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(n-2-p)}|\boldsymbol{z}_{\boldsymbol{\epsilon}}^{(s-1)}),\boldsymbol{x}^{(n-1-p)}\Big)\\ &+2M_{prod}C_{0,t}^{N-1}\sum_{q=1}^{M^{(s)}}|\epsilon_{q}^{(s)}|. \end{split}$$

Proof. By using the same argument as in the proof of Lemma C.11, the following holds with probability at least $1 - \delta$:

$$\begin{split} &|\sigma_{m,t}^{(n)}(\tilde{z}_{0,t}^{(n-1)}(x^{(s)},\ldots,x^{(n-1)}|z_{\epsilon}^{(s-1)}),x^{(n)}) - \sigma_{m,t}^{(n)}(\tilde{z}_{0,t}^{(n-1)}(x^{(s+1)},\ldots,x^{(n-1)}|z_{\epsilon}^{(s)}),x^{(n)})| \\ &\leq 2\beta_{t}^{1/2}L_{\sigma}\sum_{j=1}^{M^{(n-1)}}\sigma_{j,t}^{(n-1)}\left(\tilde{z}_{0,t}^{(n-2)}(x^{(s+1)},\ldots,x^{(n-2)}|z_{\epsilon}^{(s)}),x^{(n-1)}\right) + L_{\sigma}M^{(n-1)}(L_{f}+\beta_{t}^{1/2}L_{\sigma}) \\ &\cdot \sum_{i=1}^{M^{(n-2)}}\left[|\tilde{z}_{0,i,t}^{(n-2)}(x^{(s)},\ldots,x^{(n-2)}|z_{\epsilon}^{(s-1)}) - \tilde{z}_{0,i,t}^{(n-2)}(x^{(s+1)},\ldots,x^{(n-2)}|z_{\epsilon}^{(s)})|\right] \\ &\leq 2\beta_{t}^{1/2}L_{\sigma}\sum_{j=1}^{M^{(n-1)}}\sigma_{j,t}^{(n-1)}(\tilde{z}_{0,t}^{(n-2)}(x^{(s)},\ldots,x^{(n-2)}|z_{\epsilon}^{(s-1)}),x^{(n-1)}) \\ &+ 2\beta_{t}^{1/2}L_{\sigma}M^{(n-1)}(L_{f}+\beta_{t}^{1/2}L_{\sigma})\sum_{i=1}^{M^{(n-2)}}\sigma_{i,t}^{(n-2)}(\tilde{z}_{0,t}^{(n-3)}(x^{(s)},\ldots,x^{(n-3)}|z_{\epsilon}^{(s-1)}),x^{(n-2)}) \\ &+ L_{\sigma}M^{(n-1)}M^{(n-2)}(L_{f}+\beta_{t}^{1/2}L_{\sigma})\sum_{i=1}^{M^{(n-2)}}\sigma_{i,t}^{(n-2)}(\tilde{z}_{0,t}^{(n-3)}(x^{(s)},\ldots,x^{(n-3)}|z_{\epsilon}^{(s-1)}),x^{(n-2)}) \\ &+ \sum_{q=1}^{M^{(n-3)}}\left[|\tilde{z}_{0,q,t}^{(n-3)}(x^{(s)},\ldots,x^{(n-3)}|z_{\epsilon}^{(s-1)}) - \tilde{z}_{0,q,t}^{(n-3)}(x^{(s+1)},\ldots,x^{(n-3)}|z_{\epsilon}^{(s)})|\right] \\ &\leq \\ \vdots \\ &\leq 2\beta_{t}^{1/2}L_{\sigma}M_{\mathrm{prod}}(L_{f}+\beta_{t}^{1/2}L_{\sigma}+1)^{N-2} \\ &\sum_{p=0}^{n-s-2}\sum_{i=1}^{M^{(n-1-p)}}\left[\sigma_{i,t}^{(n-1-p)}(\tilde{z}_{0,t}^{(n-2-p)}(x^{(s)},\ldots,x^{(n-2-p)}|z_{\epsilon}^{(s-1)},x^{(s)}) - f_{q}^{(s)}(z_{\epsilon}^{(s-1)},x^{(s)}) - \epsilon_{q}^{(s)}|\right] \\ &\leq 2M_{\mathrm{prod}}(L_{f}+\beta_{t}^{1/2}L_{\sigma}+1)^{N-1} \\ &\sum_{p=0}^{n-s-1}\sum_{i=1}^{M^{(n-1-p)}}\left[\sigma_{i,t}^{(n-1-p)}(\tilde{z}_{0,t}^{(n-2-p)}(x^{(s)},\ldots,x^{(n-2-p)}|z_{\epsilon}^{(s-1)}),x^{(n-1-p)})\right] \\ &+ 2M_{\mathrm{prod}}(L_{f}+\beta_{t}^{1/2}L_{\sigma}+1)^{N-1}\sum_{q=1}^{M^{(s)}}|\epsilon_{q}^{(s)}| \end{aligned}$$

$$= 2M_{\text{prod}}C_{0,t}^{N-1} \sum_{p=0}^{n-s-1} \sum_{i=1}^{M^{(n-1-p)}} \left[\sigma_{i,t}^{(n-1-p)}(\tilde{\boldsymbol{z}}_{\mathbf{0},t}^{(n-2-p)}(\boldsymbol{x}^{(s)},\dots,\boldsymbol{x}^{(n-2-p)}|\boldsymbol{z}_{\boldsymbol{\epsilon}}^{(s-1)}),\boldsymbol{x}^{(n-1-p)}) \right] \\ + 2M_{\text{prod}}C_{0,t}^{N-1} \sum_{q=1}^{M^{(s)}} |\epsilon_q^{(s)}|.$$

Lemma D.16. Assume that the same condition as in Theorem D.14 holds. Then, for any $s \in \{1, ..., N-1\}$, $j \ge 0$ with $s+j \le N$, iteration $t \ge 1$, realization ϵ and input $\boldsymbol{x}^{(1)}, ..., \boldsymbol{x}^{(N)}$, the following holds with probability at least $1-\delta$:

$$\begin{split} &\tilde{\sigma}_{\mathbf{0},t}^{(N-j)}(\boldsymbol{x}^{(s)},\dots,\boldsymbol{x}^{(N-j)}|\boldsymbol{z}_{\epsilon}^{(s-1)}) \\ &\leq C_{2,t}\tilde{\sigma}_{\mathbf{0},t}^{(N-j)}(\boldsymbol{x}^{(s+1)},\dots,\boldsymbol{x}^{(N-j)}|\boldsymbol{z}_{\epsilon}^{(s)}) + C_{2,t}\tilde{\sigma}_{\mathbf{0},t}^{(N-j-1)}(\boldsymbol{x}^{(s)},\dots,\boldsymbol{x}^{(N-j-1)}|\boldsymbol{z}_{\epsilon}^{(s-1)}) \\ &+ C_{2,t}\sum_{i=1}^{M^{(s)}}\sigma_{i,t}^{(s)}(\boldsymbol{z}_{\epsilon}^{(s-1)},\boldsymbol{x}^{(s)}) + C_{2,t}\sum_{i=1}^{M^{(s)}}|\epsilon_{i}^{(s)}|, \end{split}$$

where

$$\begin{split} & \tilde{\sigma}_{\mathbf{0},t}^{(N-j)}(\boldsymbol{x}^{(s)}, \dots, \boldsymbol{x}^{(N-j)} | \boldsymbol{z}_{\boldsymbol{\epsilon}}^{(s-1)}) \\ & = \sum_{p=j}^{N-s} \prod_{q=1}^{p} M^{(N-q+1)} L_f^p \sum_{i=1}^{M^{(N-p)}} \left[\sigma_{i,t}^{(N-p)}(\tilde{\boldsymbol{z}}_{\mathbf{0},t}^{(N-p-1)}(\boldsymbol{x}^{(s)}, \dots, \boldsymbol{x}^{(N-p-1)} | \boldsymbol{z}_{\boldsymbol{\epsilon}}^{(s-1)}), \boldsymbol{x}^{(N-p)}) \right]. \end{split}$$

Proof. From the definition of $\tilde{\sigma}_{\mathbf{0},t}^{(N-j)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(N-j)}|\boldsymbol{z}_{\epsilon}^{(s-1)})$, the following inequality holds with probability at least $1-\delta$:

$$\begin{split} &\tilde{\sigma}_{\mathbf{0},t}^{(N-j)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(N-j)}|\boldsymbol{z}_{\epsilon}^{(s-1)}) \\ &= \sum_{p=j}^{N-s} \prod_{q=1}^{p} M^{(N-q+1)} L_{f}^{p} \sum_{i=1}^{M^{(N-p)}} \left[\sigma_{i,t}^{(N-p)}(\tilde{\boldsymbol{z}}_{\mathbf{0},t}^{(N-p-1)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(N-p-1)}|\boldsymbol{z}_{\epsilon}^{(s-1)}),\boldsymbol{x}^{(N-p)}) \right] \\ &\leq M_{\text{prod}} C_{0}^{N-1} \sum_{p=j}^{N-s} \sum_{i=1}^{M^{(N-p)}} \left[\sigma_{i,t}^{(N-p)}(\tilde{\boldsymbol{z}}_{\mathbf{0},t}^{(N-p-1)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(N-p-1)}|\boldsymbol{z}_{\epsilon}^{(s-1)}),\boldsymbol{x}^{(N-p)}) \right] \\ &= M_{\text{prod}} C_{0}^{N-1} \sum_{p=j}^{N-s-1} \sum_{i=1}^{M^{(N-p)}} \left[\sigma_{i,t}^{(N-p)}(\tilde{\boldsymbol{z}}_{\mathbf{0},t}^{(N-p-1)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N-p-1)}|\boldsymbol{z}_{\epsilon}^{(s)}),\boldsymbol{x}^{(N-p)}) \right] \\ &+ M_{\text{prod}} C_{0}^{N-1} \sum_{p=j}^{N-s-1} \sum_{i=1}^{M^{(N-p)}} \left[\left(\sigma_{i,t}^{(N-p)}(\tilde{\boldsymbol{z}}_{\mathbf{0},t}^{(N-p-1)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(N-p-1)}|\boldsymbol{z}_{\epsilon}^{(s-1)}),\boldsymbol{x}^{(N-p)}) \right] \\ &- \sigma_{i,t}^{(N-p)}(\tilde{\boldsymbol{z}}_{\mathbf{0},t}^{(N-p-1)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N-p-1)}|\boldsymbol{z}_{\epsilon}^{(s)}),\boldsymbol{x}^{(N-p)}) \right) + M_{\text{prod}} C_{0}^{N-1} \sum_{i=1}^{M^{(s)}} \sigma_{i,t}^{(s)}(\boldsymbol{z}_{\epsilon}^{(s-1)},\boldsymbol{x}^{(s)}). \end{split}$$

Hence, from Lemma D.15, it follows that

$$\begin{split} &|\sigma_{i,t}^{(N-p)}(\tilde{\boldsymbol{z}}_{\mathbf{0},t}^{(N-p-1)}(\boldsymbol{x}^{(s:N-p-1)}|\boldsymbol{z}_{\epsilon}^{(s-1)}),\boldsymbol{x}^{(N-p)}) - \sigma_{i,t}^{(N-p)}(\tilde{\boldsymbol{z}}_{\mathbf{0},t}^{(N-p-1)}(\boldsymbol{x}^{(s+1:N-p-1)}|\boldsymbol{z}_{\epsilon}^{(s)}),\boldsymbol{x}^{(N-p)})|\\ &\leq 2M_{\mathrm{prod}}C_{0}^{N-1}\sum_{r=0}^{N-p-s-1}\sum_{j=1}^{M^{(N-p-1-r)}}\left[\sigma_{j,t}^{(N-p-1-r)}\left(\tilde{\boldsymbol{z}}_{\mathbf{0},t}^{(N-p-2-r)}(\boldsymbol{x}^{(s:N-p-2-r)}|\boldsymbol{z}_{\epsilon}^{(s-1)}),\boldsymbol{x}^{(N-p-1-r)}\right)\right]\\ &+ 2M_{\mathrm{prod}}C_{0}^{N-1}\sum_{q=1}^{M^{(s)}}|\epsilon_{q}^{(s)}|. \end{split}$$

Hence, using the same argument as in the proof of Lemma C.12, we have the desired result.

