

Supplementary Material

Adversarially Robust Optimization with Gaussian Processes

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A Illustration of STABLEOPT's Execution

The following figure gives an example of the selection procedure of STABLEOPT at two different time steps:

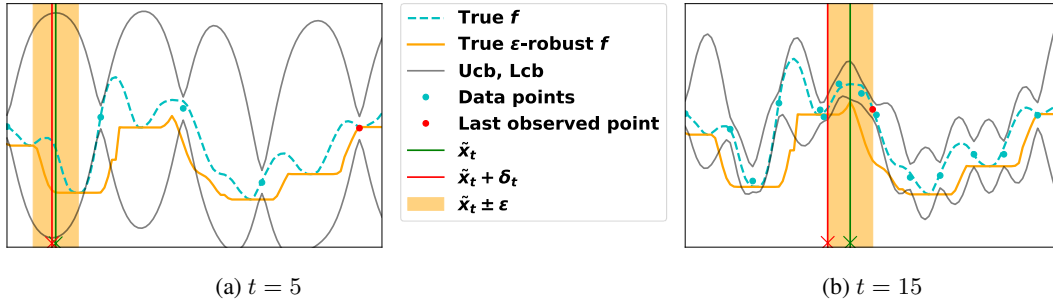
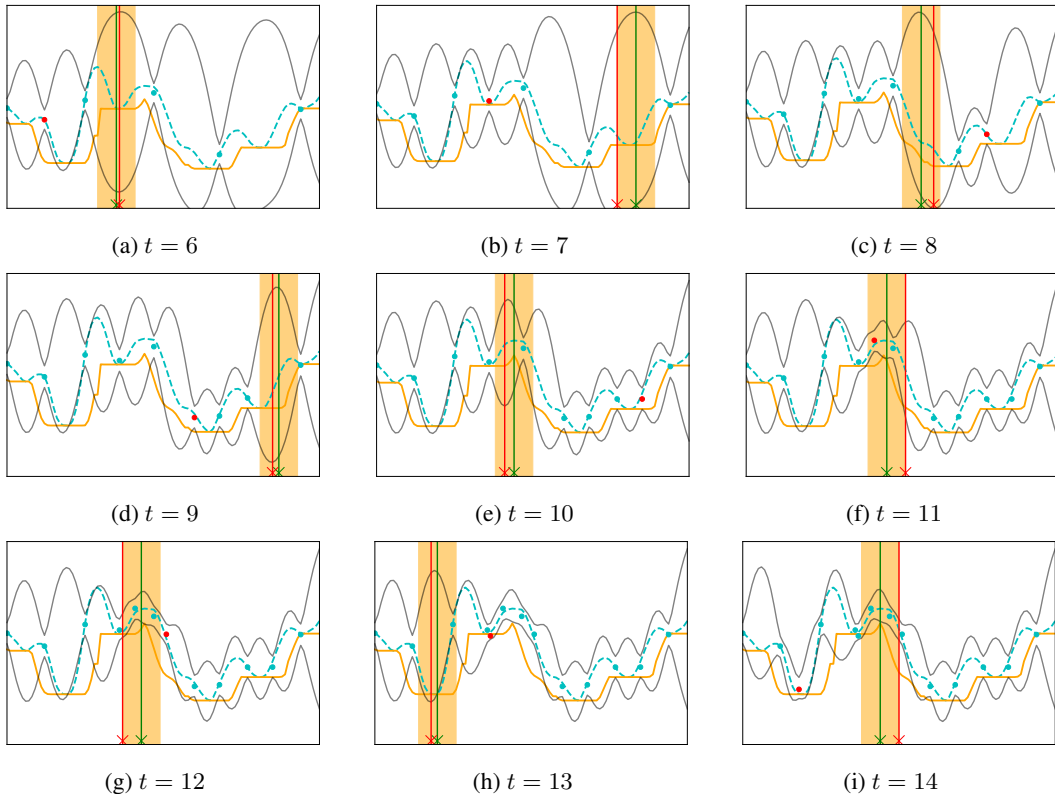


Figure 4: An execution of STABLEOPT on the running example. We observe that after $t = 15$ steps, \tilde{x}_t obtained in Eq. 13 corresponds to x_ϵ^* .

