Appendix

A. Proofs

A.1. Proof of Theorem 4.1

In this section, we prove Theorem 4.1. First, we show two lemmas.

Lemma A.1. Let $\delta \in (0,1)$, and define $\beta_t = 2\log(|\mathcal{X} \times \Omega|\pi^2 t^2/(6\delta))$. Then, with a probability of at least $1-\delta$, the following inequality holds:

$$|f(\boldsymbol{x},\boldsymbol{w}) - \mu_{t-1}(\boldsymbol{x},\boldsymbol{w})| \le \beta_t^{1/2}\sigma_{t-1}(\boldsymbol{x},\boldsymbol{w}), \quad {}^{\forall}(\boldsymbol{x},\boldsymbol{w}) \in \mathcal{X} \times \Omega, {}^{\forall} t \ge 1.$$

Proof. By replacing D and π_t in Lemma 5.1 of [23] with $\mathcal{X} \times \Omega$ and $\pi^2 t^2/6$, respectively, we have Lemma A.1. $\square$

Lemma A.2. Let $\delta \in (0,1)$, $\xi > 0$ and $\eta = \min\left\{\frac{\xi\sigma_{0,min}}{2}, \frac{\xi^2\delta\sigma_{0,min}}{8|\mathcal{X}\times\Omega|}\right\}$. Then, with a probability of at least $1-\delta/2$, the following holds for any $\boldsymbol{x} \in \mathcal{X}$ and $p(\boldsymbol{w}) \in \mathcal{A}$:

$$\tilde{F}_{\eta,p}(\boldsymbol{x}) \equiv \sum_{\boldsymbol{w}\in\Omega} \mathbb{1}[h \ge f(\boldsymbol{x},\boldsymbol{w}) > h-\eta]p(\boldsymbol{w}) < \xi.$$

Proof. From Chebyshev's inequality, for any $\nu > 0$ and $(\boldsymbol{x},\boldsymbol{w}) \in \mathcal{X} \times \Omega$, the following inequality holds:

$$\mathbb{P}(|g_\eta(\boldsymbol{x},\boldsymbol{w}) - \mu^{(g_\eta)}(\boldsymbol{x},\boldsymbol{w})| \ge \nu) \le \frac{\mathbb{V}[g_\eta(\boldsymbol{x},\boldsymbol{w})]}{\nu^2},$$

where $g_\eta(\boldsymbol{x},\boldsymbol{w}) = \mathbb{1}[h \ge f(\boldsymbol{x},\boldsymbol{w}) > h-\eta]$ and $\mu^{(g_\eta)}(\boldsymbol{x},\boldsymbol{w}) = \mathbb{E}[g_\eta(\boldsymbol{x},\boldsymbol{w})]$. Hence, by replacing ν with $(\delta/(2|\mathcal{X} \times \Omega|))^{-1/2}(\mathbb{V}[g_\eta(\boldsymbol{x},\boldsymbol{w})])^{1/2}$, with a probability of at least $1-\delta/2$, the following holds for any $(\boldsymbol{x},\boldsymbol{w}) \in \mathcal{X} \times \Omega$:

$$|g_\eta(\boldsymbol{x},\boldsymbol{w}) - \mu^{(g_\eta)}(\boldsymbol{x},\boldsymbol{w})| < \frac{\sqrt{\mathbb{V}[g_\eta(\boldsymbol{x},\boldsymbol{w})]}}{\sqrt{\delta/(2|\mathcal{X}\times\Omega|)}}.$$

This implies that

$$g_\eta(\boldsymbol{x},\boldsymbol{w}) < \mu^{(g_\eta)}(\boldsymbol{x},\boldsymbol{w}) + \frac{\sqrt{\mathbb{V}[g_\eta(\boldsymbol{x},\boldsymbol{w})]}}{\sqrt{\delta/(2|\mathcal{X}\times\Omega|)}}. \tag{A.1}$$

Moreover, noting that $g_\eta(\boldsymbol{x},\boldsymbol{w})$ follows Bernoulli distribution, we get

$$\mathbb{V}[g_\eta(\boldsymbol{x},\boldsymbol{w})] = \mathbb{E}[g_\eta(\boldsymbol{x},\boldsymbol{w})](1-\mathbb{E}[g_\eta(\boldsymbol{x},\boldsymbol{w})]) \le \mathbb{E}[g_\eta(\boldsymbol{x},\boldsymbol{w})] = \mu^{(g_\eta)}(\boldsymbol{x},\boldsymbol{w}). \tag{A.2}$$

In addition, $\mu^{(g_\eta)}(\boldsymbol{x},\boldsymbol{w})$ can be expressed as

$$\mu^{(g_\eta)}(\boldsymbol{x},\boldsymbol{w}) = \Phi\left(\frac{h}{\sigma_0(\boldsymbol{x},\boldsymbol{w})}\right) - \Phi\left(\frac{h-\eta}{\sigma_0(\boldsymbol{x},\boldsymbol{w})}\right).$$

Furthermore, by using Taylor's expansion, for any $a < b$ it holds that

$$\Phi(b) = \Phi(a) + \phi(c)(b-a) \le \Phi(a) + \phi(0)(b-a) \le \Phi(a) + (b-a),$$

where $c \in (a,b)$. Thus, we obtain

$$\mu^{(g_\eta)}(\boldsymbol{x},\boldsymbol{w}) \le \frac{\eta}{\sigma_0(\boldsymbol{x},\boldsymbol{w})} \le \frac{\eta}{\sigma_{0,min}}. \tag{A.3}$$

Thus, by substituting (A.2) and (A.3) into (A.1), we have

$$g_\eta(\boldsymbol{x},\boldsymbol{w}) < \frac{\eta}{\sigma_{0,min}} + \sqrt{\frac{2\eta|\mathcal{X}\times\Omega|}{\delta\sigma_{0,min}}}.$$

Hence, from the definition of η, we get

$$g_\eta(\boldsymbol{x},\boldsymbol{w}) < \frac{\xi}{2} + \sqrt{\frac{\xi^2}{4}} = \xi.$$

Therefore, for any $p(\boldsymbol{w}) \in \mathcal{A}$, the following holds:

$$\tilde{F}_{\eta,p}(\boldsymbol{x}) = \sum_{\boldsymbol{w}\in\Omega} g_\eta(\boldsymbol{x},\boldsymbol{w})p(\boldsymbol{w}) < \sum_{\boldsymbol{w}\in\Omega} \xi p(\boldsymbol{w}) = \xi.$$

$\square$

By using Lemma A.1 and A.2, we prove Theorem 4.1.

Proof. Let $\delta \in (0,1)$ and $\beta_t = 2\log(|\mathcal{X} \times \Omega|\pi^2 t^2/(3\delta))$. Then, from Lemma A.1, with a probability of at least $1 - \delta/2$ the following holds:

$$l_t(\boldsymbol{x}, \boldsymbol{w}) \le f(\boldsymbol{x}, \boldsymbol{w}) \le u_t(\boldsymbol{x}, \boldsymbol{w}), \quad {}^\forall(\boldsymbol{x}, \boldsymbol{w}) \in \mathcal{X} \times \Omega, {}^\forall t \ge 1. \tag{A.4}$$

Thus, from the definition of $\tilde{Q}_t(\boldsymbol{x}, \boldsymbol{w}; \eta)$, it holds that

$$\mathbb{1}[f(\boldsymbol{x}, \boldsymbol{w}) > h] \le \tilde{u}_t(\boldsymbol{x}, \boldsymbol{w}; \eta).$$

This implies that

$$F(\boldsymbol{x}) = \inf_{p(\boldsymbol{w}) \in \mathcal{A}} \sum_{\boldsymbol{w} \in \Omega} \mathbb{1}[f(\boldsymbol{x}, \boldsymbol{w}) > h] p(\boldsymbol{w}) \le \inf_{p(\boldsymbol{w}) \in \mathcal{A}} \sum_{\boldsymbol{w} \in \Omega} \tilde{u}_t(\boldsymbol{x}, \boldsymbol{w}; \eta) p(\boldsymbol{w}) = u_t^{(F)}(\boldsymbol{x}; \eta).$$

Therefore, noting that the definition of L_t, we have

$$\boldsymbol{x} \in L_t \Rightarrow F(\boldsymbol{x}) \le u_t^{(F)}(\boldsymbol{x}; \eta) \le \alpha. \tag{A.5}$$

On the other hand, for any $\boldsymbol{x} \in \mathcal{X}$ and $p(\boldsymbol{w}) \in \mathcal{A}$, it holds that

$$\sum_{\boldsymbol{w} \in \Omega} \mathbb{1}[f(\boldsymbol{x}, \boldsymbol{w}) > h] p(\boldsymbol{w}) + \tilde{F}_{\eta,p}(\boldsymbol{x}) = \sum_{\boldsymbol{w} \in \Omega} \mathbb{1}[f(\boldsymbol{x}, \boldsymbol{w}) > h - \eta] p(\boldsymbol{w}).$$

Moreover, from Lemma A.2, with a probability of at least $1 - \delta/2$, the following holds:

$$\sum_{\boldsymbol{w} \in \Omega} \mathbb{1}[f(\boldsymbol{x}, \boldsymbol{w}) > h] p(\boldsymbol{w}) + \xi > \sum_{\boldsymbol{w} \in \Omega} \mathbb{1}[f(\boldsymbol{x}, \boldsymbol{w}) > h - \eta] p(\boldsymbol{w}). \tag{A.6}$$