Lemma D.17. Assume that the same condition as in Theorem D.14 holds. Then, for any $s \in \{1, ..., N-1\}$, iteration $t \geq 1$, realization ϵ and input $x^{(1)}, ..., x^{(N)}$, the following holds with probability at least $1 - \delta$:

$$\begin{split} &\tilde{\sigma}_{\mathbf{0},1,t}^{(N)}(\boldsymbol{x}^{(s)},\dots,\boldsymbol{x}^{(N)}|\boldsymbol{z}_{\boldsymbol{\epsilon}}^{(s-1)}) \\ &\leq C_{3,t}\tilde{\sigma}_{\mathbf{0},1,t}^{(N)}(\boldsymbol{x}^{(s+1)},\dots,\boldsymbol{x}^{(N)}|\boldsymbol{z}_{\boldsymbol{\epsilon}}^{(s)}) + C_{3,t}\sum_{i=1}^{M^{(s)}}\sigma_{i,t}^{(s)}(\boldsymbol{z}_{\boldsymbol{\epsilon}}^{(s-1)},\boldsymbol{x}^{(s)}) + C_{3,t}\sum_{i=1}^{M^{(s)}}|\epsilon_{i}^{(s)}|. \end{split}$$

Proof. By repeating Lemma D.16, the following holds with probability at least $1 - \delta$:

$$\begin{split} &\tilde{\sigma}_{0,1,t}^{(N)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(N)}|\boldsymbol{z}_{\epsilon}^{(s-1)}) \\ &= \tilde{\sigma}_{0,t}^{(N-0)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(N-0)}|\boldsymbol{z}_{\epsilon}^{(s-1)}) \\ &\leq C_{2,t}\tilde{\sigma}_{0,t}^{(N-0)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N-0)}|\boldsymbol{z}_{\epsilon}^{(s)}) + C_{2,t}\sum_{i=1}^{M^{(s)}} \sigma_{i,t}^{(s)}(\boldsymbol{z}_{\epsilon}^{(s-1)},\boldsymbol{x}^{(s)}) + C_{2,t}\sum_{i=1}^{M^{(s)}} |\epsilon_{i}^{(s)}| \\ &+ C_{2,t}\tilde{\sigma}_{0,t}^{(N-1)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(N-1)}|\boldsymbol{z}_{\epsilon}^{(s-1)}) \\ &\leq C_{2,t}\tilde{\sigma}_{0,t}^{(N-0)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N-0)}|\boldsymbol{z}_{\epsilon}^{(s)}) + C_{2,t}\sum_{i=1}^{M^{(s)}} \sigma_{i,t}^{(s)}(\boldsymbol{z}_{\epsilon}^{(s-1)},\boldsymbol{x}^{(s)}) + C_{2,t}\sum_{i=1}^{M^{(s)}} |\epsilon_{i}^{(s)}| \\ &+ C_{2,t}^{2}\tilde{\sigma}_{0,t}^{(N-1)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N-1)}|\boldsymbol{z}_{\epsilon}^{(s)}) + C_{2,t}^{2}\sum_{i=1}^{M^{(s)}} \sigma_{i,t}^{(s)}(\boldsymbol{z}_{\epsilon}^{(s-1)},\boldsymbol{x}^{(s)}) + C_{2,t}^{2}\sum_{i=1}^{M^{(s)}} |\epsilon_{i}^{(s)}| \\ &+ C_{2,t}^{2}\tilde{\sigma}_{0,t}^{(N-2)}(\boldsymbol{x}^{(s)},\ldots,\boldsymbol{x}^{(N-2)}|\boldsymbol{z}_{\epsilon}^{(s-1)}) \\ &\leq \\ \vdots \\ &\leq (C_{2,t}+C_{2,t}^{2}+\cdots+C_{2,t}^{N})\tilde{\sigma}_{0,t}^{(N-0)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N-0)}|\boldsymbol{z}_{\epsilon}^{(s)}) \\ &+ (C_{2,t}+C_{2,t}^{2}+\cdots+C_{2,t}^{N})\sum_{i=1}^{M^{(s)}} \sigma_{i,t}^{(s)}(\boldsymbol{z}_{\epsilon}^{(s-1)},\boldsymbol{x}^{(s)}) + (C_{2,t}+C_{2,t}^{2}+\cdots+C_{2,t}^{N})\sum_{i=1}^{M^{(s)}} |\epsilon_{i}^{(s)}| \\ &\leq NC_{2,t}^{N}\tilde{\sigma}_{0,1,t}^{(N)}(\boldsymbol{x}^{(s+1)},\ldots,\boldsymbol{x}^{(N)}|\boldsymbol{z}_{\epsilon}^{(s)}) + NC_{2,t}^{N}\sum_{i=1}^{M^{(s)}} \sigma_{i,t}^{(s)}(\boldsymbol{z}_{\epsilon}^{(s-1)},\boldsymbol{x}^{(s)}) + NC_{2,t}^{N}\sum_{i=1}^{M^{(s)}} |\epsilon_{i}^{(s)}|. \end{split}$$

Lemma D.18. Assume that the same condition as in Theorem D.14 holds. Then, for any $n \in [N]$, iteration $t \ge 1$, $y^{(n-1)} \in \tilde{\mathcal{Y}}^{(n-1)}$ and input $x^{(n)} \in \mathcal{X}^{(n)}$, the following holds:

$$\eta_t \hat{b}_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) \leq \hat{c}_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)}) \leq (2\beta_t^{1/2} + \eta_t)\hat{b}_t^{(n)}(\boldsymbol{x}^{(n)}|\boldsymbol{y}^{(n-1)})$$

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Proof. By using the same argument as in the proof of Lemma C.14, we get Lemma D.18.

Using these lemmas we prove Theorem D.14.

Proof. Let $t \in N\mathbb{Z}_{\geq 0}$. Then, from Lemma D.18, $\boldsymbol{x}_{t+1}^{(1)}$ satisfies that

$$\hat{c}_{t}^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0}) \leq (2\beta_{t}^{1/2} + \eta_{t})\hat{b}_{t}^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0}) = (2\beta_{t}^{1/2} + \eta_{t})\tilde{\sigma}_{\boldsymbol{0},1,t}^{(N)}(\boldsymbol{x}_{t+1}^{(1)}, \tilde{\boldsymbol{x}}^{(2)}, \dots, \tilde{\boldsymbol{x}}^{(N)}|\boldsymbol{0}). \tag{D.18}$$

In addition, from (D.18) and Lemma D.17, using the same argument as in the proof of Theorem C.10, with probability at least $1 - \delta$, $\hat{c}_t^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0})$ can be bounded as follows:

$$\hat{c}_{t}^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0}) \leq (2\beta_{t}^{1/2} + \eta_{t})C_{3,t} \sum_{i=1}^{M^{(1)}} \sigma_{\boldsymbol{0},i,t}^{(1)}(\boldsymbol{0},\boldsymbol{x}_{t+1}^{(1)}) + (2\beta_{t}^{1/2} + \eta_{t})C_{3,t} \sum_{i=1}^{M^{(1)}} |\epsilon_{i}^{(1)}|$$

$$+ (2\beta_{t}^{1/2} + \eta_{t})C_{3,t} \tilde{\sigma}_{\boldsymbol{0},1,t}^{(N)}(\tilde{\boldsymbol{x}}^{(2)}, \dots, \tilde{\boldsymbol{x}}^{(N)}|\boldsymbol{y}_{t+1}^{(1)})$$

$$\leq (2\beta_{t}^{1/2} + \eta_{t})C_{3,t} \sum_{i=1}^{M^{(1)}} \sigma_{\boldsymbol{0},i,t}^{(1)}(\boldsymbol{0},\boldsymbol{x}_{t+1}^{(1)}) + (2\beta_{t}^{1/2} + \eta_{t})C_{3,t} \sum_{i=1}^{M^{(1)}} |\epsilon_{i}^{(1)}|$$

$$+ (2\beta_{t}^{1/2} + \eta_{t})^{2}C_{3,t}\eta_{t}^{-1}\tilde{\sigma}_{\boldsymbol{0},1,t}^{(N)}(\boldsymbol{x}_{t+2}^{(2)}, \dots, \tilde{\boldsymbol{x}}^{(N)}|\boldsymbol{y}_{t+1}^{(1)}).$$

By using Lemma D.17 again, it follows that

$$\hat{c}_{t}^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0}) \leq (2\beta_{t}^{1/2} + \eta_{t} + 1)^{N} C_{3,t}^{N} \eta_{t}^{-N} \sum_{n=1}^{N} \sum_{i=1}^{M^{(n)}} \sigma_{\boldsymbol{0},i,t}^{(n)}(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}_{t+n}^{(n)})$$

$$+ (2\beta_{t}^{1/2} + \eta_{t} + 1)^{N} C_{3,t}^{N} \eta_{t}^{-N} \sum_{n=1}^{N} \sum_{i=1}^{M^{(n)}} |\epsilon_{i}^{(n)}|$$

$$\leq (2\beta_{t}^{1/2} + 1 + 1)^{N} C_{3,t}^{N} \eta_{t}^{-N} \sum_{n=1}^{N} \sum_{i=1}^{M^{(n)}} \sigma_{\boldsymbol{0},i,t}^{(n)}(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}_{t+n}^{(n)})$$

$$+ (2\beta_{t}^{1/2} + 1 + 1)^{N} C_{3,t}^{N} \eta_{t}^{-N} \sum_{n=1}^{N} \sum_{i=1}^{M^{(n)}} |\epsilon_{i}^{(n)}|.$$

Thus, multiplying both sides by $2\beta_t^{1/2}\eta_t^{-1}$, we get

$$2\beta_{t}^{1/2}\eta_{t}^{-1}\hat{c}_{t}^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0}) \leq 2\beta_{t}^{1/2}\eta_{t}^{-1}(2\beta_{t}^{1/2}+2)^{N}C_{3,t}^{N}\eta_{t}^{-N}\sum_{n=1}^{N}\sum_{i=1}^{M^{(n)}}\sigma_{\mathbf{0},i,t}^{(n)}(\boldsymbol{y}^{(n-1)},\boldsymbol{x}_{t+n}^{(n)})$$

$$+2\beta_{t}^{1/2}\eta_{t}^{-1}(2\beta_{t}^{1/2}+2)^{N}C_{3,t}^{N}\eta_{t}^{-N}\sum_{n=1}^{N}\sum_{i=1}^{M^{(n)}}|\epsilon_{i}^{(n)}|$$

$$=C_{9,t}\sum_{n=1}^{N}\sum_{i=1}^{M^{(n)}}\sigma_{\mathbf{0},i,t}^{(n)}(\boldsymbol{y}^{(n-1)},\boldsymbol{x}_{t+n}^{(n)})+C_{9,t}\sum_{n=1}^{N}\sum_{i=1}^{M^{(n)}}|\epsilon_{i}^{(n)}|.$$

Here, using $(a+b)^2 \le 2a^2 + 2b^2$ and the Cauchy–Schwarz inequality, we obtain

$$(2\beta_t^{1/2}\eta_t^{-1}\hat{c}_t^{(1)}(\boldsymbol{x}_{t+1}^{(1)}|\boldsymbol{0}))^2 \leq 2C_{9,t}^2M_{\text{sum}}\sum_{n=1}^N\sum_{i=1}^{M^{(n)}}\sigma_{\boldsymbol{0},i,t}^{(n)2}(\boldsymbol{y}^{(n-1)},\boldsymbol{x}_{t+n}^{(n)}) + 2C_{9,t}^2M_{\text{sum}}\epsilon_{\text{sum}}.$$

Next, we show the existence of the sequence $T_0 < T_1 < \cdots$ satisfying

$$\mathbb{P}(\exists t \in N\mathbb{Z}_{\geq 0} \text{ s.t. } T_{k-1} \leq t \leq T_k, \ 2C_{9,t}^2 M_{\text{sum}} \epsilon_{\text{sum},t} < \xi^2/2) > 1 - \frac{6\delta}{\pi^2 k^2}.$$

From Assumption D.12, we have

$$\mathbb{P}(2C_{9,t}^2 M_{\text{sum}} \epsilon_{\text{sum},t} < \xi^2/2) = \mathbb{P}(\epsilon_{\text{sum},t} < M_{\text{sum}}^{-1} C_{9,t}^{-2} \xi^2/4) > \frac{C\xi^2}{4M_{\text{sum}} C_{9,t}^2}$$

This implies that

$$1 - \mathbb{P}(2C_{9,t}^2 M_{\text{sum}} \epsilon_{\text{sum},t} < \xi^2/2) \le 1 - \frac{C\xi^2}{4M_{\text{sum}}C_{9,t}^2}.$$

Therefore, using $1 + x \le e^x$ we get

$$\prod_{q=t}^{t'} (1 - \mathbb{P}(2C_{9,q}^2 M_{\text{sum}} \epsilon_{\text{sum},q} < \xi^2/2)) \leq \prod_{q=t}^{t'} \left(1 - \frac{C\xi^2}{4M_{\text{sum}}C_{9,q}^2} \right) \\
\leq \prod_{q=t}^{t'} \exp\left(-\frac{C\xi^2}{4M_{\text{sum}}C_{9,q}^2} \right) \\
= \exp\left(-\frac{C\xi^2}{4M_{\text{sum}}} \sum_{q=t}^{t'} C_{9,q}^{-2} \right). \tag{D.19}$$

Moreover, from Assumption D.13, the right hand side of (D.19) tends to zero when $t' \to \infty$. Thus, we can construct the sequence T_1, T_2, \ldots satisfying (D.17). Then, with probability at least $1 - \delta$, the following holds:

$$\forall k \in \mathbb{N}, \ \exists \tilde{T}_k \quad \text{s.t.} \quad T_{k-1} \leq \tilde{T}_k \leq T_k, \ 2C_{9,\tilde{T}_k}^2 M_{\text{sum}} \epsilon_{\text{sum},\tilde{T}_k} < \xi^2/2.$$

On the other hand, for the positive number K satisfying the theorem's inequality, we define

$$\hat{T} = \operatorname*{arg\,min}_{1 \leq k \leq K} (2\beta_{\tilde{T}_k}^{1/2} \eta_{\tilde{T}_k}^{-1} \hat{c}_{\tilde{T}_k}^{(1)} (\boldsymbol{x}_{\tilde{T}_k+1}^{(1)} | \boldsymbol{0}))^2.$$

Then, it follows that

$$\begin{split} K(2\beta_{\hat{T}}^{1/2}\eta_{\hat{T}}^{-1}\hat{c}_{\hat{T}}^{(1)}(\boldsymbol{x}_{\hat{T}+1}^{(1)}|\boldsymbol{0}))^{2} &\leq \sum_{k=1}^{K}(2\beta_{\tilde{T}_{k}}^{1/2}\eta_{\tilde{T}_{k}}^{-1}\hat{c}_{\tilde{T}_{k}}^{(1)}(\boldsymbol{x}_{\tilde{T}_{k}+1}^{(1)}|\boldsymbol{0}))^{2} \\ &\leq K\xi^{2}/2 + 2C_{9,T_{K}}^{2}M_{\text{sum}}\sum_{t=1}^{T_{K}}\sum_{n=1}^{N}\sum_{i=1}^{M^{(n)}}\sigma_{\boldsymbol{0},i,t}^{(n)2}(\boldsymbol{y}^{(n-1)},\boldsymbol{x}_{t+n}^{(n)}) \\ &\leq K\xi^{2}/2 + \frac{4C_{9,T_{K}}^{2}M_{\text{sum}}^{2}}{\log(1+\sigma^{-2})}\tilde{\gamma}_{T_{K}}. \end{split}$$