The intermediate time steps are illustrated as follows:



B Proofs of Theoretical Results

B.1 Proof of Theorem 1 (upper bound)

Recall that $\tilde{\mathbf{x}}_t$ is the point computed by STABLEOPT in (13) at time t , and that $\boldsymbol{\delta}_t$ corresponds to the perturbation obtained in STABLEOPT (Line 3) at time t . In the following, we condition on the event in Lemma 1 holding true, meaning that ucb_t and lcb_t provide valid confidence bounds as per (15). As stated in the lemma, this holds with probability at least $1 - \xi$.

By the definition of ϵ -instant regret, we have

$$r_\epsilon(\tilde{\mathbf{x}}_t) = \max_{\mathbf{x} \in D} \min_{\boldsymbol{\delta} \in \Delta_\epsilon(\mathbf{x})} f(\mathbf{x} + \boldsymbol{\delta}) - \min_{\boldsymbol{\delta} \in \Delta_\epsilon(\tilde{\mathbf{x}}_t)} f(\tilde{\mathbf{x}}_t + \boldsymbol{\delta}) \quad (32)$$

$$\leq \max_{\mathbf{x} \in D} \min_{\boldsymbol{\delta} \in \Delta_\epsilon(\mathbf{x})} f(\mathbf{x} + \boldsymbol{\delta}) - \min_{\boldsymbol{\delta} \in \Delta_\epsilon(\tilde{\mathbf{x}}_t)} \text{lcb}_{t-1}(\tilde{\mathbf{x}}_t + \boldsymbol{\delta}) \quad (33)$$

$$= \max_{\mathbf{x} \in D} \min_{\boldsymbol{\delta} \in \Delta_\epsilon(\mathbf{x})} f(\mathbf{x} + \boldsymbol{\delta}) - \text{lcb}_{t-1}(\tilde{\mathbf{x}}_t + \boldsymbol{\delta}_t) \quad (34)$$

$$\leq \max_{\mathbf{x} \in D} \min_{\boldsymbol{\delta} \in \Delta_\epsilon(\mathbf{x})} \text{ucb}_{t-1}(\mathbf{x} + \boldsymbol{\delta}) - \text{lcb}_{t-1}(\tilde{\mathbf{x}}_t + \boldsymbol{\delta}_t) \quad (35)$$

$$= \min_{\boldsymbol{\delta} \in \Delta_\epsilon(\tilde{\mathbf{x}}_t)} \text{ucb}_{t-1}(\tilde{\mathbf{x}}_t + \boldsymbol{\delta}) - \text{lcb}_{t-1}(\tilde{\mathbf{x}}_t + \boldsymbol{\delta}_t) \quad (36)$$

$$\leq \text{ucb}_{t-1}(\tilde{\mathbf{x}}_t + \boldsymbol{\delta}_t) - \text{lcb}_{t-1}(\tilde{\mathbf{x}}_t + \boldsymbol{\delta}_t) \quad (37)$$

$$= 2\beta_t^{1/2} \sigma_{t-1}(\tilde{\mathbf{x}}_t + \boldsymbol{\delta}_t), \quad (38)$$

where (33) and (35) follow from Lemma 1, (34) follows since $\boldsymbol{\delta}_t$ minimizes lcb_{t-1} by definition, (36) follows since $\tilde{\mathbf{x}}_t$ maximizes the robust upper confidence bound by definition, (37) follows by upper bounding the minimum by the specific choice $\boldsymbol{\delta}_t \in \Delta_\epsilon(\tilde{\mathbf{x}}_t)$, and (38) follows since the upper and lower confidence bounds are separated by $2\beta_t^{1/2} \sigma_{t-1}(\cdot)$ according to their definitions in (12).