Thus, we get the following inequality:

$$\inf_{p(\boldsymbol{w}) \in \mathcal{A}} \left(\sum_{\boldsymbol{w} \in \Omega} \mathbb{1}[f(\boldsymbol{x}, \boldsymbol{w}) > h] p(\boldsymbol{w}) + \xi \right) = F(\boldsymbol{x}) + \xi > \inf_{p(\boldsymbol{w}) \in \mathcal{A}} \sum_{\boldsymbol{w} \in \Omega} \mathbb{1}[f(\boldsymbol{x}, \boldsymbol{w}) > h - \eta] p(\boldsymbol{w}). \tag{A.7}$$

Furthermore, from the definition of $\tilde{Q}_t(\boldsymbol{x}, \boldsymbol{w}; \eta)$, the following inequality holds:

$$\mathbb{1}[f(\boldsymbol{x}, \boldsymbol{w}) > h - \eta] \ge \tilde{l}_t(\boldsymbol{x}, \boldsymbol{w}; \eta).$$

Therefore, we have

$$\inf_{p(\boldsymbol{w}) \in \mathcal{A}} \sum_{\boldsymbol{w} \in \Omega} \mathbb{1}[f(\boldsymbol{x}, \boldsymbol{w}) > h - \eta] p(\boldsymbol{w}) \ge \inf_{p(\boldsymbol{w}) \in \mathcal{A}} \sum_{\boldsymbol{w} \in \Omega} \tilde{l}_t(\boldsymbol{x}, \boldsymbol{w}; \eta) p(\boldsymbol{w}) = l_t^{(F)}(\boldsymbol{x}; \eta). \tag{A.8}$$

Hence, by combining (A.7) and (A.8), we obtain

$$l_t^{(F)}(\boldsymbol{x}; \eta) < F(\boldsymbol{x}) + \xi.$$

Thus, from the definition of H_t, it holds that

$$\boldsymbol{x} \in H_t \Rightarrow \alpha < F(\boldsymbol{x}) + \xi \Rightarrow \alpha - \xi < F(\boldsymbol{x}). \tag{A.9}$$

Hence, from (A.5), (A.9) and the definition of $e_\alpha(\boldsymbol{x})$, the following inequality holds:

$$\max_{\boldsymbol{x} \in \mathcal{X}} e_\alpha(\boldsymbol{x}) \le \xi.$$

Finally, since both (A.4) and (A.6) hold with a probability of at least $1 - \delta$, the following holds for any $t \ge 1$:

$$\mathbb{P}\left(\max_{\boldsymbol{x} \in \mathcal{X}} e_\alpha(\boldsymbol{x}) \le \xi \right) \ge 1 - \delta.$$

$\square$

A.2. Proof of Theorem 4.2 and 4.3

In this section, we prove Theorem 4.2 and 4.3. First, we show related lemmas.

Lemma A.3. Let $\eta > 0$ and $\beta_t > 0$. Suppose that the following holds for some $T \geq 1$:

$$2\beta_T^{1/2}\sigma_{T-1}(\boldsymbol{x},\boldsymbol{w}) < \eta, \quad {}^\forall(\boldsymbol{x},\boldsymbol{w}) \in \mathcal{X}\times\Omega. \tag{A.10}$$

Then, Algorithm 1 terminates after at most T iterations.

Proof. From the definition of $\tilde{Q}_t(\boldsymbol{x},\boldsymbol{w};\eta)$, if $l_T(\boldsymbol{x},\boldsymbol{w}) > h-\eta$, then $\tilde{l}_T(\boldsymbol{x},\boldsymbol{w};\eta) = \tilde{u}_T(\boldsymbol{x},\boldsymbol{w};\eta) = 1$. On the other hand, noting that $u_T(\boldsymbol{x},\boldsymbol{w}) - l_T(\boldsymbol{x},\boldsymbol{w}) = 2\beta_T^{1/2}\sigma_{T-1}(\boldsymbol{x},\boldsymbol{w})$ and (A.10), if $l_T(\boldsymbol{x},\boldsymbol{w}) \leq h-\eta$, then $u_T(\boldsymbol{x},\boldsymbol{w}) \leq h$. This implies that $\tilde{l}_T(\boldsymbol{x},\boldsymbol{w};\eta) = \tilde{u}_T(\boldsymbol{x},\boldsymbol{w};\eta) = 0$. Thus, under (A.10), the following holds for any $(\boldsymbol{x},\boldsymbol{w}) \in \mathcal{X}\times\Omega$:

$$\tilde{l}_T(\boldsymbol{x},\boldsymbol{w};\eta) = \tilde{u}_T(\boldsymbol{x},\boldsymbol{w};\eta).$$

Hence, from the definitions of $l_t^{(F)}(\boldsymbol{x};\eta)$ and $u_t^{(F)}(\boldsymbol{x};\eta)$, we have $l_t^{(F)}(\boldsymbol{x};\eta) = u_t^{(F)}(\boldsymbol{x};\eta)$. Therefore, for any $\boldsymbol{x}\in\mathcal{X}$, $\boldsymbol{x}$ satisfies $\boldsymbol{x}\in H_T$ or $\boldsymbol{x}\in L_T$, i.e., $U_T = \emptyset$. □

Lemma A.4. Let $\eta > 0$ and $\beta_t > 0$. Suppose that the following inequalities hold for some $(\boldsymbol{x}^*,\boldsymbol{w}^*) \in \mathcal{X}\times\Omega$:

$$\sigma^{-2}\sigma_{t-1}^2(\boldsymbol{x}^*,\boldsymbol{w}^*)\beta_t^{1/2} < \frac{\eta}{2}, \tag{A.11}$$

$$\sigma^{-2}\sigma_{t-1}^2(\boldsymbol{x}^*,\boldsymbol{w}^*) < \eta^2/4. \tag{A.12}$$

Then, (3.2) can be bounded as

$$a_{t-1}(\boldsymbol{x}^*,\boldsymbol{w}^*) \leq |\mathcal{X}|2^{|\Omega|}\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{\sigma^2\eta^2}{8\sigma_{t-1}^2(\boldsymbol{x}^*,\boldsymbol{w}^*)}\right).$$

Proof. First, we define the set $\mathcal{B}$ as

$$\mathcal{B} = \left\{\boldsymbol{b} = (b_1,\ldots,b_{|\Omega|}) \in \{0,1\}^{|\Omega|} \;\middle|\; \inf_{p(\boldsymbol{w})\in\mathcal{A}}\sum_{j=1}^{|\Omega|}p(\boldsymbol{w}_j)b_j > \alpha\right\}.$$

Moreover, for each $\boldsymbol{b}\in\mathcal{B}$, let $N^{(\boldsymbol{b})}$ be a subset of $\{1,\ldots,|\Omega|\}$ satisfying

$${}^\forall s \in N^{(\boldsymbol{b})},\ b_s = 1.$$

Then, the following holds for any $\boldsymbol{x}\in U_t$:

$$\begin{aligned}
&\mathbb{E}_{y^*}[\mathbb{1}[l_t^{(F)}(\boldsymbol{x};0|\boldsymbol{x}^*,\boldsymbol{w}^*,y^*) > \alpha]] \\
&= \mathbb{P}_{y^*}[(\mathbb{1}[l_t(\boldsymbol{x},\boldsymbol{w}_1|\boldsymbol{x}^*,\boldsymbol{w}^*,y^*) > h],\ldots,\mathbb{1}[l_t(\boldsymbol{x},\boldsymbol{w}_{|\Omega|}|\boldsymbol{x}^*,\boldsymbol{w}^*,y^*) > h])^\top \in \mathcal{B}] \\
&= \sum_{\boldsymbol{b}\in\mathcal{B}}\mathbb{P}_{y^*}[\mathbb{1}[l_t(\boldsymbol{x},\boldsymbol{w}_1|\boldsymbol{x}^*,\boldsymbol{w}^*,y^*) > h] = b_1,\ldots,\mathbb{1}[l_t(\boldsymbol{x},\boldsymbol{w}_{|\Omega|}|\boldsymbol{x}^*,\boldsymbol{w}^*,y^*) > h] = b_{|\Omega|}] \\
&\leq \sum_{\boldsymbol{b}\in\mathcal{B}}\mathbb{P}_{y^*}[{}^\forall s\in N^{(\boldsymbol{b})}, \mathbb{1}[l_t(\boldsymbol{x},\boldsymbol{w}_s|\boldsymbol{x}^*,\boldsymbol{w}^*,y^*) > h] = b_s],
\end{aligned} \tag{A.13}$$

where $l_t(\boldsymbol{x},\boldsymbol{w}_j|\boldsymbol{x}^*,\boldsymbol{w}^*,y^*)$ is the lower confidence bound of $f(\boldsymbol{x},\boldsymbol{w}_j)$ after adding $(\boldsymbol{x}^*,\boldsymbol{w}^*,y^*)$ to $\{(\boldsymbol{x}_i,\boldsymbol{w}_i,y_i)\}_{i=1}^t$. Next, for any $N^{(\boldsymbol{b})}$, there exists $s_{\boldsymbol{b}}\in N^{(\boldsymbol{b})}$ such that

$$l_t(\boldsymbol{x},\boldsymbol{w}_{s_{\boldsymbol{b}}}) \leq h-\eta. \tag{A.14}$$