By dividing both sides by K, we obtain

$$(2\beta_{\hat{T}}^{1/2}\eta_{\hat{T}}^{-1}\hat{c}_{\hat{T}}^{(1)}(\boldsymbol{x}_{\hat{T}+1}^{(1)}|\boldsymbol{0}))^{2} \leq \xi^{2}/2 + \frac{4C_{9,T_{K}}^{2}M_{\text{sum}}^{2}}{\log(1+\sigma^{-2})}\tilde{\gamma}_{T_{K}}K^{-1}$$
$$< \xi^{2}/2 + \xi^{2}/2 = \xi^{2}.$$

This implies that

$$2\beta_{\hat{T}}^{1/2}\eta_{\hat{T}}^{-1}\hat{c}_{\hat{T}}^{(1)}(\boldsymbol{x}_{\hat{T}+1}^{(1)}|\mathbf{0}) < \xi. \tag{D.20}$$

Finally, from the definition of the estimated solution and CIs, $F(\cdot)$ can be bounded as follows:

$$\begin{split} F(\boldsymbol{x}_{F,*}^{(1)}, \dots, \boldsymbol{x}_{F,*}^{(N)}) &\leq \min_{t \in N\mathbb{Z}_{\geq 0}, t \leq T_K} \widehat{\mathrm{UCB}}_t^{(F)}(\boldsymbol{x}_{F,*}^{(1)}, \dots, \boldsymbol{x}_{F,*}^{(N)}) \\ &\leq \widehat{\mathrm{UCB}}_{\hat{T}}^{(F)}(\boldsymbol{x}_{F,*}^{(1)}, \dots, \boldsymbol{x}_{F,*}^{(N)}), \\ F(\hat{\boldsymbol{x}}_{F,T_K}^{(1)}, \dots, \hat{\boldsymbol{x}}_{F,T_K}^{(N)}) &\geq \max_{t \in N\mathbb{Z}_{\geq 0}, t \leq T_K} \widehat{\mathrm{LCB}}_t^{(F)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(N)}) \\ &\geq \widehat{\mathrm{LCB}}_{\hat{T}}^{(F)}(\boldsymbol{x}_{F,*}^{(1)}, \dots, \boldsymbol{x}_{F,*}^{(N)}). \end{split}$$

Therefore, the following holds with probability at least $1-2\delta$:

$$F(\boldsymbol{x}_{F,*}^{(1)}, \dots, \boldsymbol{x}_{F,*}^{(N)}) - F(\hat{\boldsymbol{x}}_{F,T_{K}}^{(1)}, \dots, \hat{\boldsymbol{x}}_{F,T_{K}}^{(N)}) \leq 2\beta_{\hat{T}}^{1/2} \tilde{\sigma}_{\mathbf{0},1,\hat{T}}^{(N)}(\boldsymbol{x}_{F,*}^{(1)}, \dots, \boldsymbol{x}_{F,*}^{(N)})$$

$$\leq 2\beta_{\hat{T}}^{1/2} \hat{b}_{\hat{T}}^{(1)}(\boldsymbol{x}_{F,*}^{(1)}|\mathbf{0})$$

$$\leq 2\beta_{\hat{T}}^{1/2} \eta_{\hat{T}}^{-1} \hat{c}_{\hat{T}}^{(1)}(\boldsymbol{x}_{F,*}^{(1)}|\mathbf{0}) \leq 2\beta_{\hat{T}}^{1/2} \eta_{\hat{T}}^{-1} \hat{c}_{\hat{T}}^{(1)}(\boldsymbol{x}_{\hat{T}+1}^{(1)}|\mathbf{0}). \tag{D.21}$$

Hence, by substituting (D.20) into (D.21), we have Theorem D.14.

E Sufficient Conditions and Modifications for the Proposed Method

In this section, we consider theorem's conditions and its modifications. First, in the noiseless setting, we assume that $\tilde{\mu}_t^{(m)}(x^{(n)},\ldots,x^{(m)}|y^{(n-1)})\in\mathcal{Y}^{(m)}$ to construct the valid CI . For this assumption, the following sufficient condition exists.

Theorem E.1. Assume that each $\mathcal{X}^{(n)}$ is a compact set, and each observation is noiseless. Also assume that each $f_m^{(n)}$ is a function defined on $[-2B_{n-1}, 2B_{n-1}]^{M^{(n-1)}} \times \mathcal{X}^{(n)}$ and satisfies $f_m^{(n)} \in \mathcal{H}_{k^{(n)}}$, where B_n is some positive constant satisfying $\|f_m^{(n)}\|_{\mathcal{H}_{k^{(n)}}} \leq B_n$ and $B_0 = 0$. Then, $\tilde{\boldsymbol{\mu}}_t^{(n)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n)}) \in [-2B_n, 2B_n]^{M^{(n)}}$ for any $n \in [N]$, t > 1 and $\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n)}$.

Proof. From the reproducing property of $k^{(n)}$, noting that $k^{(n)}(\boldsymbol{a}, \boldsymbol{a}) \leq 1$ we have

$$|f_m^{(1)}(\boldsymbol{a})| = |\langle f_m^{(1)}(\cdot), k^{(1)}(\cdot, \boldsymbol{a}) \rangle_{\mathcal{H}_{k(1)}}|$$

$$\leq ||f_m^{(1)}||_{\mathcal{H}_{k(1)}} k^{(1)}(\boldsymbol{a}, \boldsymbol{a})^{1/2} \leq B_1.$$

In addition, since $\mathcal{X}^{(1)}$ is the compact set, $[-2B_0,2B_0]^{M^{(0)}} \times \mathcal{X}^{(1)}$ is also the compact set. Hence, from Lemma C.2 the following holds for any $m \in [M^{(1)}]$, $t \geq 1$ and $(\boldsymbol{w}, \boldsymbol{x}) \in [-2B_0, 2B_0]^{M^{(0)}} \times \mathcal{X}^{(1)}$:

$$|\mu_{m,t}^{(1)}(\boldsymbol{w},\boldsymbol{x})| = |\mu_{m,t}^{(1)}(\boldsymbol{w},\boldsymbol{x}) - f_m^{(n)}(\boldsymbol{w},\boldsymbol{x}) + f_m^{(n)}(\boldsymbol{w},\boldsymbol{x})|$$

$$\leq |\mu_{m,t}^{(1)}(\boldsymbol{w},\boldsymbol{x}) - f_m^{(n)}(\boldsymbol{w},\boldsymbol{x})| + |f_m^{(n)}(\boldsymbol{w},\boldsymbol{x})|$$

$$\leq B_1 + B_1 = 2B_1.$$

This implies that $\mu_t^{(1)}(\mathbf{0}, \mathbf{x}^{(1)}) = \tilde{\mu}_t^{(1)}(\mathbf{x}^{(1)}) \in [-2B_1, 2B_1]^{M^{(1)}}$. By repeating this process, we get

$$\boldsymbol{\mu}_t^{(n)}(\tilde{\boldsymbol{\mu}}_t^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) = \tilde{\boldsymbol{\mu}}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}) \in [-2B_n,2B_n]^{M^{(n)}}.$$

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Theorem E.1 implies that by defining $\mathcal{Y}^{(n)}$ as $[-2B_n, 2B_n]^{M^{(n)}}$ and $B = \max_{1 \leq n \leq N} B_n$, we obtain Assumption C.1 and $\tilde{\mu}_t^{(n)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n)}) \in \mathcal{Y}^{(n)}$. Similarly, under the same assumption we have $\tilde{\mu}_t^{(m)}(\boldsymbol{x}^{(n)}, \dots, \boldsymbol{x}^{(m)}|\boldsymbol{y}^{(n-1)}) \in \mathcal{Y}^{(m)}$.

Next, we consider the condition $\tilde{\boldsymbol{z}}_{\epsilon,t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)})\in\tilde{\mathcal{Y}}^{(n)}$ for the noisy observation setting. In the noisy setting, it is not easy to give a sufficient condition for this condition to be satisfied. Nevertheless, we can avoid this condition by modifying the definition of $\tilde{\boldsymbol{z}}_{\epsilon,t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)})$. Let $\mathcal{L}=[-L,L]^d$ be a d-dimensional hypercube. For each $\boldsymbol{a}=(a_1,\ldots,a_d)\in\mathbb{R}^d$, suppose that $\mathcal{P}(\mathcal{M},\boldsymbol{a})$ is a projection of \boldsymbol{a} onto \mathcal{M} , where the i-th element of $\mathcal{P}(\mathcal{M},\boldsymbol{a})$, $\mathcal{P}_i(\mathcal{M},\boldsymbol{a})$, is given by

$$\mathcal{P}_i(\mathcal{M}, \boldsymbol{a}) = \underset{l \in [-L, L]}{\operatorname{arg \, min}} |a_i - l|.$$

Then, the following theorem holds.

Theorem E.2. Assume that each $\mathcal{X}^{(n)}$ is a compact set, and each observation noise $\epsilon_m^{(n)}$ is a zero mean random variable with $-A \leq \epsilon_m^{(n)} \leq A$. Also assume that each $f_m^{(n)}$ is a function defined on $[-A_{n-1} - B_{n-1}, A_{n-1} + B_{n-1}]^{M^{(n-1)}} \times \mathcal{X}^{(n)}$ and satisfies $f_m^{(n)} \in \mathcal{H}_{k^{(n)}}$, where $A_0 = B_0 = 0$, $A_n = A$ and B_n is some positive constant satisfying $||f_m^{(n)}||_{\mathcal{H}_{k^{(n)}}} \leq B_n$. For each $t \geq 1$ and $(\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)})$, define

$$\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}) = \begin{cases} \boldsymbol{\epsilon}^{(1)} + \mathcal{P}(\mathcal{Y}^{(1)},\boldsymbol{\mu}_t^{(1)}(\boldsymbol{0},\boldsymbol{x}^{(1)})) & (n=1), \\ \boldsymbol{\epsilon}^{(n)} + \mathcal{P}(\mathcal{Y}^{(n)},\boldsymbol{\mu}_t^{(n)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n-1)}(\boldsymbol{x}^{(1:n-1)}),\boldsymbol{x}^{(n)})) & (n \geq 2), \end{cases}$$

where $\mathcal{Y}^{(n)} = [-B_n, B_n]^{M^{(n)}}$. Then, $\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon}, t}^{(n)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n)}) \in [-A_n - B_n, A_n + B_n]^{M^{(n)}} = \tilde{\mathcal{Y}}^{(n)}$ for all $n \in [N]$, $t \geq 1$, $\boldsymbol{\epsilon}$ and $(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n)})$. Moreover, $\boldsymbol{f}^{(n)}$ satisfies $\boldsymbol{f}^{(n)}(\boldsymbol{w}, \boldsymbol{x}) + \boldsymbol{\epsilon}^{(n)} \in \tilde{\mathcal{Y}}^{(n)}$ for all $\boldsymbol{w} \in \tilde{\mathcal{Y}}^{(n-1)}$, $\boldsymbol{x} \in \mathcal{X}^{(n)}$ and $\boldsymbol{\epsilon}^{(n)}$.

Proof. From the reproducing property of $k^{(n)}(\cdot,\cdot)$, and the assumptions $k^{(n)}(\cdot,\cdot) \leq 1$ and $||f_m^{(n)}||_{\mathcal{H}_{k^{(n)}}} \leq B_n$, we have $f_m^{(n)}(\boldsymbol{w},\boldsymbol{x}) \in [-B_n,B_n]$. Therefore, noting that $-A \leq \epsilon_m^{(n)} \leq A$, we get $\boldsymbol{f}^{(n)}$ satisfies $\boldsymbol{f}^{(n)}(\boldsymbol{w},\boldsymbol{x}) + \boldsymbol{\epsilon}^{(n)} \in \tilde{\mathcal{Y}}^{(n)}$. Similarly, from the definition of $\mathcal{P}(\mathcal{Y}^{(n)},\boldsymbol{a})$, it follows that

$$\mathcal{P}(\mathcal{Y}^{(n)}, \boldsymbol{\mu}_t^{(n)}(\hat{\boldsymbol{z}}_{\epsilon,t}^{(n-1)}(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n-1)}), \boldsymbol{x}^{(n)})) \in \mathcal{Y}^{(n)} = [-B_n, B_n]^{M^{(n)}}.$$

Thus, we obtain $\hat{m{z}}_{m{\epsilon},t}^{(n)}(m{x}^{(1)},\ldots,m{x}^{(n)})\in \mathcal{Y}^{(n)}.$

In this modified $\hat{z}_{\epsilon,t}^{(n)}(x^{(1)},\ldots,x^{(n)})$, similar results given in Theorem D.4 hold.