In fact, the analysis from (33) to (38) shows that the following *pessimistic estimate* of $r_\epsilon(\tilde{\mathbf{x}}_t)$ is upper bounded by $2\beta_t^{1/2} \sigma_{t-1}(\tilde{\mathbf{x}}_t + \boldsymbol{\delta}_t)$:

$$\bar{r}_\epsilon(\tilde{\mathbf{x}}_t) = \max_{\mathbf{x} \in D} \min_{\boldsymbol{\delta} \in \Delta_\epsilon(\mathbf{x})} f(\mathbf{x} + \boldsymbol{\delta}) - \min_{\boldsymbol{\delta} \in \Delta_\epsilon(\tilde{\mathbf{x}}_t)} \text{lcb}_{t-1}(\tilde{\mathbf{x}}_t + \boldsymbol{\delta}). \quad (39)$$

Unlike $r_\epsilon(\tilde{\mathbf{x}}_t)$, the algorithm has the required knowledge to identify the value of $t \in \{1, \dots, T\}$ with the smallest $\bar{r}_\epsilon(\tilde{\mathbf{x}}_t)$. Specifically, the first term on the right-hand side of (39) does not depend on t , so the smallest $\bar{r}_\epsilon(\tilde{\mathbf{x}}_t)$ is achieved by $\mathbf{x}^{(T)}$ defined in (17). Since the minimum is upper bounded by the average, it follows that

$$r_\epsilon(\mathbf{x}^{(T)}) \leq \bar{r}_\epsilon(\mathbf{x}^{(T)}) \quad (40)$$

$$\leq \frac{1}{T} \sum_{t=1}^T 2\beta_t^{1/2} \sigma_{t-1}(\tilde{\mathbf{x}}_t + \boldsymbol{\delta}_t) \quad (41)$$

$$\leq \frac{2\beta_T^{1/2}}{T} \sum_{t=1}^T \sigma_{t-1}(\tilde{\mathbf{x}}_t + \boldsymbol{\delta}_t), \quad (42)$$

where (41) uses (38), and (42) uses the monotonicity of β_T . Next, we claim that

$$2 \sum_{t=1}^T \sigma_{t-1}(\tilde{\mathbf{x}}_t + \boldsymbol{\delta}_t) \leq \sqrt{C_1 T \gamma_T}, \quad (43)$$

where $C_1 = 8/\log(1 + \sigma^{-2})$. In fact, this is a special case of the well-known result [31, Lemma 5.4]⁴ which upper bounds the sum of posterior standard deviations of sampled points in terms of the information gain γ_T (recall that STABLEOPT samples at location $\tilde{\mathbf{x}}_t + \boldsymbol{\delta}_t$). Combining (42)–(43) and re-arranging, we deduce that after T satisfies $\frac{T}{\beta_T \gamma_T} \geq \frac{C_1}{\eta^2}$, the ϵ -instant regret is at most η , thus completing the proof.

⁴More precisely, [31, Lemma 5.4] alongside an application of the Cauchy-Schwarz inequality as in [31].

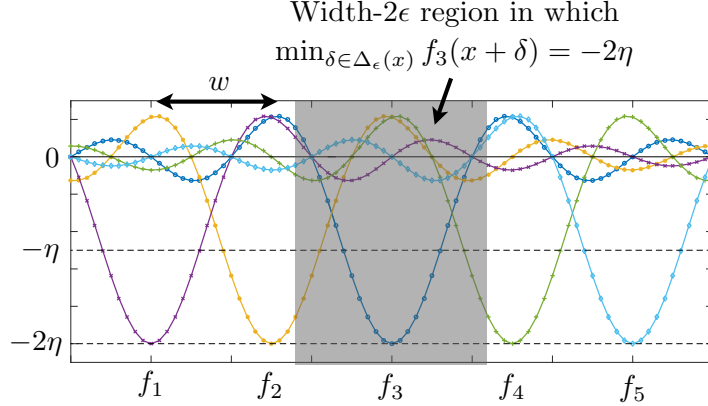


Figure 6: Illustration of functions f_1, \dots, f_5 equal to a common function shifted by various multiples of a given parameter w . In the ϵ -stable setting, there is a wide region (shown in gray for the dark blue curve f_3) within which the perturbed function value equals -2η .

B.2 Proof of Theorem 2 (lower bound)

Our lower bounding analysis builds heavily on that of the non-robust optimization setting with $f \in \mathcal{F}_k(B)$ studied in [27], but with important differences. Roughly speaking, the analysis of [27] is based on the difficulty of finding a very narrow “bump” of height 2η in a function whose values are mostly close to zero. In the ϵ -stable setting, however, even the points around such a bump will be adversarially perturbed to another point whose function value is nearly zero. Hence, all points are essentially equally bad.