In fact, if $l_t(\boldsymbol{x},\boldsymbol{w}_{s_{\boldsymbol{b}}}) > h-\eta$ for any $s\in N^{(\boldsymbol{b})}$, then we get

$$(\mathbb{1}[l_t(\boldsymbol{x},\boldsymbol{w}_1) > h-\eta],\ldots,\mathbb{1}[l_t(\boldsymbol{x},\boldsymbol{w}_{|\Omega|}) > h-\eta])^\top \in \mathcal{B},$$

which contradicts $\boldsymbol{x}\in U_t$. Furthermore, from Lemma 2 of [30], $\mathbb{P}_{y^*}[l_t(\boldsymbol{x},\boldsymbol{w}_{s_{\boldsymbol{b}}}|\boldsymbol{x}^*,\boldsymbol{w}^*,y^*) > h]$ can be calculated as

$$\mathbb{P}_{y^*}[l_t(\boldsymbol{x},\boldsymbol{w}_{s_{\boldsymbol{b}}}|\boldsymbol{x}^*,\boldsymbol{w}^*,y^*) > h] = \Phi\left(\frac{\sqrt{\sigma_{t-1}^2(\boldsymbol{x}^*,\boldsymbol{w}^*)+\sigma^2}}{|k_{t-1}((\boldsymbol{x},\boldsymbol{w}_{s_{\boldsymbol{b}}}),(\boldsymbol{x}^*,\boldsymbol{w}^*))|}(\mu_{t-1}(\boldsymbol{x},\boldsymbol{w}_{s_{\boldsymbol{b}}}) - \beta_t^{1/2}\sigma_{t-1}(\boldsymbol{x},\boldsymbol{w}_{s_{\boldsymbol{b}}}|\boldsymbol{x}^*,\boldsymbol{w}^*) - h)\right), \tag{A.15}$$

where $\sigma_{t-1}(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}}|\boldsymbol{x}^*, \boldsymbol{w}^*)$ is the posterior variance of $f(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}})$ after adding $(\boldsymbol{x}^*, \boldsymbol{w}^*, y^*)$ to $\{(\boldsymbol{x}_i, \boldsymbol{w}_i, y_i)\}_{i=1}^t$. Moreover, by using (A.14) we obtain

$$\begin{aligned}
&\mu_{t-1}(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}}) - \beta_t^{1/2}\sigma_{t-1}(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}}|\boldsymbol{x}^*, \boldsymbol{w}^*) - h \\
&= \mu_{t-1}(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}}) - \beta_t^{1/2}\sigma_{t-1}(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}}) + \beta_t^{1/2}\sigma_{t-1}(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}}) - \beta_t^{1/2}\sigma_{t-1}(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}}|\boldsymbol{x}^*, \boldsymbol{w}^*) - h \\
&= l_t(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}}) + \beta_t^{1/2}\sigma_{t-1}(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}}) - \beta_t^{1/2}\sigma_{t-1}(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}}|\boldsymbol{x}^*, \boldsymbol{w}^*) - h \\
&\le -\eta + \beta_t^{1/2}(\sigma_{t-1}(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}}) - \sigma_{t-1}(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}}|\boldsymbol{x}^*, \boldsymbol{w}^*)). \qquad \text{(A.16)}
\end{aligned}$$

In addition, the following three inequalities hold:

$$\sigma \le \sqrt{\sigma_{t-1}^2(\boldsymbol{x}^*, \boldsymbol{w}^*) + \sigma^2}, \qquad \text{(A.17)}$$

$$|k_{t-1}((\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}}), (\boldsymbol{x}^*, \boldsymbol{w}^*))| \le \sigma_{t-1}(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}})\sigma_{t-1}(\boldsymbol{x}^*, \boldsymbol{w}^*) \le \sigma_0(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}})\sigma_{t-1}(\boldsymbol{x}^*, \boldsymbol{w}^*) \le \sigma_{t-1}(\boldsymbol{x}^*, \boldsymbol{w}^*), \qquad \text{(A.18)}$$

$$\sigma_{t-1}(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}}) - \sigma_{t-1}(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}}|\boldsymbol{x}^*, \boldsymbol{w}^*) \le \frac{\sigma_{t-1}(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}})\sigma_{t-1}^2(\boldsymbol{x}^*, \boldsymbol{w}^*)}{\sigma_{t-1}^2(\boldsymbol{x}^*, \boldsymbol{w}^*) + \sigma^2} \le \frac{\sigma_0(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}})\sigma_{t-1}^2(\boldsymbol{x}^*, \boldsymbol{w}^*)}{\sigma^2} \le \frac{\sigma_{t-1}^2(\boldsymbol{x}^*, \boldsymbol{w}^*)}{\sigma^2}, \qquad \text{(A.19)}$$

where the first, second and third inequalities in (A.18) can be derived from Hölder's inequality, monotonicity of the posterior variance and the assumption $\max_{(\boldsymbol{x}, \boldsymbol{w}) \in \mathcal{X} \times \Omega} \sigma_0^2(\boldsymbol{x}, \boldsymbol{w}) \le 1$, respectively. Similarly, the first inequality in (A.19) can be derived from the equation (39) of [30]. Therefore, by substituting (A.16)–(A.19) and (A.11) into (A.15), we obtain the following inequality:

$$\mathbb{P}_{y^*}[l_t(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}}|\boldsymbol{x}^*, \boldsymbol{w}^*, y^*) > h] \le \Phi\left(\frac{\sigma}{\sigma_{t-1}(\boldsymbol{x}^*, \boldsymbol{w}^*)}(-\eta/2)\right), \qquad \text{(A.20)}$$

Moreover, noting that the assumption (A.12) is equal to the condition $1 < \sigma\sigma_{t-1}^{-1}(\boldsymbol{x}^*, \boldsymbol{w}^*)(\eta/2)$, the right hand side in (A.20) can be bounded as

$$\begin{aligned}
\Phi\left(\frac{\sigma}{\sigma_{t-1}(\boldsymbol{x}^*, \boldsymbol{w}^*)}(-\eta/2)\right) &= \int_{-\infty}^{\frac{\sigma}{\sigma_{t-1}(\boldsymbol{x}^*, \boldsymbol{w}^*)}(-\eta/2)} \phi(z)\mathrm{d}z \\
&= \int_{\frac{\sigma}{\sigma_{t-1}(\boldsymbol{x}^*, \boldsymbol{w}^*)}(\eta/2)}^{\infty} \phi(z)\mathrm{d}z \\
&\le \int_{\frac{\sigma}{\sigma_{t-1}(\boldsymbol{x}^*, \boldsymbol{w}^*)}(\eta/2)}^{\infty} z\phi(z)\mathrm{d}z \\
&= [-\phi(z)]_{\frac{\sigma}{\sigma_{t-1}(\boldsymbol{x}^*, \boldsymbol{w}^*)}(\eta/2)}^{\infty} \\
&= \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2\eta^2}{8\sigma_{t-1}^2(\boldsymbol{x}^*, \boldsymbol{w}^*)}\right). \qquad \text{(A.21)}
\end{aligned}$$

Finally, from (A.13), (A.20) and (A.21), $\mathbb{E}_{y^*}[\mathbb{1}[l_t^{(F)}(\boldsymbol{x}; 0|\boldsymbol{x}^*, \boldsymbol{w}^*, y^*) > \alpha]]$ can be bounded as

$$\begin{aligned}
&\mathbb{E}_{y^*}[\mathbb{1}[l_t^{(F)}(\boldsymbol{x}; 0|\boldsymbol{x}^*, \boldsymbol{w}^*, y^*) > \alpha]] \\
&\le \sum_{\boldsymbol{b} \in \mathcal{B}} \mathbb{P}_{y^*}[{}^\forall s \in N^{(\boldsymbol{b})}, \mathbb{1}[l_t(\boldsymbol{x}, \boldsymbol{w}_s|\boldsymbol{x}^*, \boldsymbol{w}^*, y^*) > h] = b_s] \\
&\le \sum_{\boldsymbol{b} \in \mathcal{B}} \mathbb{P}_{y^*}[\mathbb{1}[l_t(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}}|\boldsymbol{x}^*, \boldsymbol{w}^*, y^*) > h] = b_{s_{\boldsymbol{b}}}] \\
&= \sum_{\boldsymbol{b} \in \mathcal{B}} \mathbb{P}_{y^*}[l_t(\boldsymbol{x}, \boldsymbol{w}_{s_{\boldsymbol{b}}}|\boldsymbol{x}^*, \boldsymbol{w}^*, y^*) > h] \\
&\le \sum_{\boldsymbol{b} \in \mathcal{B}} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2\eta^2}{8\sigma_{t-1}^2(\boldsymbol{x}^*, \boldsymbol{w}^*)}\right) \\
&= |\mathcal{B}| \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2\eta^2}{8\sigma_{t-1}^2(\boldsymbol{x}^*, \boldsymbol{w}^*)}\right) \le 2^{|\Omega|} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2\eta^2}{8\sigma_{t-1}^2(\boldsymbol{x}^*, \boldsymbol{w}^*)}\right).
\end{aligned}$$