Theorem E.3. Assume that the same condition as in Theorem E.2 holds. Given $\delta \in (0,1)$, define $B = \max_{1 \le n \le N} B_n$ and β_t as in (D.2). Moreover, assume that Assumptions C.3 and C.4 hold. Then, with probability at least $1 - \delta$, the following holds for any realization of ϵ :

$$|z_{\epsilon,m}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}) - \hat{z}_{\epsilon,m,t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)})| \leq \beta_t^{1/2} \hat{\sigma}_{\epsilon,m,t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)})$$

$$\forall n \in [N], m \in [M^{(n)}], t \geq 1,$$

where $\hat{z}^{(n)}_{\epsilon,m,t}$ is the m-th element of $\hat{z}^{(n)}_{\epsilon,t}$, and $\hat{\sigma}^{(n)}_{\epsilon,m,t}(x^{(1)},\dots,x^{(n)})$ is given by

$$\hat{\sigma}^{(n)}_{\boldsymbol{\epsilon},m,t}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)}) =$$

$$\sigma_{m,t}^{(n)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) + L_f \sum_{s=1}^{M^{(n-1)}} \hat{\sigma}_{\boldsymbol{\epsilon},s,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),$$

and
$$\hat{\sigma}_{\epsilon,s,t}^{(1)}(x^{(1)}) = \sigma_{s,t}^{(1)}(\mathbf{0}, x^{(1)}).$$

Proof. For any $t \ge 1$, $n \in [N]$, $m \in [M^{(n)}]$, $\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n)}$ and realization of $\boldsymbol{\epsilon}$, it follows that

$$\begin{split} &|f_m^{(n)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) - \boldsymbol{\mu}_{m,t}^{(n)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)})| \\ &= |f_m^{(n)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) - \mathcal{P}_m(\mathcal{Y}^{(n)},\boldsymbol{\mu}_t^{(n)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}))| \\ &+ |\mathcal{P}_m(\mathcal{Y}^{(n)},\boldsymbol{\mu}_t^{(n)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)})) - \boldsymbol{\mu}_{m,t}^{(n)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)})| \\ &\geq |f_m^{(n)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}) - \mathcal{P}_m(\mathcal{Y}^{(n)},\boldsymbol{\mu}_t^{(n)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)}))|, \end{split}$$

where the first equality is derived by $f_m^{(n)}(\hat{\boldsymbol{z}}_{\epsilon,t}^{(n-1)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}),\boldsymbol{x}^{(n)})\in\mathcal{Y}^{(n)}$ and the definition of $\mathcal{P}(\mathcal{Y}^{(n)},\boldsymbol{a})$. Thus, for $i\in[M^{(2)}]$ and $(\boldsymbol{x}^{(1)},\boldsymbol{x}^{(2)})$, the following inequality holds with probability at least $1-\delta$:

$$\begin{split} &|z_{\boldsymbol{\epsilon},i}^{(2)}(\boldsymbol{x}^{(1)},\boldsymbol{x}^{(2)}) - \hat{z}_{\boldsymbol{\epsilon},i,t}^{(2)}(\boldsymbol{x}^{(1)},\boldsymbol{x}^{(2)})| \\ &\leq |f_{i}^{(2)}(\boldsymbol{z}_{\boldsymbol{\epsilon}}^{(1)}(\boldsymbol{x}^{(1)}),\boldsymbol{x}^{(2)}) - f_{i}^{(2)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(1)}(\boldsymbol{x}^{(1)}),\boldsymbol{x}^{(2)})| \\ &+ |f_{i}^{(2)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(1)}(\boldsymbol{x}^{(1)}),\boldsymbol{x}^{(2)}) - \mathcal{P}_{i}(\mathcal{Y}^{(2)},\boldsymbol{\mu}_{t}^{(2)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(1)}(\boldsymbol{x}^{(1)}),\boldsymbol{x}^{(2)}))| \\ &\leq L_{f}\|\boldsymbol{f}^{(1)}(\boldsymbol{0},\boldsymbol{x}^{(1)}) - \mathcal{P}(\mathcal{Y}^{(1)},\boldsymbol{\mu}_{t}^{(1)}(\boldsymbol{0},\boldsymbol{x}^{(1)}))\|_{1} \\ &+ |f_{i}^{(2)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(1)}(\boldsymbol{x}^{(1)}),\boldsymbol{x}^{(2)}) - \mathcal{P}_{i}(\mathcal{Y}^{(2)},\boldsymbol{\mu}_{t}^{(2)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(1)}(\boldsymbol{x}^{(1)}),\boldsymbol{x}^{(2)}))| \\ &\leq L_{f}\sum_{j=1}^{M^{(1)}}|f_{j}^{(1)}(\boldsymbol{0},\boldsymbol{x}^{(1)}) - \mathcal{P}_{j}(\mathcal{Y}^{(1)},\boldsymbol{\mu}_{t}^{(1)}(\boldsymbol{0},\boldsymbol{x}^{(1)}))| \\ &+ |f_{i}^{(2)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(1)}(\boldsymbol{x}^{(1)}),\boldsymbol{x}^{(2)}) - \mathcal{P}_{i}(\mathcal{Y}^{(2)},\boldsymbol{\mu}_{t}^{(2)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(1)}(\boldsymbol{x}^{(1)}),\boldsymbol{x}^{(2)}))| \\ &\leq L_{f}\sum_{j=1}^{M^{(1)}}|f_{j}^{(1)}(\boldsymbol{0},\boldsymbol{x}^{(1)}) - \mu_{j,t}^{(1)}(\boldsymbol{0},\boldsymbol{x}^{(1)})| \\ &+ |f_{i}^{(2)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(1)}(\boldsymbol{x}^{(1)}),\boldsymbol{x}^{(2)}) - \mu_{i,t}^{(2)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(1)}(\boldsymbol{x}^{(1)}),\boldsymbol{x}^{(2)})| \\ &\leq \beta_{t}^{1/2}\sigma_{i,t}^{(2)}(\hat{\boldsymbol{z}}_{\boldsymbol{\epsilon},t}^{(1)}(\boldsymbol{x}^{(1)}),\boldsymbol{x}^{(2)}) + L_{f}\beta_{t}^{1/2}\sum_{j=1}^{M^{(1)}}\sigma_{j,t}^{(1)}(\boldsymbol{0},\boldsymbol{x}^{(1)}) \\ &= \beta_{t}^{1/2}\hat{\sigma}_{\boldsymbol{\epsilon},i,t}^{(2)}(\boldsymbol{x}^{(1)},\boldsymbol{x}^{(2)}). \end{split}$$

Therefore, by repeating this process up to n, we get the desired inequality.

We emphasize that by using the same technique as used in this proof, it can also be shown that Theorems D.6, D.9 and D.14 hold when using $\hat{\boldsymbol{z}}_{\epsilon,t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)})$ instead of $\tilde{\boldsymbol{z}}_{\epsilon,t}^{(n)}(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)})$.

Finally, we provide the sufficient condition for the Lipschitz continuity assumption (L2).

Theorem E.4. Let $k(x, y) : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ be one of the following kernel functions:

Linear kernel: $k(x, y) = a^2 x^{\top} y$, where a is a positive parameter.

Gaussian kernel: $k(x, y) = a^2 \exp(-\|x - y\|^2/(2\rho^2))$, where a and ρ are positive parameters.

Matérn kernel:

$$k(\boldsymbol{x}, \boldsymbol{y}) = a^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu} \frac{\|\boldsymbol{x} - \boldsymbol{y}\|}{\rho} \right)^{\nu} K_{\nu} \left(\sqrt{2\nu} \frac{\|\boldsymbol{x} - \boldsymbol{y}\|}{\rho} \right),$$

where a and ρ are positive parameters, ν is a degree of freedom with $\nu > 1$, Γ is the gamma function, and K_{ν} is the modified Bessel function of the second kind.

Moreover, assume that a user-specified variance parameter σ^2 is positive. Then, for any $t \geq 1$ and observed points x_1, \ldots, x_t , the posterior standard deviation $\sigma_t(x)$ satisfies that

$$\forall \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d, |\sigma_t(\boldsymbol{x}) - \sigma_t(\boldsymbol{y})| \le C \|\boldsymbol{x} - \boldsymbol{y}\|_1,$$
(E.1)

where C is a positive constant given by

$$C = \left\{ \begin{array}{ll} a & \text{if } k(\boldsymbol{x}, \boldsymbol{y}) \text{ is the linear kernel}, \\ \frac{\sqrt{2}a}{\rho} & \text{if } k(\boldsymbol{x}, \boldsymbol{y}) \text{ is the Gaussian kernel}, \\ \frac{\sqrt{2}a}{\rho} \sqrt{\frac{\nu}{\nu-1}} & \text{if } k(\boldsymbol{x}, \boldsymbol{y}) \text{ is the Matérn kernel}. \end{array} \right.$$

Proof. First, we show the case of the linear kernel. Let the matrix X_t be $X_t = (x_1, \dots, x_t)^{\top}$. Then, $\sigma_t^2(x)$ is given by

$$\begin{split} \sigma_t^2(\boldsymbol{x}) &= a^2 \boldsymbol{x}^\top \boldsymbol{x} - a^4 \boldsymbol{x}^\top \boldsymbol{X}_t^\top (a^2 \boldsymbol{X}_t \boldsymbol{X}_t^\top + \sigma^2 \boldsymbol{I}_t)^{-1} \boldsymbol{X}_t \boldsymbol{x} \\ &= a^2 \boldsymbol{x}^\top \boldsymbol{x} - a^2 \boldsymbol{x}^\top \boldsymbol{X}_t^\top (\boldsymbol{X}_t \boldsymbol{X}_t^\top + a^{-2} \sigma^2 \boldsymbol{I}_t)^{-1} \boldsymbol{X}_t \boldsymbol{x} \\ &= a^2 \boldsymbol{x}^\top (\boldsymbol{I}_d - \boldsymbol{X}_t^\top (\boldsymbol{X}_t \boldsymbol{X}_t^\top + a^{-2} \sigma^2 \boldsymbol{I}_t)^{-1} \boldsymbol{X}_t) \boldsymbol{x}. \end{split}$$

The matrix X_t can be decomposed as

$$X_t = H' \Lambda H^{\top}$$
,

where $\boldsymbol{H}' = (\boldsymbol{h}_1', \dots, \boldsymbol{h}_t')^{\top}$ and $\boldsymbol{H} = (\boldsymbol{h}_1, \dots, \boldsymbol{h}_d)^{\top}$ are orthogonal matrices, and $\boldsymbol{\Lambda}$ is the $t \times d$ rectangular diagonal matrix whose (j,j) element is the jth singular value $s_j \geq 0$ of \boldsymbol{X}_t . Thus, $\boldsymbol{I}_d - \boldsymbol{X}_t^{\top} (\boldsymbol{X}_t \boldsymbol{X}_t^{\top} + a^{-2} \sigma^2 \boldsymbol{I}_t)^{-1} \boldsymbol{X}_t$ can be rewritten as follows:

$$I_d - X_t^{\top} (X_t X_t^{\top} + a^{-2} \sigma^2 I_t)^{-1} X_t = H \Theta H^{\top},$$

where Θ is the diagonal matrix whose (j,j) element is $1 - s_j^2/(s_j^2 + a^{-2}\sigma^2)$. Thus, the posterior standard deviation $\sigma_t(\boldsymbol{x})$ can be expressed as

$$\sigma_t(\boldsymbol{x}) = \sqrt{a^2 \boldsymbol{x}^\top \boldsymbol{H} \boldsymbol{\Theta} \boldsymbol{H}^\top \boldsymbol{x}} = a \| \boldsymbol{\Theta}^{1/2} \boldsymbol{H}^\top \boldsymbol{x} \|.$$

Hence, using the triangle inequality we have

$$|\sigma_t(\boldsymbol{x}) - \sigma_t(\boldsymbol{y})| = a|\|\boldsymbol{\Theta}^{1/2}\boldsymbol{H}^{\top}\boldsymbol{x}\| - \|\boldsymbol{\Theta}^{1/2}\boldsymbol{H}^{\top}\boldsymbol{y}\||$$

$$\leq a\|\boldsymbol{\Theta}^{1/2}\boldsymbol{H}^{\top}\boldsymbol{x} - \boldsymbol{\Theta}^{1/2}\boldsymbol{H}^{\top}\boldsymbol{y}\|$$

$$= a\|\boldsymbol{\Theta}^{1/2}\boldsymbol{H}^{\top}(\boldsymbol{x} - \boldsymbol{y})\|.$$
(E.2)

Noting that the diagonal element θ_j of Θ satisfies $0 \le \theta_j \le 1$, from $\|x - y\| \le \|x - y\|_1$ we get

$$\|\mathbf{\Theta}^{1/2} \boldsymbol{H}^{\top} (\boldsymbol{x} - \boldsymbol{y})\| = \sqrt{(\boldsymbol{x} - \boldsymbol{y})^{\top} \boldsymbol{H} \boldsymbol{\Theta} \boldsymbol{H}^{\top} (\boldsymbol{x} - \boldsymbol{y})}$$

$$\leq \sqrt{(\boldsymbol{x} - \boldsymbol{y})^{\top} \boldsymbol{H} \boldsymbol{I}_{d} \boldsymbol{H}^{\top} (\boldsymbol{x} - \boldsymbol{y})} = \|\boldsymbol{x} - \boldsymbol{y}\| \leq \|\boldsymbol{x} - \boldsymbol{y}\|_{1}. \tag{E.3}$$

Therefore, by substituting (E.3) into (E.2), we have the desired result.