To overcome this challenge, we consider the reverse scenario: Most of the function values are still nearly zero, but there exists a narrow *valley* of depth -2η . This means that every point within an ϵ -ball around the function minimizer will be perturbed to the point with value -2η . Hence, a constant fraction of the volume is still 2η -suboptimal, and it is impossible to avoid this region with high probability unless the time horizon T is sufficiently large. An illustration is given in Figure 6, with further details below.

We now proceed with the formal proof.

B.2.1 Preliminaries

Recall that we are considering an arbitrary given (deterministic) GP optimization algorithm. More precisely, such an algorithm consists of a sequence of decision functions that return a sampling location \mathbf{x}_t based on y_1, \dots, y_{t-1} , and an additional decision function that reports the final point $\mathbf{x}^{(T)}$ based on y_1, \dots, y_T . The points $\mathbf{x}_1, \dots, \mathbf{x}_{t-1}$ (or $\mathbf{x}_1, \dots, \mathbf{x}_T$) do not need to be treated as additional inputs to these functions, since $(\mathbf{x}_1, \dots, \mathbf{x}_{t-1})$ is a deterministic function of (y_1, \dots, y_{t-1}) .

We first review several useful results and techniques from [27]:

- We lower bound the worst-case ϵ -regret within $\mathcal{F}_k(B)$ by the ϵ -regret averaged over a suitably-designed finite collection $\{f_1, \dots, f_M\} \subset \mathcal{F}_k(B)$ of size M .
- We choose each $f_m(\mathbf{x})$ to be a shifted version of a common function $g(\mathbf{x})$ on \mathbb{R}^p . Specifically, each $f_m(\mathbf{x})$ is obtained by shifting $g(\mathbf{x})$ by a different amount, and then cropping to $D = [0, 1]^p$. For our purposes, we require $g(\mathbf{x})$ to satisfy the following properties:
 1. The RKHS norm in \mathbb{R}^p is bounded, $\|g\|_k \leq B$;
 2. We have (i) $g(\mathbf{x}) \in [-2\eta, 2\eta]$ with minimum value $g(0) = -2\eta$, and (ii) there is a “width” w such that $g(\mathbf{x}) > -\eta$ for all $\|\mathbf{x}\|_\infty \geq w$;
 3. There are absolute constants $h_0 > 0$ and $\zeta > 0$ such that $g(\mathbf{x}) = \frac{2\eta}{h_0} h\left(\frac{\mathbf{x}\zeta}{w}\right)$ for some function $h(\mathbf{z})$ that decays faster than any finite power of $\|\mathbf{z}\|_2$ as $\|\mathbf{z}\|_2 \rightarrow \infty$.

Letting $g(\mathbf{x})$ be such a function, we construct the M functions by shifting $g(\mathbf{x})$ so that each $f_m(\mathbf{x})$ is centered on a unique point in a uniform grid, with points separated by w in each dimension. Since $D = [0, 1]^p$, one can construct

$$M = \left\lfloor \left(\frac{1}{w} \right)^p \right\rfloor \quad (44)$$

such functions. We will use this construction with $w \ll 1$, so that there is no risk of having $M = 0$, and in fact M can be assumed larger than any desired absolute constant.

- It is shown in [27] that the above properties⁵ can be achieved with

$$M = \left\lfloor \left(\frac{r \sqrt{\log \frac{B(2\pi l^2)^{p/4} h(0)}{2\eta}}}{\zeta \pi l} \right)^p \right\rfloor \quad (45)$$

in the case of the SE kernel, and with

$$M = \left\lfloor \left(\frac{Bc_3}{\eta} \right)^{p/\nu} \right\rfloor \quad (46)$$

in the case of the Matérn kernel, where

$$c_3 := \left(\frac{r}{\zeta} \right)^\nu \cdot \left(\frac{c_2^{-1/2}}{2(8\pi^2)^{(\nu+p/2)/2}} \right), \quad (47)$$

and where $c_2 > 0$ is an absolute constant. Note that these values of M amount to choosing w in (44), and the assumption of sufficiently small $\frac{\eta}{B}$ in the theorem statement ensures that $M \gg 1$ (or equivalently $w \ll 1$) as stated above.