Therefore, from the definition of $a_{t-1}(\boldsymbol{x}^*, \boldsymbol{w}^*)$, we have

$$
\begin{aligned}
a_{t-1}(\boldsymbol{x}^*, \boldsymbol{w}^*) &= \sum_{\boldsymbol{x} \in U_t} \mathbb{E}_{y^*}[\mathbb{1}[l_t^{(F)}(\boldsymbol{x}; 0 | \boldsymbol{x}^*, \boldsymbol{w}^*, y^*) > \alpha]] \\
&\leq \sum_{\boldsymbol{x} \in U_t} 2^{|\Omega|} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2 \eta^2}{8\sigma_{t-1}^2(\boldsymbol{x}^*, \boldsymbol{w}^*)}\right) \\
&= |U_t| 2^{|\Omega|} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2 \eta^2}{8\sigma_{t-1}^2(\boldsymbol{x}^*, \boldsymbol{w}^*)}\right) \leq |\mathcal{X}| 2^{|\Omega|} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2 \eta^2}{8\sigma_{t-1}^2(\boldsymbol{x}^*, \boldsymbol{w}^*)}\right).
\end{aligned}
$$

□

Lemma A.5. Let $\eta > 0$, $\beta_t > 0$ and $\gamma > 0$. Also let $(\boldsymbol{x}_t, \boldsymbol{w}_t) \in \mathcal{X} \times \Omega$ be a maximum point of $a_{t-1}^{(1)}(\boldsymbol{x}^*, \boldsymbol{w}^*)$. Assume that the following inequalities hold for some $T \geq 1$:

$$\sigma^{-2} \sigma_{T-1}^2(\boldsymbol{x}_T, \boldsymbol{w}_T) \beta_T^{1/2} < \frac{\eta}{2}, \tag{A.22}$$

$$\sigma^{-2} \sigma_{T-1}^2(\boldsymbol{x}_T, \boldsymbol{w}_T) < \eta^2/4, \tag{A.23}$$

$$\sigma_{T-1}^2(\boldsymbol{x}_T, \boldsymbol{w}_T) \beta_T < \eta^2/4, \tag{A.24}$$

$$\frac{1}{2} \log \beta_T - \frac{\eta^2 \sigma^2}{8\sigma_{T-1}^2(\boldsymbol{x}_T, \boldsymbol{w}_T)} < \log(|\mathcal{X}|^{-1} 2^{-|\Omega|} \eta \gamma 2^{-1} \sqrt{2\pi}). \tag{A.25}$$

Then, Algorithm 1 terminates after at most T iterations.

Proof. From the definitions of $a_{t-1}^{(1)}(\boldsymbol{x}^*, \boldsymbol{w}^*)$ and $(\boldsymbol{x}_t, \boldsymbol{w}_t)$, the following holds for any $(\boldsymbol{x}, \boldsymbol{w}) \in \mathcal{X} \times \Omega$:

$$\gamma \sigma_{T-1}(\boldsymbol{x}, \boldsymbol{w}) \leq a_{T-1}^{(1)}(\boldsymbol{x}, \boldsymbol{w}) \leq a_{T-1}^{(1)}(\boldsymbol{x}_T, \boldsymbol{w}_T) = \max\{a_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T), \gamma \sigma_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T)\}. \tag{A.26}$$

In addition, from (A.22), (A.23) and Lemma A.4, $a_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T)$ can be bounded as

$$a_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T) \leq |\mathcal{X}| 2^{|\Omega|} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2 \eta^2}{8\sigma_{T-1}^2(\boldsymbol{x}_T, \boldsymbol{w}_T)}\right). \tag{A.27}$$

Thus, by substituting (A.27) into (A.26), we have

$$\gamma \sigma_{T-1}(\boldsymbol{x}, \boldsymbol{w}) \leq \max\left\{|\mathcal{X}| 2^{|\Omega|} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2 \eta^2}{8\sigma_{T-1}^2(\boldsymbol{x}_T, \boldsymbol{w}_T)}\right), \gamma \sigma_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T)\right\}.$$

This implies that

$$\beta_T^{1/2} \sigma_{T-1}(\boldsymbol{x}, \boldsymbol{w}) \leq \max\left\{\gamma^{-1} \beta_T^{1/2} |\mathcal{X}| 2^{|\Omega|} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2 \eta^2}{8\sigma_{T-1}^2(\boldsymbol{x}_T, \boldsymbol{w}_T)}\right), \beta_T^{1/2} \sigma_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T)\right\}. \tag{A.28}$$

On the other hand, (A.24) and (A.25) are equal to the following inequalities, respectively:

$$\beta_T^{1/2} \sigma_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T) < \eta/2, \tag{A.29}$$

$$\exp\left(-\frac{\eta^2 \sigma^2}{8\sigma_{T-1}^2(\boldsymbol{x}_T, \boldsymbol{w}_T)}\right) < \frac{|\mathcal{X}|^{-1} 2^{-|\Omega|} \eta \gamma 2^{-1} \sqrt{2\pi}}{\beta_T^{1/2}}. \tag{A.30}$$

Hence, by combining (A.28), (A.29) and (A.30), we get $\beta_T^{1/2} \sigma_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T) < \eta/2$. Therefore, from Lemma A.3, we have Lemma A.5. □

Lemma A.6. Let $\eta > 0$ and $\beta_t > 0$. Assume that (A.11) and (A.12) hold for some $(\boldsymbol{x}^*, \boldsymbol{w}^*) \in \mathcal{X} \times \Omega$. Then, $\mathrm{MILE}_{t-1}(\boldsymbol{x}^*, \boldsymbol{w}^*)$ can be bounded as

$$\mathrm{MILE}_{t-1}(\boldsymbol{x}^*, \boldsymbol{w}^*) \leq |\mathcal{X} \times \Omega| \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2 \eta^2}{8\sigma_{t-1}^2(\boldsymbol{x}^*, \boldsymbol{w}^*)}\right).$$

Proof. From Lemma 2 of [30] and the definition of $\mathrm{MILE}_{t-1}(\boldsymbol{x}, \boldsymbol{w})$, the following holds:

$$
\begin{aligned}
&\mathrm{MILE}_{t-1}(\boldsymbol{x}^*, \boldsymbol{w}^*) \\
&= \sum_{(\boldsymbol{x},\boldsymbol{w})\in U_t\times\Omega} \mathbb{E}_{y^*}[\mathbb{1}[l_t(\boldsymbol{x},\boldsymbol{w}|\boldsymbol{x}^*,\boldsymbol{w}^*,y^*) > h]] - |\{(\boldsymbol{x},\boldsymbol{w}) \in U_t\times\Omega \mid l_t(\boldsymbol{x},\boldsymbol{w}) > h-\eta\}| \\
&= \sum_{(\boldsymbol{x},\boldsymbol{w})\in U_t\times\Omega} \mathbb{P}_{y^*}[l_t(\boldsymbol{x},\boldsymbol{w}|\boldsymbol{x}^*,\boldsymbol{w}^*,y^*) > h] - |\{(\boldsymbol{x},\boldsymbol{w}) \in U_t\times\Omega \mid l_t(\boldsymbol{x},\boldsymbol{w}) > h-\eta\}| \\
&\leq \sum_{(\boldsymbol{x},\boldsymbol{w})\in U_t\times\Omega} \Phi\left(\frac{\sqrt{\sigma^2_{t-1}(\boldsymbol{x}^*,\boldsymbol{w}^*)+\sigma^2}}{|k_{t-1}((\boldsymbol{x},\boldsymbol{w}),(\boldsymbol{x}^*,\boldsymbol{w}^*))|}(\mu_{t-1}(\boldsymbol{x},\boldsymbol{w}) - \beta_t^{1/2}\sigma_{t-1}(\boldsymbol{x},\boldsymbol{w}|\boldsymbol{x}^*,\boldsymbol{w}^*) - h)\right) \\
&\quad - |\{(\boldsymbol{x},\boldsymbol{w}) \in U_t\times\Omega \mid l_t(\boldsymbol{x},\boldsymbol{w}) > h-\eta\}|. \\
&= \sum_{(\boldsymbol{x},\boldsymbol{w})\in U_t\times\Omega} \left\{ \Phi\left(\frac{\sqrt{\sigma^2_{t-1}(\boldsymbol{x}^*,\boldsymbol{w}^*)+\sigma^2}}{|k_{t-1}((\boldsymbol{x},\boldsymbol{w}),(\boldsymbol{x}^*,\boldsymbol{w}^*))|}(\mu_{t-1}(\boldsymbol{x},\boldsymbol{w}) - \beta_t^{1/2}\sigma_{t-1}(\boldsymbol{x},\boldsymbol{w}|\boldsymbol{x}^*,\boldsymbol{w}^*) - h)\right) - \mathbb{1}[l_t(\boldsymbol{x},\boldsymbol{w}) > h-\eta] \right\}.
\end{aligned} \tag{A.31}
$$