Next, we show the case of the Gaussian kernel. From Bochner's theorem, the Gaussian kernel can be rewritten as follows (see, e.g., section 4.2.1 in (Rasmussen and Williams, 2005)):

$$k(\boldsymbol{x}, \boldsymbol{y}) = a^2 \int_{\mathbb{R}^d} e^{2\pi \mathrm{i}(\boldsymbol{x} - \boldsymbol{y})^{\top} \boldsymbol{\lambda}} (2\pi \rho^2)^{d/2} e^{-2\pi^2 \rho^2 \|\boldsymbol{\lambda}\|^2} d\boldsymbol{\lambda},$$

where i is the imaginary unit. Furthermore, for each natural number $s \in \mathbb{N}$, let \mathcal{I}_s and \mathcal{C}_s be families of sets given by

$$\mathcal{I}_s = \left\{ \left[-s + \frac{j-1}{2^s}, -s + \frac{j}{2^s} \right) \mid j = 1, \dots, 2s2^s \right\},$$

$$\mathcal{C}_s = \left\{ I_1 \times \dots \times I_d \mid I_1, \dots, I_d \in \mathcal{I}_s \right\}.$$

In addition, for each element $C_{s,k} = [a_{s,k}^{(1)}, b_{s,k}^{(1)}) \times \cdots [a_{s,k}^{(d)}, b_{s,k}^{(d)})$ of \mathcal{C}_s , $(k = 1, \dots, (2s2^s)^d)$, we define the representative point $\lambda_{s,k}$ of $C_{s,k}$ as

$$\boldsymbol{\lambda}_{s,k} = \left(\frac{a_{s,k}^{(1)} + b_{s,k}^{(1)}}{2}, \dots, \frac{a_{s,k}^{(d)} + b_{s,k}^{(d)}}{2}\right)^{\top} = (\lambda_{s,k}^{(1)}, \dots, \lambda_{s,k}^{(d)})^{\top}.$$

Moreover, let $\phi_s(x)$ be the $(2s2^s)^d$ -dimensional vector whose kth element $\phi_{s,k}(x)$ is given by

$$\phi_{s,k}(\mathbf{x}) = ae^{2\pi i \mathbf{x}^{\top} \lambda_{s,k}} (2\pi \rho^2)^{d/4} e^{-\pi^2 \rho^2 \|\lambda_{s,k}\|^2} \left(\frac{1}{2^s}\right)^{d/2}.$$

Then, the inner product $\langle \phi_s(x), \phi_s(y) \rangle \equiv \overline{\phi_s(x)}^{\top} \phi_s(y)$ satisfies

$$\lim_{s \to \infty} \langle \boldsymbol{\phi}_s(\boldsymbol{x}), \boldsymbol{\phi}_s(\boldsymbol{y}) \rangle = \lim_{s \to \infty} \sum_{k=1}^{(2s2^s)^d} a^2 e^{2\pi i (-\boldsymbol{x}+\boldsymbol{y})^\top \boldsymbol{\lambda}_{s,k}} (2\pi\rho^2)^{d/2} e^{-2\pi^2\rho^2 \|\boldsymbol{\lambda}_{s,k}\|^2} \left(\frac{1}{2^s}\right)^d$$

$$= a^2 \int_{\mathbb{R}^d} e^{2\pi i (-\boldsymbol{x}+\boldsymbol{y})^\top \boldsymbol{\lambda}} (2\pi\rho^2)^{d/2} e^{-2\pi^2\rho^2 \|\boldsymbol{\lambda}\|^2} d\boldsymbol{\lambda}$$

$$= a^2 \int_{\mathbb{R}^d} e^{2\pi i (\boldsymbol{x}-\boldsymbol{y})^\top \boldsymbol{\lambda}} (2\pi\rho^2)^{d/2} e^{-2\pi^2\rho^2 \|\boldsymbol{\lambda}\|^2} d\boldsymbol{\lambda} = k(\boldsymbol{x}, \boldsymbol{y}).$$

Furthermore, we define $\check{\sigma}_{t,s}^2({m x})$ and $\epsilon_{t,s}({m x})$ as

$$egin{aligned} \check{\sigma}_{t,s}^2(oldsymbol{x}) &= \langle oldsymbol{\phi}_s(oldsymbol{x}), oldsymbol{\phi}_s(oldsymbol{x})
angle - (\langle oldsymbol{\phi}_s(oldsymbol{x}), oldsymbol{\phi}_s(oldsymbol{x}_1)
angle, \ldots, \langle oldsymbol{\phi}_s(oldsymbol{x}), oldsymbol{\phi}_s(oldsymbol{x}_t)
angle, \\ &(oldsymbol{K}_{t,s} + \sigma^2 oldsymbol{I}_t)^{-1} (\langle oldsymbol{\phi}_s(oldsymbol{x}), oldsymbol{\phi}_s(oldsymbol{x}_1)
angle, \ldots, \langle oldsymbol{\phi}_s(oldsymbol{x}), oldsymbol{\phi}_s(oldsymbol{x}_t)
angle^{\top}, \\ &= k(oldsymbol{x}, oldsymbol{x}) - (k(oldsymbol{x}, oldsymbol{x}_1), \ldots, k(oldsymbol{x}, oldsymbol{x}_t)) (oldsymbol{K}_t + \sigma^2 oldsymbol{I}_t)^{-1} (k(oldsymbol{x}, oldsymbol{x}_1), \ldots, k(oldsymbol{x}, oldsymbol{x}_t))^{\top} \\ &- \check{\sigma}_{t,s}^2(oldsymbol{x}) \\ &= \sigma_t^2(oldsymbol{x}) - \check{\sigma}_{t,s}^2(oldsymbol{x}), \end{aligned}$$

where $K_{t,s}$ and K_t are $t \times t$ matrices whose (i,j) elements are given by $\langle \phi_s(\boldsymbol{x}_i), \phi_s(\boldsymbol{x}_j) \rangle$ and $\langle \phi_s(\boldsymbol{x}_i), \phi_s(\boldsymbol{x}_j) \rangle$, respectively. Then, noting that $\lim_{s \to \infty} \langle \phi_s(\boldsymbol{x}), \phi_s(\boldsymbol{y}) \rangle = k(\boldsymbol{x}, \boldsymbol{y})$ we get

$$\lim_{s \to \infty} \check{\sigma}_{t,s}^2(\boldsymbol{x}) = \sigma_t^2(\boldsymbol{x}), \quad \lim_{s \to \infty} \epsilon_{t,s}(\boldsymbol{x}) = 0.$$

We now consider $\sigma_t(x)$ and $\sigma_t(y)$. Without loss of generality, we can assume that $\sigma_t(x) \ge \sigma_t(y)$. Then, we have

$$|\sigma_t(\mathbf{x}) - \sigma_t(\mathbf{y})| = \sigma_t(\mathbf{x}) - \sigma_t(\mathbf{y}). \tag{E.4}$$

In addition, the following inequality holds:

$$\sigma_{t}(\boldsymbol{x}) = \sqrt{\tilde{\sigma}_{t,s}^{2}(\boldsymbol{x})} = \sqrt{\tilde{\sigma}_{t,s}^{2}(\boldsymbol{x}) + \epsilon_{t,s}(\boldsymbol{x})} \leq \sqrt{\tilde{\sigma}_{t,s}^{2}(\boldsymbol{x}) + |\epsilon_{t,s}(\boldsymbol{x})|} \leq \sqrt{\tilde{\sigma}_{t,s}^{2}(\boldsymbol{x}) + \sqrt{|\epsilon_{t,s}(\boldsymbol{x})|}}.$$
(E.5)

Similarly, if $\epsilon_{t,s}(\boldsymbol{y}) > 0$, then $\sigma_t(\boldsymbol{y})$ satisfies

$$\sigma_t(oldsymbol{y}) = \sqrt{\check{\sigma}_{t,s}^2(oldsymbol{y}) + \epsilon_{t,s}(oldsymbol{y})} \geq \sqrt{\check{\sigma}_{t,s}^2(oldsymbol{y})} \geq \sqrt{\check{\sigma}_{t,s}^2(oldsymbol{y})} - \sqrt{|\epsilon_{t,s}(oldsymbol{y})|}$$

On the other hand, if $\epsilon_{t,s}(\boldsymbol{y}) \leq 0$, then $\sigma_t(\boldsymbol{y})$ satisfies

$$\sigma_t(\boldsymbol{y}) = \sqrt{\check{\sigma}_{t,s}^2(\boldsymbol{y}) + \epsilon_{t,s}(\boldsymbol{y})} = \sqrt{\check{\sigma}_{t,s}^2(\boldsymbol{y}) - |\epsilon_{t,s}(\boldsymbol{y})|} \geq \sqrt{\check{\sigma}_{t,s}^2(\boldsymbol{y})} - \sqrt{|\epsilon_{t,s}(\boldsymbol{y})|},$$

where the last inequality is given by $\sqrt{u}-\sqrt{v} \leq \sqrt{u-v}$, $(u \geq v \geq 0)$. Hence, for both cases, the following holds:

$$\sigma_t(\boldsymbol{y}) \ge \sqrt{\check{\sigma}_{t,s}^2(\boldsymbol{y})} - \sqrt{|\epsilon_{t,s}(\boldsymbol{y})|}.$$
 (E.6)

Thus, by substituting (E.5) and (E.6) into (E.4), we obtain

$$|\sigma_t(\boldsymbol{x}) - \sigma_t(\boldsymbol{y})| \le \sqrt{\check{\sigma}_{t,s}^2(\boldsymbol{x})} - \sqrt{\check{\sigma}_{t,s}^2(\boldsymbol{y})} + \sqrt{|\epsilon_{t,s}(\boldsymbol{x})|} + \sqrt{|\epsilon_{t,s}(\boldsymbol{y})|}.$$
 (E.7)

Furthermore, we define the matrix $X_{t,s}$ as $X_{t,s} = (\phi_s(x_1), \dots, \phi_s(x_t))^*$, where A^* is the conjugate transpose of A. Then, $\check{\sigma}_{t,s}^2(x)$ can be rewritten as follows:

$$\check{\sigma}_{t,s}^2(\boldsymbol{x}) = \overline{\phi_s(\boldsymbol{x})}^{\top} (\boldsymbol{I}_{(2s2^s)^d} - \boldsymbol{X}_{t,s}^* (\boldsymbol{X}_{t,s} \boldsymbol{X}_{t,s}^* + \sigma^2 \boldsymbol{I}_t)^{-1} \boldsymbol{X}_{t,s}) \phi_s(\boldsymbol{x}).$$

Therefore, by using the singular decomposition of $X_{t,s}$, we have

$$\check{\sigma}_{t,s}^2(oldsymbol{x}) = \overline{oldsymbol{\phi}_s(oldsymbol{x})}^ op oldsymbol{U}oldsymbol{\Theta}oldsymbol{U}^*oldsymbol{\phi}_s(oldsymbol{x}),$$

where U and Θ are unitary and diagonal matrices, respectively. By using the same argument as in the case of the linear kernel, it can be shown that the (k,k) element θ_k of Θ satisfies $0 \le \theta_k \le 1$. Hence, noting that

$$\check{\sigma}_{t,s}(oldsymbol{x}) = \sqrt{\check{\sigma}_{t,s}^2(oldsymbol{x})} = \|oldsymbol{\Theta}^{1/2}oldsymbol{U}^*oldsymbol{\phi}_s(oldsymbol{x})\|$$

and (E.7), from the triangle inequality we get

$$|\sigma_{t}(\boldsymbol{x}) - \sigma_{t}(\boldsymbol{y})| \leq \|\boldsymbol{\Theta}^{1/2}\boldsymbol{U}^{*}\boldsymbol{\phi}_{s}(\boldsymbol{x})\| - \|\boldsymbol{\Theta}^{1/2}\boldsymbol{U}^{*}\boldsymbol{\phi}_{s}(\boldsymbol{y})\| + \sqrt{|\epsilon_{t,s}(\boldsymbol{x})|} + \sqrt{|\epsilon_{t,s}(\boldsymbol{y})|}$$

$$\leq \|\boldsymbol{\Theta}^{1/2}\boldsymbol{U}^{*}\boldsymbol{\phi}_{s}(\boldsymbol{x}) - \boldsymbol{\Theta}^{1/2}\boldsymbol{U}^{*}\boldsymbol{\phi}_{s}(\boldsymbol{y})\| + \sqrt{|\epsilon_{t,s}(\boldsymbol{x})|} + \sqrt{|\epsilon_{t,s}(\boldsymbol{y})|}$$

$$= \|\boldsymbol{\Theta}^{1/2}\boldsymbol{U}^{*}(\boldsymbol{\phi}_{s}(\boldsymbol{x}) - \boldsymbol{\phi}_{s}(\boldsymbol{y}))\| + \sqrt{|\epsilon_{t,s}(\boldsymbol{x})|} + \sqrt{|\epsilon_{t,s}(\boldsymbol{y})|}$$

$$\leq \|\boldsymbol{\phi}_{s}(\boldsymbol{x}) - \boldsymbol{\phi}_{s}(\boldsymbol{y})\| + \sqrt{|\epsilon_{t,s}(\boldsymbol{x})|} + \sqrt{|\epsilon_{t,s}(\boldsymbol{y})|}, \tag{E.8}$$

where the last inequality is given by $0 \le \theta_k \le 1$. Moreover, for each j with $1 \le j \le d-1$, let $\boldsymbol{x}[j] = (y_1, \dots, y_j, x_{j+1}, \dots, x_d)^\top$, and let $\boldsymbol{x}[0] \equiv \boldsymbol{x}$ and $\boldsymbol{x}[d] \equiv \boldsymbol{y}$. Then, the following inequality holds:

$$\|\phi_{s}(\boldsymbol{x}) - \phi_{s}(\boldsymbol{y})\| = \left\| \sum_{j=1}^{d} \{\phi_{s}(\boldsymbol{x}[j-1]) - \phi_{s}(\boldsymbol{x}[j])\} \right\|$$

$$\leq \sum_{j=1}^{d} \|\phi_{s}(\boldsymbol{x}[j-1]) - \phi_{s}(\boldsymbol{x}[j])\|. \tag{E.9}$$

Thus, by substituting (E.9) into (E.8), we obtain

$$|\sigma_t(\boldsymbol{x}) - \sigma_t(\boldsymbol{y})| \le \sum_{j=1}^a \|\phi_s(\boldsymbol{x}[j-1]) - \phi_s(\boldsymbol{x}[j])\| + \sqrt{|\epsilon_{t,s}(\boldsymbol{x})|} + \sqrt{|\epsilon_{t,s}(\boldsymbol{y})|}.$$
(E.10)