- Property 2 above ensures that the “robust” function value $\min_{\delta \in \Delta_\epsilon(\mathbf{x})} f(\mathbf{x})$ equals -2η for any \mathbf{x} whose ϵ -neighborhood includes the minimizer \mathbf{x}_{\min} of f , while being $-\eta$ or higher for any input whose entire ϵ -neighborhood is separated from \mathbf{x}_{\min} by at least w . For $w \ll 1$ and $\epsilon < 0.5$, a point of the latter type is guaranteed to exist, which implies

$$r_\epsilon(\mathbf{x}) \geq \eta \quad (48)$$

for any \mathbf{x} whose ϵ -neighborhood includes \mathbf{x}_{\min} .

In addition, we introduce the following notation, also used in [27]:

- The probability density function of the output sequence $\mathbf{y} = (y_1, \dots, y_T)$ when the underlying function is f_m is denoted by $P_m(\mathbf{y})$. We also define $f_0(\mathbf{x}) = 0$ to be the zero function, and define $P_0(\mathbf{y})$ analogously for the case that the optimization algorithm is run on f_0 . Expectations and probabilities (with respect to the noisy observations) are similarly written as $\mathbb{E}_m, \mathbb{P}_m, \mathbb{E}_0,$ and \mathbb{P}_0 when the underlying function is f_m or f_0 . On the other hand, in the absence of a subscript, $\mathbb{E}[\cdot]$ and $\mathbb{P}[\cdot]$ are taken with respect to the noisy observations *and* the random function f drawn uniformly from $\{f_1, \dots, f_M\}$ (recall that we are lower bounding the worst case by this average).
- Let $\{\mathcal{R}_m\}_{m=1}^M$ be a partition of the domain into M regions according the above-mentioned uniform grid, with f_m taking its minimum value of -2η in the centre of \mathcal{R}_m . Moreover, let j_t be the index at time t such that \mathbf{x}_t falls into \mathcal{R}_{j_t} ; this can be thought of as a quantization of \mathbf{x}_t .
- Define the maximum (absolute) function value within a given region \mathcal{R}_j as

$$\bar{v}_m^j := \max_{\mathbf{x} \in \mathcal{R}_j} |f_m(\mathbf{x})|, \quad (49)$$

and the maximum KL divergence to P_0 within the region as

$$\bar{D}_m^j := \max_{\mathbf{x} \in \mathcal{R}_j} D(P_0(\cdot|\mathbf{x}) \| P_m(\cdot|\mathbf{x})), \quad (50)$$

where $P_m(y|\mathbf{x})$ is the distribution of an observation y for a given selected point \mathbf{x} under the function f_m , and similarly for $P_0(y|\mathbf{x})$.

⁵Here $g(\mathbf{x})$ plays the role of $-g(\mathbf{x})$ in [27] due to the discussion at the start of this appendix, but otherwise the construction is identical.

- Let $N_j \in \{0, \dots, T\}$ be a random variable representing the number of points from \mathcal{R}_j that are selected throughout the T rounds.

Next, we present several useful lemmas. The following well-known change-of-measure result, which can be viewed as a form of Le Cam’s method, has been used extensively in both discrete and continuous bandit problems.

Lemma 2. [1, p. 27] *For any function $a(\mathbf{y})$ taking values in a bounded range $[0, A]$, we have*

$$|\mathbb{E}_m[a(\mathbf{y})] - \mathbb{E}_0[a(\mathbf{y})]| \leq A d_{\text{TV}}(P_0, P_m) \quad (51)$$

$$\leq A \sqrt{D(P_0 \| P_m)}, \quad (52)$$

where $d_{\text{TV}}(P_0, P_m) = \frac{1}{2} \int_{\mathbb{R}^T} |P_0(\mathbf{y}) - P_m(\mathbf{y})| d\mathbf{y}$ is the total variation distance.

We briefly remark on some slight differences here compared to [1, p. 27]. There, only $\mathbb{E}_m[a(\mathbf{y})] - \mathbb{E}_0[a(\mathbf{y})]$ is upper bounded in terms of $d_{\text{TV}}(P_0, P_m)$, but one easily obtains the same upper bound on $\mathbb{E}_0[a(\mathbf{y})] - \mathbb{E}_m[a(\mathbf{y})]$ by interchanging the roles of P_0 and P_m . The step (52) follows from Pinsker’s inequality, $d_{\text{TV}}(P_0, P_m) \leq \sqrt{\frac{D(P_0 \| P_m)}{2}}$, and by upper bounding $\frac{1}{\sqrt{2}} \leq 1$ to ease the notation.