Next, for each $(\boldsymbol{x},\boldsymbol{w}) \in U_t\times\Omega$, we consider the two cases of $l_t(\boldsymbol{x},\boldsymbol{w}) > h-\eta$ and $l_t(\boldsymbol{x},\boldsymbol{w}) \leq h-\eta$. If $l_t(\boldsymbol{x},\boldsymbol{w}) > h-\eta$, then the following inequality holds:

$$
\begin{aligned}
&\Phi\left(\frac{\sqrt{\sigma^2_{t-1}(\boldsymbol{x}^*,\boldsymbol{w}^*)+\sigma^2}}{|k_{t-1}((\boldsymbol{x},\boldsymbol{w}),(\boldsymbol{x}^*,\boldsymbol{w}^*))|}(\mu_{t-1}(\boldsymbol{x},\boldsymbol{w}) - \beta_t^{1/2}\sigma_{t-1}(\boldsymbol{x},\boldsymbol{w}|\boldsymbol{x}^*,\boldsymbol{w}^*) - h)\right) - \mathbb{1}[l_t(\boldsymbol{x},\boldsymbol{w}) > h-\eta] \\
&\leq 0 \leq \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2\eta^2}{8\sigma^2_{t-1}(\boldsymbol{x}^*,\boldsymbol{w}^*)}\right).
\end{aligned}
$$

On the other hand, if $l_t(\boldsymbol{x},\boldsymbol{w}) \leq h-\eta$, then using (A.15)–(A.21) we have

$$
\begin{aligned}
&\Phi\left(\frac{\sqrt{\sigma^2_{t-1}(\boldsymbol{x}^*,\boldsymbol{w}^*)+\sigma^2}}{|k_{t-1}((\boldsymbol{x},\boldsymbol{w}),(\boldsymbol{x}^*,\boldsymbol{w}^*))|}(\mu_{t-1}(\boldsymbol{x},\boldsymbol{w}) - \beta_t^{1/2}\sigma_{t-1}(\boldsymbol{x},\boldsymbol{w}|\boldsymbol{x}^*,\boldsymbol{w}^*) - h)\right) - \mathbb{1}[l_t(\boldsymbol{x},\boldsymbol{w}) > h-\eta] \\
&= \Phi\left(\frac{\sqrt{\sigma^2_{t-1}(\boldsymbol{x}^*,\boldsymbol{w}^*)+\sigma^2}}{|k_{t-1}((\boldsymbol{x},\boldsymbol{w}),(\boldsymbol{x}^*,\boldsymbol{w}^*))|}(\mu_{t-1}(\boldsymbol{x},\boldsymbol{w}) - \beta_t^{1/2}\sigma_{t-1}(\boldsymbol{x},\boldsymbol{w}|\boldsymbol{x}^*,\boldsymbol{w}^*) - h)\right) \leq \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2\eta^2}{8\sigma^2_{t-1}(\boldsymbol{x}^*,\boldsymbol{w}^*)}\right).
\end{aligned}
$$

Therefore, in both cases, the following inequality holds:

$$
\begin{aligned}
&\Phi\left(\frac{\sqrt{\sigma^2_{t-1}(\boldsymbol{x}^*,\boldsymbol{w}^*)+\sigma^2}}{|k_{t-1}((\boldsymbol{x},\boldsymbol{w}),(\boldsymbol{x}^*,\boldsymbol{w}^*))|}(\mu_{t-1}(\boldsymbol{x},\boldsymbol{w}) - \beta_t^{1/2}\sigma_{t-1}(\boldsymbol{x},\boldsymbol{w}|\boldsymbol{x}^*,\boldsymbol{w}^*) - h)\right) - \mathbb{1}[l_t(\boldsymbol{x},\boldsymbol{w}) > h-\eta] \\
&\leq \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2\eta^2}{8\sigma^2_{t-1}(\boldsymbol{x}^*,\boldsymbol{w}^*)}\right).
\end{aligned} \tag{A.32}
$$

Thus, by substituting (A.32) into (A.31), we obtain

$$
\begin{aligned}
\mathrm{MILE}_{t-1}(\boldsymbol{x}^*,\boldsymbol{w}^*) \leq \sum_{(\boldsymbol{x},\boldsymbol{w})\in U_t\times\Omega} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2\eta^2}{8\sigma^2_{t-1}(\boldsymbol{x}^*,\boldsymbol{w}^*)}\right) &= |U_t\times\Omega| \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2\eta^2}{8\sigma^2_{t-1}(\boldsymbol{x}^*,\boldsymbol{w}^*)}\right) \\
&\leq |\mathcal{X}\times\Omega| \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2\eta^2}{8\sigma^2_{t-1}(\boldsymbol{x}^*,\boldsymbol{w}^*)}\right).
\end{aligned}
$$

□

Lemma A.7. Let $\eta > 0$, $\beta_t > 0$, $\gamma > 0$ and $\tilde{\gamma} > 0$. Also let $(\boldsymbol{x}_t, \boldsymbol{w}_t) \in \mathcal{X}\times\Omega$ be a maximum point of $a^{(2)}_{t-1}(\boldsymbol{x}^*,\boldsymbol{w}^*)$. Assume that the inequalities (A.22), (A.23) and (A.24) hold for some $T \geq 1$. In addition, assume that the following inequalities hold:

$$
\frac{1}{2}\log\beta_T - \frac{\eta^2\sigma^2}{8\sigma^2_{T-1}(\boldsymbol{x}_T,\boldsymbol{w}_T)} < \log(|\mathcal{X}|^{-1}2^{-|\Omega|}\eta\gamma\tilde{\gamma}2^{-1}\sqrt{2\pi}), \tag{A.33}
$$

$$
\frac{1}{2}\log\beta_T - \frac{\eta^2\sigma^2}{8\sigma^2_{T-1}(\boldsymbol{x}_T,\boldsymbol{w}_T)} < \log(|\mathcal{X}\times\Omega|^{-1}\eta\tilde{\gamma}2^{-1}\sqrt{2\pi}). \tag{A.34}
$$

Then, Algorithm 1 terminates after at most T iterations.

Proof. From the definition of $a^{(2)}_{t-1}(\boldsymbol{x}^*, \boldsymbol{w}^*)$ and $(\boldsymbol{x}_t, \boldsymbol{w}_t)$, the following holds for any $(\boldsymbol{x}, \boldsymbol{w}) \in \mathcal{X} \times \Omega$:

$$\begin{aligned} \gamma\tilde{\gamma}\sigma_{T-1}(\boldsymbol{x}, \boldsymbol{w}) \le \gamma \mathrm{RMILE}_{T-1}(\boldsymbol{x}, \boldsymbol{w}) \le a^{(2)}_{T-1}(\boldsymbol{x}, \boldsymbol{w}) \le a^{(2)}_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T) \\ = \max\{a_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T), \gamma \mathrm{RMILE}_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T)\}. \end{aligned} \tag{A.35}$$

Furthermore, from (A.22), (A.23) and Lemma A.6, we have

$$\begin{aligned} \gamma \mathrm{RMILE}_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T) &= \max\{\gamma \mathrm{MILE}_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T), \gamma\tilde{\gamma}\sigma_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T)\} \\ &\le \max\left\{\gamma|\mathcal{X} \times \Omega| \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2\eta^2}{8\sigma^2_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T)}\right), \gamma\tilde{\gamma}\sigma_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T)\right\}. \end{aligned} \tag{A.36}$$

Moreover, from (A.24) and (A.34), we get the following inequalities:

$$\sigma_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T) < \beta_T^{-1/2}\eta/2, \tag{A.37}$$

$$|\mathcal{X} \times \Omega| \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2\eta^2}{8\sigma^2_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T)}\right) < \beta_T^{-1/2}\eta\tilde{\gamma}/2. \tag{A.38}$$

Thus, by substituting (A.37) and (A.38) into (A.36), we obtain

$$\gamma \mathrm{RMILE}_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T) \le \gamma\tilde{\gamma}\beta_T^{-1/2}\eta/2. \tag{A.39}$$

Similarly, from (A.22), (A.23), (A.33) and Lemma A.4, $a_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T)$ can be bounded as

$$a_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T) \le |\mathcal{X}| 2^{|\Omega|} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\sigma^2\eta^2}{8\sigma^2_{T-1}(\boldsymbol{x}_T, \boldsymbol{w}_T)}\right) \le \gamma\tilde{\gamma}\beta_T^{-1/2}\eta/2. \tag{A.40}$$

Hence, by combining (A.39) and (A.40) into (A.35), we get

$$\gamma\tilde{\gamma}\sigma_{T-1}(\boldsymbol{x}, \boldsymbol{w}) \le \gamma\tilde{\gamma}\beta_T^{-1/2}\eta/2.$$

This implies that $2\beta_T^{1/2}\sigma_{T-1}(\boldsymbol{x}, \boldsymbol{w}) < \eta$. Therefore, from Lemma A.3, we have Lemma A.7. □

Lemma A.8. Let $(\boldsymbol{x}_1, \boldsymbol{w}_1), \ldots, (\boldsymbol{x}_t, \boldsymbol{w}_t)$ be selected points, and define $C_1 = 2/\log(1+\sigma^{-2})$. Then, there exists a natural number $t' \le t$ such that

$$\sigma^2_{t'-1}(\boldsymbol{x}_{t'}, \boldsymbol{w}_{t'}) \le \frac{C_1\kappa_t}{t}.$$

Proof. From Lemma 5.3 in [23], the mutual information $I(\boldsymbol{y}_A; f)$ can be expressed as

$$I(\boldsymbol{y}_A; f) = \frac{1}{2}\sum_{i=1}^{t} \log(1 + \sigma^{-2}\sigma^2_{i-1}(\boldsymbol{x}_i, \boldsymbol{w}_i)). \tag{A.41}$$

Similarly, from Lemma 5.4 in [23], $\sigma^2_{i-1}(\boldsymbol{x}_i, \boldsymbol{w}_i)$ can be bounded as

$$\sigma^2_{i-1}(\boldsymbol{x}_i, \boldsymbol{w}_i) \le \frac{\log(1 + \sigma^{-2}\sigma^2_{i-1}(\boldsymbol{x}_i, \boldsymbol{w}_i))}{\log(1 + \sigma^{-2})}. \tag{A.42}$$

Hence, by using (A.41) and (A.42), we get

$$\sum_{i=1}^{t} \sigma^2_{i-1}(\boldsymbol{x}_i, \boldsymbol{w}_i) \le \frac{2}{\log(1 + \sigma^{-2})} I(\boldsymbol{y}_t; f) \le C_1\kappa_t. \tag{A.43}$$

Next, we define t' as $t' = \mathrm{argmin}_{1 \le i \le t}\, \sigma^2_{i-1}(\boldsymbol{x}_i, \boldsymbol{w}_i)$. Then, it follows that

$$t\sigma^2_{t'-1}(\boldsymbol{x}_{t'}, \boldsymbol{w}_{t'}) \le \sum_{i=1}^{t} \sigma^2_{i-1}(\boldsymbol{x}_i, \boldsymbol{w}_i). \tag{A.44}$$

Therefore, by combining (A.43) and (A.44), we have the desired inequality. □

Finally, using Lemma A.5, A.7 and A.8, we prove Theorem 4.2 and 4.3.