In addition, for any j and k with $1 \le j \le d$ and $1 \le k \le (2s2^s)^d$, from the definition of $\phi_{s,k}(x)$ we have

$$\phi_{s,k}(\boldsymbol{x}[j-1]) - \phi_{s,k}(\boldsymbol{x}[j]) = aD(2\pi\rho^2)^{d/4} e^{-\pi^2\rho^2 \|\boldsymbol{\lambda}_{s,k}\|^2} \left(\frac{1}{2^s}\right)^{d/2} \left(e^{2\pi i x_j \lambda_{s,k}^{(j)}} - e^{2\pi i y_j \lambda_{s,k}^{(j)}}\right),$$

$$D = e^{2\pi i (y_1, \dots, y_{j-1}, x_{j+1}, \dots, x_d)(\lambda_{s,k}^{(1)}, \dots, \lambda_{s,k}^{(j-1)}, \lambda_{s,k}^{(j+1)}, \dots, \lambda_{s,k}^{(d)})^\top}.$$

Hence, it follows that

$$\overline{(\phi_{s,k}(\boldsymbol{x}[j-1]) - \phi_{s,k}(\boldsymbol{x}[j]))} (\phi_{s,k}(\boldsymbol{x}[j-1]) - \phi_{s,k}(\boldsymbol{x}[j]))
= |\phi_{s,k}(\boldsymbol{x}[j-1]) - \phi_{s,k}(\boldsymbol{x}[j])|^{2}
\leq a^{2} (2\pi\rho^{2})^{d/2} e^{-2\pi^{2}\rho^{2} \|\boldsymbol{\lambda}_{s,k}\|^{2}} \left(\frac{1}{2^{s}}\right)^{d} |e^{2\pi i x_{j} \lambda_{s,k}^{(j)}} - e^{2\pi i y_{j} \lambda_{s,k}^{(j)}}|^{2}.$$
(E.11)

Thus, noting that $|\cos(u)-\cos(v)| \leq |u-v|$ and $|\sin(u)-\sin(v)| \leq |u-v|$ for any $u,v \in \mathbb{R}$, we get

$$|e^{2\pi i x_{j} \lambda_{s,k}^{(j)}} - e^{2\pi i y_{j} \lambda_{s,k}^{(j)}}|$$

$$= |\cos(2\pi x_{j} \lambda_{s,k}^{(j)}) + i \sin(2\pi x_{j} \lambda_{s,k}^{(j)}) - \cos(2\pi y_{j} \lambda_{s,k}^{(j)}) - i \sin(2\pi y_{j} \lambda_{s,k}^{(j)})|$$

$$= \sqrt{|\cos(2\pi x_{j} \lambda_{s,k}^{(j)}) - \cos(2\pi y_{j} \lambda_{s,k}^{(j)})|^{2} + |\sin(2\pi x_{j} \lambda_{s,k}^{(j)}) - \sin(2\pi y_{j} \lambda_{s,k}^{(j)})|^{2}}}$$

$$\leq \sqrt{8\pi^{2} \lambda_{s,k}^{(j)2} (x_{j} - y_{j})^{2}}.$$
(E.12)

Therefore, by substituting (E.12) into (E.11), we obtain

$$\overline{(\phi_{s,k}(\boldsymbol{x}[j-1]) - \phi_{s,k}(\boldsymbol{x}[j]))}(\phi_{s,k}(\boldsymbol{x}[j-1]) - \phi_{s,k}(\boldsymbol{x}[j]))
\leq a^2 (2\pi\rho^2)^{d/2} e^{-2\pi^2\rho^2 \|\boldsymbol{\lambda}_{s,k}\|^2} \left(\frac{1}{2^s}\right)^d 8\pi^2 \lambda_{s,k}^{(j)2} (x_j - y_j)^2.$$

This implies that

$$\|\phi_s(\boldsymbol{x}[j-1]) - \phi_s(\boldsymbol{x}[j])\|^2 \le \sum_{k=1}^{(2s2^s)^d} a^2 (2\pi\rho^2)^{d/2} e^{-2\pi^2\rho^2 \|\boldsymbol{\lambda}_{s,k}\|^2} \left(\frac{1}{2^s}\right)^d 8\pi^2 \lambda_{s,k}^{(j)2} (x_j - y_j)^2.$$
 (E.13)

Moreover, the following holds when $s \to \infty$:

$$\begin{split} &\lim_{s \to \infty} \sum_{k=1}^{(2s2^s)^d} a^2 (2\pi \rho^2)^{d/2} e^{-2\pi^2 \rho^2 \|\boldsymbol{\lambda}_{s,k}\|^2} \left(\frac{1}{2^s}\right)^d 8\pi^2 \lambda_{s,k}^{(j)2} (x_j - y_j)^2 \\ &= a^2 (2\pi \rho^2)^{d/2} 8\pi^2 (x_j - y_j)^2 \int_{\mathbb{R}^d} e^{-2\pi^2 \rho^2 \boldsymbol{\lambda}^\top \boldsymbol{\lambda}} \lambda_j^2 \mathrm{d}\boldsymbol{\lambda} \\ &= a^2 8\pi^2 (x_j - y_j)^2 \left(\int_{\mathbb{R}} (2\pi \rho^2)^{1/2} \lambda_j^2 e^{-2\pi^2 \rho^2 \lambda_j^2} \mathrm{d}\lambda_j \right) \prod_{i \neq j}^d \left(\int_{\mathbb{R}} (2\pi \rho^2)^{1/2} e^{-2\pi^2 \rho^2 \lambda_i^2} \mathrm{d}\lambda_i \right). \end{split}$$

By putting $2\pi\rho\lambda_i=u_i$ for each i with $1\leq i\leq d$, we have

$$a^{2}8\pi^{2}(x_{j} - y_{j})^{2} \left(\int_{\mathbb{R}} (2\pi\rho^{2})^{1/2} \lambda_{j}^{2} e^{-2\pi^{2}\rho^{2}\lambda_{j}^{2}} d\lambda_{j} \right) \prod_{i \neq j}^{d} \left(\int_{\mathbb{R}} (2\pi\rho^{2})^{1/2} e^{-2\pi^{2}\rho^{2}\lambda_{i}^{2}} d\lambda_{i} \right)$$

$$= a^{2}2\rho^{-2}(x_{j} - y_{j})^{2} \int_{\mathbb{R}} (2\pi)^{-1/2} u_{j}^{2} e^{-u_{j}^{2}/2} du_{j} \prod_{i \neq j}^{d} \left(\int_{\mathbb{R}} (2\pi)^{-1/2} e^{-u_{i}^{2}/2} du_{i} \right)$$

$$= \frac{2a^{2}}{\rho^{2}} (x_{j} - y_{j})^{2}. \tag{E.14}$$

Thus, (E.13) can be rewritten as follows:

$$\begin{split} &\|\phi_{s}(\boldsymbol{x}[j-1]) - \phi_{s}(\boldsymbol{x}[j])\|^{2} \\ &\leq \frac{2a^{2}}{\rho^{2}}(x_{j} - y_{j})^{2} \\ &\quad + \sum_{k=1}^{(2s2^{s})^{d}} a^{2}(2\pi\rho^{2})^{d/2}e^{-2\pi^{2}\rho^{2}\|\boldsymbol{\lambda}_{s,k}\|^{2}} \left(\frac{1}{2^{s}}\right)^{d} 8\pi^{2}\lambda_{s,k}^{(j)2}(x_{j} - y_{j})^{2} - \frac{2a^{2}}{\rho^{2}}(x_{j} - y_{j})^{2} \\ &\leq \frac{2a^{2}}{\rho^{2}}(x_{j} - y_{j})^{2} \\ &\quad + \left| \sum_{k=1}^{(2s2^{s})^{d}} a^{2}(2\pi\rho^{2})^{d/2}e^{-2\pi^{2}\rho^{2}\|\boldsymbol{\lambda}_{s,k}\|^{2}} \left(\frac{1}{2^{s}}\right)^{d} 8\pi^{2}\lambda_{s,k}^{(j)2}(x_{j} - y_{j})^{2} - \frac{2a^{2}}{\rho^{2}}(x_{j} - y_{j})^{2} \right| \\ &\equiv \frac{2a^{2}}{\rho^{2}}(x_{j} - y_{j})^{2} + \tilde{\epsilon}_{s,j}, \end{split}$$

where $\tilde{\epsilon}_{s,j}$ satisfies that $\lim_{s \to \infty} |\tilde{\epsilon}_{s,j}| = 0$ from (E.14). Hence, we get

$$\|\phi_s(x[j-1]) - \phi_s(x[j])\| \le \sqrt{\frac{2a^2}{\rho^2}(x_j - y_j)^2 + \tilde{\epsilon}_{s,j}} \le \frac{\sqrt{2}a}{\rho}|x_j - y_j| + \sqrt{\tilde{\epsilon}_{s,j}}.$$
 (E.15)

By substituting (E.15) into (E.10), we obtain

$$|\sigma_t(\boldsymbol{x}) - \sigma_t(\boldsymbol{y})| \le \frac{\sqrt{2}a}{\rho} \|\boldsymbol{x} - \boldsymbol{y}\|_1 + \sum_{j=1}^d \sqrt{\tilde{\epsilon}_{s,j}} + \sqrt{|\epsilon_{t,s}(\boldsymbol{x})|} + \sqrt{|\epsilon_{t,s}(\boldsymbol{y})|}.$$

Furthermore, because the number s is an arbitrary natural number, and

$$\lim_{s \to \infty} \left(\sum_{j=1}^{d} \sqrt{\tilde{\epsilon}_{s,j}} + \sqrt{|\epsilon_{t,s}(\boldsymbol{x})|} + \sqrt{|\epsilon_{t,s}(\boldsymbol{y})|} \right) = 0,$$

we have

$$|\sigma_t(\boldsymbol{x}) - \sigma_t(\boldsymbol{y})| \leq \frac{\sqrt{2}a}{a} \|\boldsymbol{x} - \boldsymbol{y}\|_1.$$

Finally, we show the case of the Matérn kernel. From Bochner's theorem, the Matérn kernel can be rewritten as follows (see, section 4.2.1 in (Rasmussen and Williams, 2005)):

$$k(\boldsymbol{x}, \boldsymbol{y}) = a^2 \int_{\mathbb{R}^d} e^{2\pi \mathrm{i}(\boldsymbol{x} - \boldsymbol{y})^{\top} \boldsymbol{\lambda}} \frac{2^d \pi^{d/2} \Gamma(\nu + d/2) (2\nu)^{\nu}}{\Gamma(\nu) \rho^{2\nu}} \left(\frac{2\nu}{\rho^2} + 4\pi^2 \|\boldsymbol{\lambda}\|^2 \right)^{-(\nu + d/2)} d\boldsymbol{\lambda}.$$

For each $s \in \mathbb{N}$ and k with $k = 1, \ldots, (2s2^s)^d$, we define \mathcal{I}_s , \mathcal{C}_s , the element $C_{s,k} = [a_{s,k}^{(1)}, b_{s,k}^{(1)}) \times \cdots [a_{s,k}^{(d)}, b_{s,k}^{(d)})$ of \mathcal{C}_s , and the representative point $\lambda_{s,k}$ of $C_{s,k}$ as in the case of the Gaussian kernel. Similarly, let $\phi_s(\boldsymbol{x})$ be the $(2s2^s)^d$ -dimensional vector whose kth element $\phi_{s,k}(\boldsymbol{x})$ is given by

$$\phi_{s,k}(\boldsymbol{x}) = ae^{2\pi i \boldsymbol{x}^{\top} \boldsymbol{\lambda}_{s,k}} \left(\frac{2^{d} \pi^{d/2} \Gamma(\nu + d/2) (2\nu)^{\nu}}{\Gamma(\nu) \rho^{2\nu}} \left(\frac{2\nu}{\rho^{2}} + 4\pi^{2} \|\boldsymbol{\lambda}_{s,k}\|^{2} \right)^{-(\nu + d/2)} \right)^{1/2} \left(\frac{1}{2^{s}} \right)^{d/2}.$$

Then, by using the same argument as in the case of the Gaussian kernel, we obtain the following inequality similar to (E.10):

$$|\sigma_t(\boldsymbol{x}) - \sigma_t(\boldsymbol{y})| \le \sum_{j=1}^d ||\phi_s(\boldsymbol{x}[j-1]) - \phi_s(\boldsymbol{x}[j])|| + |\epsilon_{t,s}(\boldsymbol{x}, \boldsymbol{y})|,$$
(E.16)

where $\lim_{s\to\infty} |\epsilon_{t,s}(\boldsymbol{x},\boldsymbol{y})| = 0$. Moreover, for any j and k with $1 \le j \le d$ and $1 \le k \le (2s2^s)^d$, from the definition of $\phi_{s,k}(\boldsymbol{x})$ we get

$$\begin{split} & \phi_{s,k}(\boldsymbol{x}[j-1]) - \phi_{s,k}(\boldsymbol{x}[j]) \\ &= aD \left(\frac{2^d \pi^{d/2} \Gamma(\nu + d/2) (2\nu)^{\nu}}{\Gamma(\nu) \rho^{2\nu}} \left(\frac{2\nu}{\rho^2} + 4\pi^2 \| \boldsymbol{\lambda}_{s,k} \|^2 \right)^{-(\nu + d/2)} \right)^{1/2} \left(\frac{1}{2^s} \right)^{d/2} \\ & \left(e^{2\pi i x_j \lambda_{s,k}^{(j)}} - e^{2\pi i y_j \lambda_{s,k}^{(j)}} \right), \\ & D = e^{2\pi i (y_1, \dots, y_{j-1}, x_{j+1}, \dots, x_d) (\lambda_{s,k}^{(1)}, \dots, \lambda_{s,k}^{(j-1)}, \lambda_{s,k}^{(j+1)}, \dots, \lambda_{s,k}^{(d)})^{\top}}. \end{split}$$