Proof. From Lemma A.8 and monotonicity of β_t, for any $t \geq 1$, there exists a natural number $t' \leq t$ such that

$$\begin{aligned}
\sigma^{-2}\sigma^2_{t'-1}(\boldsymbol{x}_{t'}, \boldsymbol{w}_{t'})\beta^{1/2}_{t'} &\leq \frac{\sigma^{-2}\beta^{1/2}_{t'}C_1\kappa_t}{t} \leq \frac{\sigma^{-2}\beta^{1/2}_{t}C_1\kappa_t}{t}, \\
\sigma^{-2}\sigma^2_{t'-1}(\boldsymbol{x}_{t'}, \boldsymbol{w}_{t'}) &\leq \frac{\sigma^{-2}C_1\kappa_t}{t}, \\
\sigma^2_{t'-1}(\boldsymbol{x}_{t'}, \boldsymbol{w}_{t'})\beta_{t'} &\leq \frac{C_1\beta_{t'}\kappa_t}{t} \leq \frac{C_1\beta_t\kappa_t}{t}, \\
\frac{1}{2}\log\beta_{t'} - \frac{\eta^2\sigma^2}{8\sigma^2_{t'-1}(\boldsymbol{x}_{t'}, \boldsymbol{w}_{t'})} &\leq \frac{1}{2}\log\beta_{t'} - \frac{T\eta^2\sigma^2}{8C_1\kappa_t} \leq \frac{1}{2}\log\beta_t - \frac{T\eta^2\sigma^2}{8C_1\kappa_t}.
\end{aligned} \tag{A.45}$$

Hence, from (A.45), if the inequality conditions in Theorem 4.2 hold, then the inequality conditions in Lemma A.5 also hold for some $\tilde{T} \leq T$. Therefore, from Lemma A.5, Algorithm 1 terminates after at most $\tilde{T}$ iterations, i.e., Theorem 4.2 holds. By using the same argument, Theorem 4.3 can also be proved. □

A.3. Proof of Lemma 3.1 and 3.2

First, we prove Lemma 3.1

Proof. From GP properties, the posterior mean $\mu_{t-1}(\boldsymbol{x}, \boldsymbol{w}|\boldsymbol{x}^*, \boldsymbol{w}^*, y^*)$ and the posterior variance $\sigma^2_{t-1}(\boldsymbol{x}, \boldsymbol{w}|\boldsymbol{x}^*, \boldsymbol{w}^*)$ of $f(\boldsymbol{x}, \boldsymbol{w})$ after adding $(\boldsymbol{x}^*, \boldsymbol{w}^*, y^*)$ can be written as follows (see, e.g., [29]):

$$\begin{aligned}
\mu_{t-1}(\boldsymbol{x}, \boldsymbol{w}|\boldsymbol{x}^*, \boldsymbol{w}^*, y^*) &= \mu_{t-1}(\boldsymbol{x}, \boldsymbol{w}) - \frac{k_{t-1}((\boldsymbol{x}, \boldsymbol{w}), (\boldsymbol{x}^*, \boldsymbol{w}^*))}{\sigma^2_{t-1}(\boldsymbol{x}^*, \boldsymbol{w}^*) + \sigma^2}(y^* - \mu_{t-1}(\boldsymbol{x}^*, \boldsymbol{w}^*)), \\
\sigma^2_{t-1}(\boldsymbol{x}, \boldsymbol{w}|\boldsymbol{x}^*, \boldsymbol{w}^*) &= \sigma^2_{t-1}(\boldsymbol{x}, \boldsymbol{w}) - \frac{k^2_{t-1}((\boldsymbol{x}, \boldsymbol{w}), (\boldsymbol{x}^*, \boldsymbol{w}^*))}{\sigma^2_{t-1}(\boldsymbol{x}^*, \boldsymbol{w}^*) + \sigma^2}.
\end{aligned}$$

Thus, $l_t(\boldsymbol{x}, \boldsymbol{w}|\boldsymbol{x}^*, \boldsymbol{w}^*, y^*)$ is a linear function with respect to (w.r.t.) y^*. Hence, the indicator function $\mathbb{1}[l_t(\boldsymbol{x}, \boldsymbol{w}_j|\boldsymbol{x}^*, \boldsymbol{w}^*, y^*) > h]$ is a piecewise constant function w.r.t. y^*, where the breakpoint is $y^* = r_j$. Therefore, for any $s \in \{1, \ldots, |\Omega| + 1\}$, the following holds:

$$\begin{aligned}
&(\mathbb{1}[l_t(\boldsymbol{x}, \boldsymbol{w}_1|\boldsymbol{x}^*, \boldsymbol{w}^*, c) > h], \ldots, \mathbb{1}[l_t(\boldsymbol{x}, \boldsymbol{w}_{|\Omega|}|\boldsymbol{x}^*, \boldsymbol{w}^*, c) > h])^\top \\
&= (\mathbb{1}[l_t(\boldsymbol{x}, \boldsymbol{w}_1|\boldsymbol{x}^*, \boldsymbol{w}^*, c') > h], \ldots, \mathbb{1}[l_t(\boldsymbol{x}, \boldsymbol{w}_{|\Omega|}|\boldsymbol{x}^*, \boldsymbol{w}^*, c') > h])^\top, \quad {}^\forall c, c' \in R_s.
\end{aligned}$$

This implies that

$$l^{(F)}_t(\boldsymbol{x}; 0|\boldsymbol{x}^*, \boldsymbol{w}^*, c) = l^{(F)}_t(\boldsymbol{x}; 0|\boldsymbol{x}^*, \boldsymbol{w}^*, c'), \quad {}^\forall c, c' \in R_s.$$

Hence, using this we have

$$\begin{aligned}
&\mathbb{E}_{y^*}[\mathbb{1}[l^{(F)}_t(\boldsymbol{x}; 0|\boldsymbol{x}^*, \boldsymbol{w}^*, y^*) > \alpha]] \\
&= \int \mathbb{1}[l^{(F)}_t(\boldsymbol{x}; 0|\boldsymbol{x}^*, \boldsymbol{w}^*, y^*) > \alpha]p(y^*)\mathrm{d}y^* \\
&= \sum_{s=1}^{|\Omega|+1} \int_{y^* \in R_s} \mathbb{1}[l^{(F)}_t(\boldsymbol{x}; 0|\boldsymbol{x}^*, \boldsymbol{w}^*, y^*) > \alpha]p(y^*)\mathrm{d}y^* \\
&= \sum_{s=1}^{|\Omega|+1} \mathbb{1}[l^{(F)}_t(\boldsymbol{x}; 0|\boldsymbol{x}^*, \boldsymbol{w}^*, c_s) > \alpha] \int_{y^* \in R_s} p(y^*)\mathrm{d}y^* \\
&= \sum_{s=1}^{|\Omega|+1} \mathbb{P}(y^* \in R_s)\mathbb{1}[l^{(F)}_t(\boldsymbol{x}; 0|\boldsymbol{x}^*, \boldsymbol{w}^*, c_s) > \alpha].
\end{aligned}$$

□

Next, we prove Lemma 3.2.

Proof. From the definition of $l^{(F)}_t(\boldsymbol{x}; 0|\boldsymbol{x}^*, \boldsymbol{w}^*, c_s)$, $l^{(F)}_t(\boldsymbol{x}; 0|\boldsymbol{x}^*, \boldsymbol{w}^*, c_s)$ can be expressed as

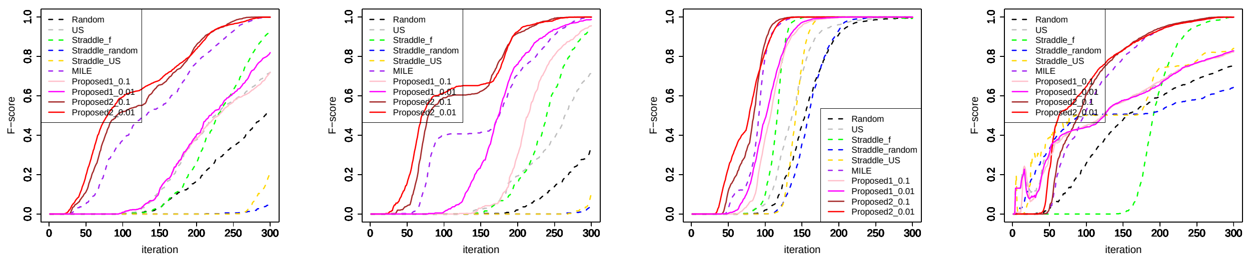
$$l^{(F)}_t(\boldsymbol{x}; 0|\boldsymbol{x}^*, \boldsymbol{w}^*, c_s) = \inf_{p(\boldsymbol{w}) \in \mathcal{A}} \sum_{\boldsymbol{w} \in \Omega} \mathbb{1}[l_t(\boldsymbol{x}, \boldsymbol{w}|\boldsymbol{x}^*, \boldsymbol{w}^*, c_s) > h]p(\boldsymbol{w}).$$

Moreover, since $p^*(\boldsymbol{w}) \in \mathcal{A}$, the following holds:

$$\inf_{p(\boldsymbol{w}) \in \mathcal{A}} \sum_{\boldsymbol{w} \in \Omega} \mathbb{1}[l_t(\boldsymbol{x}, \boldsymbol{w}|\boldsymbol{x}^*, \boldsymbol{w}^*, c_s) > h]p(\boldsymbol{w}) \leq \sum_{\boldsymbol{w} \in \Omega} \mathbb{1}[l_t(\boldsymbol{x}, \boldsymbol{w}|\boldsymbol{x}^*, \boldsymbol{w}^*, c_s) > h]p^*(\boldsymbol{w}).$$

Table 2: Parameter setting in synthetic data experiments

	$L1$-Uniform	$L1$-Normal	$L2$-Uniform	$L2$-Normal
Booth	$h = 100$, $\alpha = 0.62$ $\sigma^2 = 10^{-4}$, $\sigma_f^2 = 1300^2$, $L = 4$, $\beta_t^{1/2} = 2$, $\epsilon = 0.65$, $L_1 = -10$, $U_1 = 10$, $L_2 = -10$, $U_2 = 10$	$h = 100$, $\alpha = 0.5$, $\sigma^2 = 10^{-4}$, $\sigma_f^2 = 1300^2$, $L = 4$, $\beta_t^{1/2} = 2$, $\epsilon = 0.65$, $L_1 = -10$, $U_1 = 10$, $L_2 = -10$, $U_2 = 10$	$h = 100$, $\alpha = 0.5$, $\sigma^2 = 10^{-4}$, $\sigma_f^2 = 1300^2$, $L = 4$, $\beta_t^{1/2} = 2$, $\epsilon = 0.05$, $L_1 = -10$, $U_1 = 10$, $L_2 = -10$, $U_2 = 10$	$h = 100$, $\alpha = 0.5$, $\sigma^2 = 10^{-4}$, $\sigma_f^2 = 1300^2$, $L = 4$, $\beta_t^{1/2} = 2$, $\epsilon = 0.1$, $L_1 = -10$, $U_1 = 10$, $L_2 = -10$, $U_2 = 10$
Matyas	$h = 5$, $\alpha = 0.53$ $\sigma^2 = 10^{-4}$, $\sigma_f^2 = 50^2$, $L = 4$, $\beta_t^{1/2} = 2$, $\epsilon = 0.15$, $L_1 = -10$, $U_1 = 10$, $L_2 = -10$, $U_2 = 10$	$h = 5$, $\alpha = 0.53$, $\sigma^2 = 10^{-4}$, $\sigma_f^2 = 50^2$, $L = 4$, $\beta_t^{1/2} = 2$, $\epsilon = 0.15$, $L_1 = -10$, $U_1 = 10$, $L_2 = -10$, $U_2 = 10$	$h = 5$, $\alpha = 0.5$, $\sigma^2 = 10^{-4}$, $\sigma_f^2 = 50^2$, $L = 4$, $\beta_t^{1/2} = 2$, $\epsilon = 0.05$, $L_1 = -10$, $U_1 = 10$, $L_2 = -10$, $U_2 = 10$	$h = 5$, $\alpha = 0.5$, $\sigma^2 = 10^{-4}$, $\sigma_f^2 = 50^2$, $L = 4$, $\beta_t^{1/2} = 2$, $\epsilon = 0.1$, $L_1 = -10$, $U_1 = 10$, $L_2 = -10$, $U_2 = 10$
McCormick	$h = 1$, $\alpha = 0.57$ $\sigma^2 = 10^{-4}$, $\sigma_f^2 = 20^2$, $L = 1$, $\beta_t^{1/2} = 3$, $\epsilon = 0.25$, $L_1 = -1.5$, $U_1 = 4$, $L_2 = -3$, $U_2 = 4$	$h = 1$, $\alpha = 0.59$, $\sigma^2 = 10^{-6}$, $\sigma_f^2 = 20^2$, $L = 1$, $\beta_t^{1/2} = 3$, $\epsilon = 0.15$, $L_1 = -1.5$, $U_1 = 4$, $L_2 = -3$, $U_2 = 4$	$h = 2$, $\alpha = 0.5$, $\sigma^2 = 10^{-6}$, $\sigma_f^2 = 20^2$, $L = 1$, $\beta_t^{1/2} = 3$, $\epsilon = 0.05$, $L_1 = -1.5$, $U_1 = 4$, $L_2 = -3$, $U_2 = 4$	$h = 1$, $\alpha = 0.55$, $\sigma^2 = 10^{-6}$, $\sigma_f^2 = 20^2$, $L = 1$, $\beta_t^{1/2} = 3$, $\epsilon = 0.07$, $L_1 = -1.5$, $U_1 = 4$, $L_2 = -3$, $U_2 = 4$
Styblinski-Tang	$h = -3990$, $\alpha = 0.61$ $\sigma^2 = 10^{-4}$, $\sigma_f^2 = 2000^2$, $L = 3$, $\beta_t^{1/2} = 2$, $\epsilon = 0.2$, $L_1 = -10$, $U_1 = 10$, $L_2 = -10$, $U_2 = 10$	$h = -3990$, $\alpha = 0.61$, $\sigma^2 = 10^{-4}$, $\sigma_f^2 = 2000^2$, $L = 3$, $\beta_t^{1/2} = 2$, $\epsilon = 0.2$, $L_1 = -10$, $U_1 = 10$, $L_2 = -10$, $U_2 = 10$	$h = -3990$, $\alpha = 0.7$, $\sigma^2 = 10^{-4}$, $\sigma_f^2 = 2000^2$, $L = 3$, $\beta_t^{1/2} = 2$, $\epsilon = 0.05$, $L_1 = -10$, $U_1 = 10$, $L_2 = -10$, $U_2 = 10$	$h = -3990$, $\alpha = 0.7$, $\sigma^2 = 10^{-4}$, $\sigma_f^2 = 2000^2$, $L = 3$, $\beta_t^{1/2} = 2$, $\epsilon = 0.1$, $L_1 = -10$, $U_1 = 10$, $L_2 = -10$, $U_2 = 10$



Booth Matyas McCormick Styblinski-Tang

Figure 4: Average F-score over 50 simulations with four benchmark functions when the distance function and reference distribution are $L2$-norm and Uniform, respectively.

Therefore, we have

$$l_t^{(F)}(\boldsymbol{x}; 0|\boldsymbol{x}^*, \boldsymbol{w}^*, c_s) \leq \sum_{\boldsymbol{w} \in \Omega} \mathbb{1}[l_t(\boldsymbol{x}, \boldsymbol{w}|\boldsymbol{x}^*, \boldsymbol{w}^*, c_s) > h] p^*(\boldsymbol{w}).$$

Hence, if the inequality assumption in Lemma 3.2 holds, then we get $l_t^{(F)}(\boldsymbol{x}; 0|\boldsymbol{x}^*, \boldsymbol{w}^*, c_s) \leq \alpha$. This implies that $\mathbb{1}[l_t^{(F)}(\boldsymbol{x}; 0|\boldsymbol{x}^*, \boldsymbol{w}^*, c_s) > \alpha] = 0$. $\square$

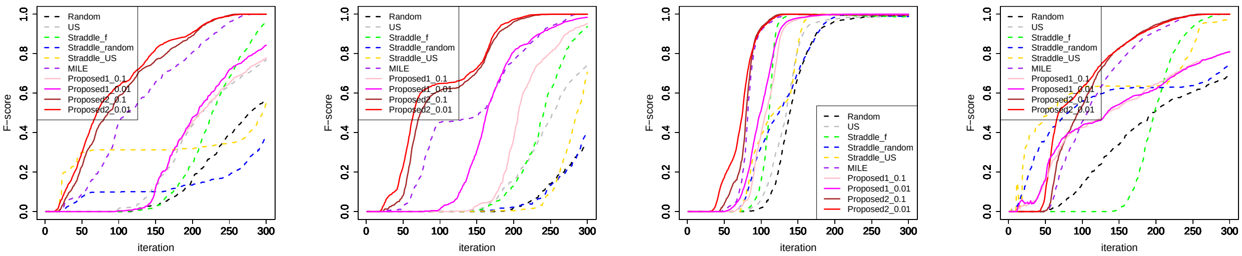
B. Additional Experiments

B.1. Synthetic and Simulation Experiments in the $L2$-norm Setting

In this section, we performed the same experiment as in Subsection 5.1 and 5.3 under the setting that the distance function is $L2$-norm. Similarly, we used Uniform and Normal as the reference distribution. Here, the parameters used in the synthetic data experiments are listed in Table 2. On the other hand, the same parameters as in Subsection 5.3 were used in infection simulation experiments. Under this setup, we took one initial point at random, and ran the algorithms until the number of iterations reached 300 (resp. 100) in the synthetic data (resp. infection simulation) experiments. We performed 50 Monte Carlo simulations and obtained the average F-score. From Figures 4 and 5, it can be confirmed that our proposed methods outperform other existing methods as well as the results of synthetic data experiments using $L1$-norm as the distance function. From Figure 6, it can also be confirmed that the same results as in Subsection 5.3 are obtained in infection simulation experiments.