It follows that

$$\overline{(\phi_{s,k}(\boldsymbol{x}[j-1]) - \phi_{s,k}(\boldsymbol{x}[j]))} (\phi_{s,k}(\boldsymbol{x}[j-1]) - \phi_{s,k}(\boldsymbol{x}[j]))
= |\phi_{s,k}(\boldsymbol{x}[j-1]) - \phi_{s,k}(\boldsymbol{x}[j])|^{2}
\leq a^{2} \frac{2^{d} \pi^{d/2} \Gamma(\nu + d/2)(2\nu)^{\nu}}{\Gamma(\nu)\rho^{2\nu}} \left(\frac{2\nu}{\rho^{2}} + 4\pi^{2} \|\boldsymbol{\lambda}_{s,k}\|^{2}\right)^{-(\nu+d/2)} \left(\frac{1}{2^{s}}\right)^{d} |e^{2\pi i x_{j} \lambda_{s,k}^{(j)}} - e^{2\pi i y_{j} \lambda_{s,k}^{(j)}}|^{2}.$$
(E.17)

By substituting (E.12) into (E.17), we have

$$\overline{(\phi_{s,k}(\boldsymbol{x}[j-1]) - \phi_{s,k}(\boldsymbol{x}[j]))}(\phi_{s,k}(\boldsymbol{x}[j-1]) - \phi_{s,k}(\boldsymbol{x}[j]))
\leq a^2 \frac{2^d \pi^{d/2} \Gamma(\nu + d/2)(2\nu)^{\nu}}{\Gamma(\nu)\rho^{2\nu}} \left(\frac{2\nu}{\rho^2} + 4\pi^2 \|\boldsymbol{\lambda}_{s,k}\|^2\right)^{-(\nu+d/2)} \left(\frac{1}{2^s}\right)^d 8\pi^2 \lambda_{s,k}^{(j)2} (x_j - y_j)^2.$$

This implies that

$$\begin{aligned} &\|\boldsymbol{\phi}_{s}(\boldsymbol{x}[j-1]) - \boldsymbol{\phi}_{s}(\boldsymbol{x}[j])\|^{2} \\ &\leq \sum_{k=1}^{(2s2^{s})^{d}} a^{2} \frac{2^{d} \pi^{d/2} \Gamma(\nu + d/2) (2\nu)^{\nu}}{\Gamma(\nu) \rho^{2\nu}} \left(\frac{2\nu}{\rho^{2}} + 4\pi^{2} \|\boldsymbol{\lambda}_{s,k}\|^{2}\right)^{-(\nu + d/2)} \left(\frac{1}{2^{s}}\right)^{d} 8\pi^{2} \lambda_{s,k}^{(j)2} (x_{j} - y_{j})^{2}. \end{aligned}$$

Furthermore, the following holds when $s \to \infty$:

$$\begin{split} &\lim_{s \to \infty} \sum_{k=1}^{(2s2^s)^d} a^2 \frac{2^d \pi^{d/2} \Gamma(\nu + d/2) (2\nu)^{\nu}}{\Gamma(\nu) \rho^{2\nu}} \left(\frac{2\nu}{\rho^2} + 4\pi^2 \| \boldsymbol{\lambda}_{s,k} \|^2 \right)^{-(\nu + d/2)} \left(\frac{1}{2^s} \right)^d 8\pi^2 \lambda_{s,k}^{(j)2} (x_j - y_j)^2 \\ &= a^2 8\pi^2 (x_j - y_j)^2 \int_{\mathbb{R}^d} \frac{2^d \pi^{d/2} \Gamma(\nu + d/2) (2\nu)^{\nu}}{\Gamma(\nu) \rho^{2\nu}} \left(\frac{2\nu}{\rho^2} + 4\pi^2 \| \boldsymbol{\lambda} \|^2 \right)^{-(\nu + d/2)} \lambda_j^2 \mathrm{d}\boldsymbol{\lambda}. \end{split}$$

In addition, by putting $2\nu = \tilde{\nu}$ and $\Sigma = (4\pi^2 \rho^2)^{-1} I_d$, we obtain

$$\begin{split} &\frac{2^{d}\pi^{d/2}\Gamma(\nu+d/2)(2\nu)^{\nu}}{\Gamma(\nu)\rho^{2\nu}}\left(\frac{2\nu}{\rho^{2}}+4\pi^{2}\|\boldsymbol{\lambda}\|^{2}\right)^{-(\nu+d/2)}\\ &=\frac{\Gamma((\tilde{\nu}+d)/2)}{\Gamma(\tilde{\nu}/2)\tilde{\nu}^{d/2}\pi^{d/2}|\boldsymbol{\Sigma}|^{1/2}}\left(1+\frac{1}{\tilde{\nu}}\boldsymbol{\lambda}^{\top}\boldsymbol{\Sigma}^{-1}\boldsymbol{\lambda}\right)^{-(\tilde{\nu}+d)/2}\equiv f(\boldsymbol{\lambda};\tilde{\nu},\boldsymbol{\Sigma}). \end{split}$$

Note that $f(\lambda; \tilde{\nu}, \Sigma)$ is the probability density function of $T_{\tilde{\nu}}(\mathbf{0}, \Sigma)$, where $T_{\tilde{\nu}}(\mathbf{0}, \Sigma)$ is the multivariate t-distribution with location parameter $\mathbf{0}$, scale matrix Σ and $\tilde{\nu}$ degrees of freedom. It is known that the mean vector and covariance matrix of $T_{\tilde{\nu}}(\mathbf{0}, \Sigma)$ are respectively given by $\mathbf{0}$ and $\frac{\tilde{\nu}}{\tilde{\nu}-2}\Sigma$ when $\tilde{\nu}>2$ (see, e.g., (Kotz and Nadarajah, 2004)). From the assumption $\nu>1$, noting that $\tilde{\nu}=2\nu>2$ we have

$$\begin{split} & \int_{\mathbb{R}^d} \frac{2^d \pi^{d/2} \Gamma(\nu + d/2) (2\nu)^{\nu}}{\Gamma(\nu) \rho^{2\nu}} \left(\frac{2\nu}{\rho^2} + 4\pi^2 \|\boldsymbol{\lambda}\|^2 \right)^{-(\nu + d/2)} \lambda_j^2 \mathrm{d}\boldsymbol{\lambda} \\ & = \int_{\mathbb{R}^d} f(\boldsymbol{\lambda}; \tilde{\nu}, \boldsymbol{\Sigma}) \lambda_j^2 \mathrm{d}\boldsymbol{\lambda} \\ & = \frac{\tilde{\nu}}{\tilde{\nu} - 2} \frac{1}{4\pi^2 \rho^2} = \frac{\nu}{\nu - 1} \frac{1}{4\pi^2 \rho^2}. \end{split}$$

This implies that

$$\begin{split} &\lim_{s \to \infty} \sum_{k=1}^{(2s2^s)^d} a^2 \frac{2^d \pi^{d/2} \Gamma(\nu + d/2) (2\nu)^{\nu}}{\Gamma(\nu) \rho^{2\nu}} \left(\frac{2\nu}{\rho^2} + 4\pi^2 \| \boldsymbol{\lambda}_{s,k} \|^2 \right)^{-(\nu + d/2)} \left(\frac{1}{2^s} \right)^d 2 \lambda_{s,k}^{(j)2} (x_j - y_j)^2 \\ &= \frac{2a^2}{\rho^2} (x_j - y_j)^2 \frac{\nu}{\nu - 1}. \end{split}$$

Therefore, by using the same argument as in the case of the Gaussian kernel, we obtain

$$\|\phi_s(x[j-1]) - \phi_s(x[j])\| \le \frac{\sqrt{2}a}{\rho} \sqrt{\frac{\nu}{\nu-1}} |x_j - y_j| + |\hat{\epsilon}_{s,j}|,$$
 (E.18)

where $\lim_{s\to\infty} |\hat{\epsilon}_{s,j}|=0$. Hence, by substituting (E.18) into (E.16), and taking $s\to\infty$ we get

$$|\sigma_t(\boldsymbol{x}) - \sigma_t(\boldsymbol{y})| \le \frac{\sqrt{2}a}{\rho} \sqrt{\frac{\nu}{\nu - 1}} \|\boldsymbol{x} - \boldsymbol{y}\|_1.$$

The condition that σ^2 in Theorem E.4 is positive is necessary only for the inverse matrix calculation. Note that σ^2 is a user-specified variance parameter of a formal GP model, and is different from the true noise variance. That is, Theorem E.4 holds even when the variance of the true noise is zero, i.e., in the noiseless setting. Also note that C in Theorem E.4 is a constant independent of σ^2 . The result for the Matérn kernel is for the case of $\nu > 1$ degrees of freedom, and it is a future work to clarify whether the same result holds for $\nu \leq 1$ as well. On the other hand, unfortunately, it can be shown that (E.1) does not hold for $\nu = 1/2$, which is often used in practice for Matérn kernels.

Theorem E.5. In the setting of Theorem E.4, the Matérn kernel with $\nu = 1/2$ does not satisfy (E.1).

Proof. Let C be an arbitrary positive number. The Matérn kernel with $\nu = 1/2$ is given by

$$k(\boldsymbol{x}, \boldsymbol{y}) = a^2 \exp(-\|\boldsymbol{x} - \boldsymbol{y}\|/\rho).$$

In addition, suppose that $x_1 = \cdots = x_t = 0$. Moreover, we define K_t as

$$\boldsymbol{K}_t = a^2 \mathbf{1}_t \mathbf{1}_t^\top + \sigma^2 \boldsymbol{I}_t.$$

Then, the inverse matrix K_t^{-1} can be expressed as

$$\boldsymbol{K}_t^{-1} = \sigma^{-2} \boldsymbol{I}_t - \frac{\frac{a^2}{\sigma^4} \boldsymbol{1}_t \boldsymbol{1}_t^\top}{1 + \frac{a^2}{\sigma^2} t}.$$

Therefore, the posterior variance at point 0 is given by

$$\sigma_t^2(\mathbf{0}) = a^2 - a^4 \mathbf{1}_t^{\top} \mathbf{K}_t^{-1} \mathbf{1}_t = a^2 - a^4 \frac{t}{\sigma^2 + a^2 t} = \frac{a^2 \sigma^2}{\sigma^2 + a^2 t}$$

Next, let s be a number with $0 < s < \rho/2$, and let $\boldsymbol{x} = (s, 0, \dots, 0)^{\top}$. Then, we have

$$\begin{split} \sigma_t^2(\boldsymbol{x}) &= a^2 - a^4 \exp(-2s/\rho) \mathbf{1}_t^\top \boldsymbol{K}_t^{-1} \mathbf{1}_t \\ &= a^2 - a^4 \exp(-2s/\rho) \frac{t}{\sigma^2 + a^2 t} \\ &= a^2 - a^4 (1 + \exp(-2s/\rho) - 1) \frac{t}{\sigma^2 + a^2 t} \\ &= \sigma_t^2(\mathbf{0}) + \frac{a^4 t}{\sigma^2 + a^2 t} (1 - \exp(-2s/\rho)) \\ &= \sigma_t^2(\mathbf{0}) \left\{ 1 + \frac{a^4 t}{\sigma_t^2(\mathbf{0})(\sigma^2 + a^2 t)} (1 - \exp(-2s/\rho)) \right\} \equiv \sigma_t^2(\mathbf{0}) (1 + u). \end{split}$$

Thus, from $u \ge 0$ we get

$$|\sigma_t(\boldsymbol{x}) - \sigma_t(\boldsymbol{0})| = \sigma_t(\boldsymbol{x}) - \sigma_t(\boldsymbol{0}) = \sigma_t(\boldsymbol{0})\sqrt{1+u} - \sigma_t(\boldsymbol{0}).$$

Furthermore, by using Taylor's expansion of $f(u) = \sqrt{1+u}$ at point u = 0, we obtain

$$\sqrt{1+u} \ge 1 + \frac{1}{2}u - \frac{1}{8}u^2.$$

Moreover, for each t, there exists a number s such that $0 < s < \rho/2$ and $u \le 1$. Therefore, it follows that

$$\sqrt{1+u} \ge 1 + \frac{1}{2}u - \frac{1}{8}u^2 \ge 1 + \frac{1}{2}u - \frac{1}{8}u = 1 + \frac{3}{8}u.$$

By using this, we have

$$|\sigma_t(\boldsymbol{x}) - \sigma_t(\boldsymbol{0})| \ge \frac{3}{8}u\sigma_t(\boldsymbol{0}) = \frac{3}{8}\frac{a^4t}{\sigma_t(\boldsymbol{0})(\sigma^2 + a^2t)}(1 - \exp(-2s/\rho)).$$

In addition, noting that $\exp(-2s/\rho) \le 1 - 2s/\rho + (2s/\rho)^2/2$ and $1 - s/\rho \ge 1/2$, we get

$$1 - \exp(-2s/\rho) \ge 2s/\rho - (2s/\rho)^2/2 = 2s/\rho(1 - s/\rho) \ge s/\rho.$$

Therefore, the following inequality holds:

$$|\sigma_t(\boldsymbol{x}) - \sigma_t(\boldsymbol{0})| \ge \frac{3}{8} \frac{a^4 t/\rho}{\sigma_t(\boldsymbol{0})(\sigma^2 + a^2 t)} s = \frac{3}{8} \frac{a^4/\rho}{\sigma_t(\boldsymbol{0})(\sigma^2/t + a^2)} \|\boldsymbol{x} - \boldsymbol{0}\|_1.$$

Hence, since $\lim_{t\to\infty} \sigma_t(\mathbf{0}) = 0$, the following inequality holds for sufficiently large t:

$$|\sigma_t(x) - \sigma_t(\mathbf{0})| \ge \frac{3}{8} \frac{a^4/\rho}{\sigma_t(\mathbf{0})(\sigma^2/t + a^2)} ||x - \mathbf{0}||_1 > C||x - \mathbf{0}||_1.$$

F Details of the Experimental Settings and Pseudo-codes

In this section, we describe the experimental settings.