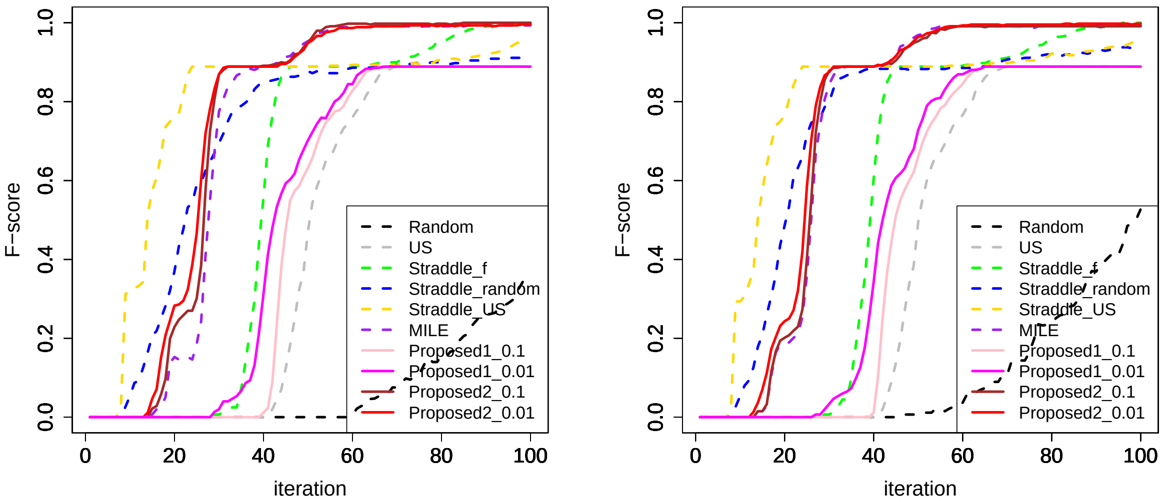
B.2. Computation Time Experiments in the Other Benchmark Function Setting

In this section, we performed the same experiment as in Subsection 5.2 for the Matyas, McCormick and Styblinski-Tang benchmark functions. We evaluated the computation time of (3.2) when we performed the



Booth Matyas McCormick Styblinski-Tang

Figure 5: Average F-score over 50 simulations with four benchmark functions when the distance function and reference distribution are $L2$-norm and Normal, respectively.



$L2$-Uniform $L2$-Normal

Figure 6: Average F-score over 50 simulations in the infection control problem when the distance function is $L2$-norm.

same experiment as in Subsection 5.2 using Proposed1_0.01 and Proposed2_0.01. Here, as for the parameter settings, we considered only the case of $L1$-Normal in Table 2. Under this setup, we took one initial point at random and ran the algorithms until the number of iterations reached to 300. Furthermore, for each trial t, we evaluated the computation time to calculate (3.2) for all candidate points $(\boldsymbol{x}^*, \boldsymbol{w}^*) \in \mathcal{X} \times \Omega$, and calculated the average computation time over 300 trials. From Tables 3, 4 and 5, it can be confirmed that the same results as in Subsection 5.2 are obtained in the three benchmark function settings.

B.3. Hyperparameter Sensitivity in the Proposed Acquisition Function

In this section, we evaluated how the performance is affected by the hyperparameter γ in the proposed acquisition function. We calculated the F-score for the cases with acquisition functions Proposed1_γ and Proposed2_γ when we performed the same experiment as in Subsection 5.1 for Booth, Matyas, McCormick and Styblinski-Tang functions. Here, Proposed1_γ and Proposed2_γ respectively represent the acquisition functions $a_t^{(1)}(\boldsymbol{x}^*, \boldsymbol{w}^*)$ and $a_t^{(2)}(\boldsymbol{x}^*, \boldsymbol{w}^*)$ with the parameter γ, and we considered γ as 0, $10^{-0.5}$, 10^{-1}, 10^{-2}, 10^{-3} and 10^{-4}. In this experiment, as for the parameter settings, we considered only the case of $L1$-Uniform in Table 2. Under this setup, we took one initial point at random and ran the algorithms until the number of iterations reached 300 (or 200). We performed 50 Monte Carlo simulations and calculated the average F-score.

From Figure 7, it can be confirmed that the acquisition function does not work for all benchmark functions when $\gamma = 0$. The reason is that $a_t(\boldsymbol{x}^*, \boldsymbol{w}^*)$ was zero for all $(\boldsymbol{x}^*, \boldsymbol{w}^*) \in \mathcal{X} \times \Omega$ when the number of data was small. Furthermore, when $\gamma > 0$, it can be seen that the performance of Proposed1_γ decreases as γ increases. One reason is that although $a_t^{(1)}(\boldsymbol{x}^*, \boldsymbol{w}^*)$ is closer to uncertainty sampling (US) as γ becomes large, US is not the acquisition function for efficiently estimating H_t. On the other hand, it can be confirmed that the performance of Proposed2_γ is not necessarily better when γ is smaller. From the definition of Proposed2_γ, when γ is large,

Table 3: Computation time (second) for the Matyas function setting

	Naive	L1	L2	L3 (10^{-4})	L3 (10^{-8})	L3 (10^{-12})
Proposed1_0.01	112403.30 ± 24588.33	6211.88 ± 1514.06	1297.19 ± 726.31	32.12 ± 7.36	32.76 ± 7.18	33.25 ± 7.06
Proposed2_0.01	98478.43 ± 19995.68	5504.84 ± 1362.62	1831.17 ± 1109.59	32.86 ± 5.43	37.50 ± 3.58	38.24 ± 4.90

Table 4: Computation time (second) for the McCormick function setting

	Naive	L1	L2	L3 (10^{-4})	L3 (10^{-8})	L3 (10^{-12})
Proposed1_0.01	83608.24 ± 39551.78	4692.96 ± 2274.72	1094.40 ± 523.81	39.66 ± 6.27	41.25 ± 6.20	42.74 ± 6.86
Proposed2_0.01	79782.95 ± 39221.70	4383.04 ± 2286.23	1525.80 ± 931.80	49.67 ± 10.33	56.79 ± 17.54	62.59 ± 23.83

$a_t^{(2)}(\boldsymbol{x}^*, \boldsymbol{w}^*)$ behaves similarly to RMILE. RMILE is the acquisition function that works to efficiently identify $(\boldsymbol{x}, \boldsymbol{w})$ that satisfies $f(\boldsymbol{x}, \boldsymbol{w}) > h$. However, since $F(\boldsymbol{x})$ is given as the function of $\mathbb{1}[f(\boldsymbol{x}, \boldsymbol{w}) > h]$, as a result, RMILE also works to efficiently estimate H_t. This is one of the reasons why Proposed2_γ sometimes has good performance even at large γ.

Table 5: Computation time (second) for the Styblinski-Tang function setting

	Naive	L1	L2	L3 (10^{-4})	L3 (10^{-8})	L3 (10^{-12})
Proposed1_0.01	118443.10 ± 16290.13	6297.18 ± 1039.76	900.67 ± 698.84	44.88 ± 18.66	47.32 ± 20.67	48.35 ± 21.82
Proposed2_0.01	96731.93 ± 25845.16	5240.58 ± 1516.16	686.64 ± 796.10	26.77 ± 10.92	27.42 ± 11.87	28.25 ± 12.78

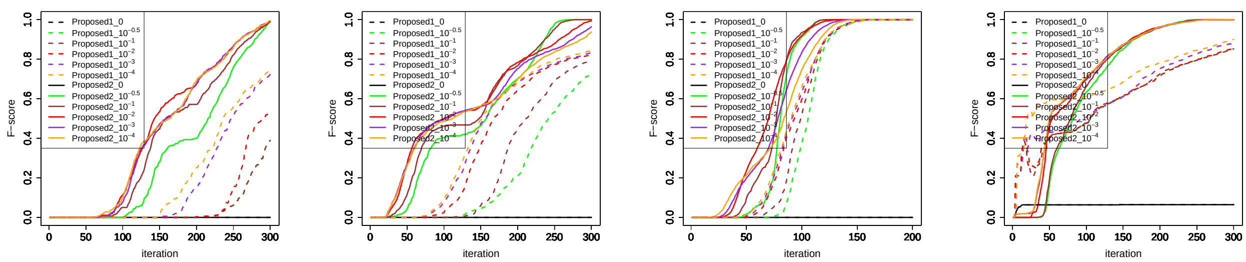


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Figure 7: Difference in average F-score for different hyperparameters with four benchmark functions when the distance function and reference distribution are $L1$-norm and Uniform, respectively.