F.1 Common Settings

We used a multi-start L-BFGS-B method (Byrd et al., 1995) (SciPy (Virtanen et al., 2020) implementation) to perform various optimization such as optimizing AFs, finding the optimal value of synthetic functions. First, we sample 1000 initial points using Latin hypercube sampling (LHS) (McKay et al., 2000). Then, we run L-BFGS-B with parameter $ftol = 10^{-3}$, $gtol = 10^{-3}$ for each initial point and pick the top 5 results. Finally, we run L-BFGS-B with default parameters for these five results and return the best result. We implemented GP models and all the comparison methods mainly using PyTorch (Paszke et al., 2019) and GPyTorch (Gardner et al., 2018). By utilizing the automatic differentiation of PyTorch, we can easily apply gradient methods to optimize AFs.

F.2 Comparison Methods

CBO In CBO, a scalar output is assumed for each stage. For each iteration t, it first chooses the controllable parameter of the final stage $x_t^{(N)}$ and desired output of previous stage $y_{\text{desire}}^{(N-1)}$ by maximizing EI:

$$(y_{\text{desire}}^{(N-1)}, \pmb{x}_t^{(N)}) = \mathop{\arg\max}_{y^{(N-1)}, \pmb{x}^{(N)}} \sigma_{t-1}^{(N)}(y^{(N-1)}, \pmb{x}^{(N)}) (Z\Phi(Z) + \phi(Z)),$$

where Φ, ϕ are the cumulative distribution function and probability density function of the standard normal distribution, respectively, Z=0 if $\sigma_{t-1}^{(N)}(y^{(N-1)}, \boldsymbol{x}^{(N)})=0$ and be $Z=(\mu_{t-1}^{(N)}(y^{(N-1)}, \boldsymbol{x}^{(N)})-F_{\mathrm{best}})/\sigma_{t-1}^{(N)}(y^{(N-1)}, \boldsymbol{x}^{(N)})$ otherwise. We could not find any description about the range of optimization parameters in (Dai Nguyen et al., 2016). We used $\mathcal{X}^{(N)}$ for the range of $\boldsymbol{x}^{(N)}$, and we used the range twice as wide as the actual range for the range of $y^{(N-1)}$, which is supposed to be unknown. Then, CBO chooses $(y_{\mathrm{desire}}^{(N-2)}, \boldsymbol{x}_t^{(N-1)})$ of stage N-1 as follows:

$$(y_{\text{desire}}^{(N-2)}, \boldsymbol{x}_t^{(N-1)}) = \underset{y^{(N-2)}, \boldsymbol{x}^{(N-1)}}{\arg\min} \left(\kappa_1 v^{-1} + \kappa_2 v \right) \|m - y_{\text{desire}}^{(N-1)}\|_2^2 + \cot(y^{(N-2)}, \boldsymbol{x}^{(N-1)}), \tag{F.1}$$

where $m=\mu_{t-1}^{(N-1)}(y^{(N-2)},\boldsymbol{x}^{(N-1)}),\ v=\sigma_{t-1}^{(N-1)\,2}(y^{(N-2)},\boldsymbol{x}^{(N-1)}),\cos(\cdot)$ is the cost function, and κ_1,κ_2 are hyperparameters. By repeating this operation, a controllable parameter of stage 1 $\boldsymbol{x}_t^{(1)}$ is determined finally. We used $\cos(\cdot)=0$ for simplicity and set $\kappa_1=1,\kappa_2=1$.

In the solar cell simulator experiments, output of stage 1 and stage 2 are vectors. To deal with vector output, we replace a predictive mean and variance in (F.1) with a mean vector and covariance matrix. Therefore, for the vector output setting, the following AF was used instead of (F.1):

$$(\boldsymbol{y}_{\text{desire}}^{(n-1)}, \boldsymbol{x}_t^{(n)}) = \operatorname*{arg\,min}_{\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(x)}} \left[\left(\boldsymbol{m} - \boldsymbol{y}_{\text{desire}}^{(n)} \right)^\top \left(\kappa_1 \boldsymbol{\Sigma}^{-1} + \kappa_2 \boldsymbol{\Sigma} \right) \left(\boldsymbol{m} - \boldsymbol{y}_{\text{desire}}^{(n)} \right) \right],$$

where $\boldsymbol{m} = \boldsymbol{\mu}_{t-1}^{(n)}(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)})$ and $\boldsymbol{\Sigma}$ is a diagonal matrix whose (i, i)-th element is defined as $\sigma_{m, t-1}^{(n) \, 2}(\boldsymbol{y}^{(n-1)}, \boldsymbol{x}^{(n)})$.

FB-EI, FB-UCB In FB-EI and FB-UCB, the next sampling point is determined by using a fully black-box GP model. To construct this model, we employed an ARD Gaussian kernel and set the noise variance of GP to 10^{-4} . The kernel parameters were estimated by maximizing the marginal likelihood. In particular, FB-UCB used GP-UCB method (Srinivas et al., 2010), and we set its exploration parameter $\beta_{\rm GP-UCB}^{1/2}=2$.

EI-based Since EI-based AF is computed through sampling, we have to use stochastic gradient methods to optimize it in a naive implementation. However, L-BFGS-B can also be applied by utilizing reparameterization-trick (Kingma and Welling, 2014). At the beginning of the optimization, we draw *base-samples* $\omega^{(n)} \in \mathbb{R}^S$ from

standard multivariate Gaussian distribution for each middle stage. Then, instead of sampling each $\{y_s^{(n)}\}_{s=1}^S$ directly from Gaussian distribution, we sample it as follows:

$$y_s^{(n)} = \mu_{y_s^{(n)}} + \sigma_{y_s^{(n)}} \omega_s^{(n)}.$$

Here, $\mu_{y_s^{(n)}}$, $\sigma_{y_s^{(n)}}$ are the mean and standard deviation of the Gaussian distribution that follows $y_s^{(n)}$, respectively. The EI-based AF becomes a deterministic and differentiable function with the above modifications, and the L-BFGS-B method can be applied. Moreover, EI-based AF can also be applied to the vector output setting. We only need to change it to sample $y_s^{(n)}$ instead of $y_s^{(n)}$ in the middle stage.

In EI-SUS-R for the suspension setting experiments, we applied the stock reduction rule (13) except for the stock obtained in the last iteration.

F.3 Synthetic functions and Solar Cell Simulator

Sample Paths: In the sample path experiments, we used random Fourier features (RFFs) to draw continuous functions from GP priors. We first sampled 1000 RFFs and built Bayesian linear regression (BLR) model. From the BLR model, we sampled weight parameters and constructed functions.

Rosenbrock Function: For any $d \ge 2$, d-dimensional Rosenbrock function is defined as follows:

$$f(\mathbf{x}) = \sum_{i=1}^{d} (100(x_{i+1} - x_i^2)^2 + (x_i - 1)^2).$$

In our experiments, we used negative Rosenbrock functions, which are multiplied by -1.

Sphere Function: For any $d \ge 2$, d-dimensional Sphere function is defined as follows:

$$f(\boldsymbol{x}) = \sum_{i=1}^{d} x_i^2.$$

In our experiments, we used negative Sphere functions, which are multiplied by -1.

Matyas Function: Matyas function (d = 2) is defined as follows:

$$f(\mathbf{x}) = 0.26(x_1^2 + x_2^2) - 0.48x_1x_2.$$

In our experiments, we used negative Matyas functions, which are multiplied by -1.

Solar Cell Simulator: The simulators for stages one and two are Python implementations of the physical models described in Section 4 of (Bentzen, 2006). The simulator of stage three is based on PC1Dmod 6.2 (Haug and Greulich, 2016), which is the software for simulating solar cells. We confirmed that PC1D sometimes caused errors due to convergence failure of the internal calculations. However, standard BO frameworks cannot handle the situation where the observation fails. Thus, we used a kernel ridge regression model constructed using the data collected from PC1D as the simulator of stage 3. To create this simulator, we ran PC1D on each of the 2000 input points sampled using the LHS, and used the 1935 data points among them that could be run without error.

Algorithm 1: Cascade process optimization in sequential observation

```
Input: Initial data \{\mathcal{D}_0^{(n)}\}_{n=1}^N, \beta, \eta_t

1 for t=0,N,2N,\ldots,T do

2 Fit GP models using \{\mathcal{D}_{t-1}^{(n)}\}_{n=1}^N

3 for n=1,\ldots,N do

4 Select \boldsymbol{x}_{t+n}^{(n)} by maximizing (5c) or (11)

Observe output \boldsymbol{y}_{t+n}^{(n)} corresponding input (\boldsymbol{y}_{t+n-1}^{(n-1)},\boldsymbol{x}_{t+n}^{(n)})

6 \mathcal{D}_{t+n}^{(n)} \leftarrow \mathcal{D}_{t+n-1}^{(n)} \cup \{((\boldsymbol{y}_{t+n-1}^{(n-1)},\boldsymbol{x}_{t+n}^{(n)}),\boldsymbol{y}_{t+n}^{(n)})\}

7 end

8 t \leftarrow t+N

9 end

Output: Estimated solution \hat{\boldsymbol{x}}_t^{(1)},\ldots,\hat{\boldsymbol{x}}_t^{(N)}
```

Algorithm 2: Cascade process optimization in suspension setting

```
Input: \{\mathcal{D}_0^{(n)}\}_{n=1}^N, \beta, \eta_t, stage \operatorname{cost} \{\lambda^{(n)}\}_{n=1}^N, budget \lambda_{\max}

1 t \leftarrow 1, \mathcal{S}_t^{(0)} \leftarrow \{\mathbf{0}\}, \{\mathcal{S}_t^{(n)} \leftarrow \emptyset\}_{n=1}^{N-1}, spend \operatorname{cost} \lambda \leftarrow 0

2 while \lambda \leq \lambda_{\max} do

3 | Fit GP models using \{\mathcal{D}_{t-1}^{(n)}\}_{n=1}^N

4 | Select n_t, \boldsymbol{y}_t^{(n_t-1)}, \boldsymbol{x}_t^{(n)} by (15)

5 | Observe \boldsymbol{y}_t^{(n_t)}

6 | \mathcal{D}_t^{(n_t)} \leftarrow \mathcal{D}_{t-1}^{(n_t)} \cup \{((\boldsymbol{y}_t^{(n_t-1)}, \boldsymbol{x}_t^{(n_t)}), \boldsymbol{y}_t^{(n_t)})\}

7 | Remove stock \mathcal{S}_t^{(n_t-1)} \leftarrow \mathcal{S}_t^{(n_t-1)} \setminus \boldsymbol{y}_t^{(n_t-1)}

8 | if n_t \neq N then

9 | Add observed stock \mathcal{S}_t^{(n_t)} \leftarrow \mathcal{S}_t^{(n_t)} \cup \{\boldsymbol{y}_t^{(n_t)}\}

10 | \lambda \leftarrow \lambda + \lambda^{(n_t)}, \ t \leftarrow t + 1

11 end

Output: Estimated solution \hat{\boldsymbol{x}}_t^{(1)}, \dots, \hat{\boldsymbol{x}}_t^{(N)}
```

Hydrogen plasma treatment process: The real-world datasets for the first and second from (Miyagawa et al., 2021a) the stages are and simulator in https://www.pvlighthouse.com.au/equivalent-circuit, respectively. For both stages, we fitted the GPs with a Gaussian kernel, in which hyperparameters are selected by the marginal likelihood maximization. Then, as with sample paths, we sampled 1000 RFFs, built BLR models, and generate continuous sample paths once. We used these sample paths as the surrogate objectives.

F.4 Pseudo-codes of the proposed methods

We describe the proposed method of section 3 in algorithm 1. Additionally, we also describe the proposed method of extension setting in algorithm 2.

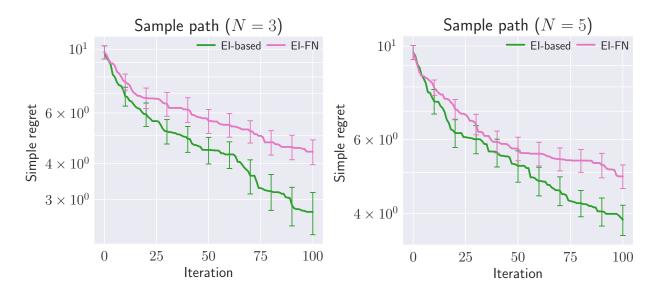


Figure 7: Results of comparison between EI-BASED and EI-FN

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G Additional Experimental Results

We additionally show the comparison between EI-BASED AF and EI-FN (Astudillo and Frazier, 2021). In this experiment, we used a three- and five-stage cascade consisting of GP pre-distributed sample paths. We set $\ell_d^{(n)}=1, \ell_w^{(n)}=1$, and the other experimental settings are the same as those described in Section 6. Figure 7 shows the results of 20 runs with different random seeds. Since the parameters $\ell_d^{(n)}$ and $\ell_w^{(n)}$ are relatively small, the sample paths can be sensitive to the input uncertainty. Therefore, in this experiment, EI-BASED AF that performs adaptive decision-making using intermediate observations clearly outperforms EI-FN, which is nonadaptive.

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