The following result simplifies the divergence term in (52).

Lemma 3. [27, Eq. (44)] *Under the preceding definitions, we have*

$$D(P_0 \| P_m) \leq \sum_{j=1}^M \mathbb{E}_0[N_j] \bar{D}_m^j. \quad (53)$$

The following well-known property gives a formula for the KL divergence between two Gaussians.

Lemma 4. [27, Eq. (36)] *For P_1 and P_2 being Gaussian with means (μ_1, μ_2) and a common variance σ^2 , we have*

$$D(P_1 \| P_2) = \frac{(\mu_1 - \mu_2)^2}{2\sigma^2}. \quad (54)$$

Finally, we have the following technical result regarding the “needle-in-haystack” type function constructed above.

Lemma 5. [27, Lemma 7] *The functions $\{f_m\}_{m=1}^M$ corresponding to (45)–(46) are such that the quantities \bar{v}_m^j satisfy $\sum_{m=1}^M (\bar{v}_m^j)^2 = O(\eta^2)$ for all j .*

B.2.2 Analysis of the average ϵ -stable regret

Let $J_{\text{bad}}(m)$ be the set of j such that all $\mathbf{x} \in \mathcal{R}_j$ yield $\min_{\boldsymbol{\delta} \in \Delta_\epsilon(\mathbf{x})} f(\mathbf{x} + \boldsymbol{\delta}) = -2\eta$ when the true function is f_m , and define $\mathcal{R}_{\text{bad}}(m) = \cup_{j \in J_{\text{bad}}(m)} \mathcal{R}_j$. By the ϵ -regret lower bound in (48), we have

$$\mathbb{E}_m[r_\epsilon(\mathbf{x}^{(T)})] \geq \eta \mathbb{P}_m[\mathbf{x}^{(T)} \in \mathcal{R}_{\text{bad}}(m)] \quad (55)$$

$$\geq \eta \left(\mathbb{P}_0[\mathbf{x}^{(T)} \in \mathcal{R}_{\text{bad}}(m)] - \sqrt{D(P_0 \| P_m)} \right) \quad (56)$$

$$\geq \eta \left(\mathbb{P}_0[\mathbf{x}^{(T)} \in \mathcal{R}_{\text{bad}}(m)] - \sqrt{\sum_{j=1}^M \mathbb{E}_0[N_j] \bar{D}_m^j} \right), \quad (57)$$

where (56) follows from Lemma 2 with $a(\mathbf{y}) = \mathbf{1}\{\mathbf{x}^{(T)} \in \mathcal{R}_{\text{bad}}(m)\}$ and $A = 1$ (recall that $\mathbf{x}^{(T)}$ is a function of $\mathbf{y} = (y_1, \dots, y_T)$), and (57) follows from Lemma 3. Averaging over m uniform on $\{1, \dots, M\}$, we obtain

$$\mathbb{E}[r_\epsilon(\mathbf{x}^{(T)})] \geq \eta \left(\frac{1}{M} \sum_{m=1}^M \mathbb{P}_0[\mathbf{x}^{(T)} \in \mathcal{R}_{\text{bad}}(m)] - \frac{1}{M} \sum_{m=1}^M \sqrt{\sum_{j=1}^M \mathbb{E}_0[N_j] \bar{D}_m^j} \right). \quad (58)$$

We proceed by bounding the two terms separately.

- We first claim that

$$\frac{1}{M} \sum_{m=1}^M \mathbb{P}_0[\mathbf{x}^{(T)} \in \mathcal{R}_{\text{bad}}(m)] \geq C_1 \quad (59)$$

for some $C_1 > 0$. To show this, it suffices to prove that any given $\mathbf{x}^{(T)} \in D$ is in at least a constant fraction of the $\mathcal{R}_{\text{bad}}(m)$ regions, of which there are M . This follows from the fact that the ϵ -ball centered at $\mathbf{x}_{m,\min} = \arg \min_{\mathbf{x} \in D} f_m(\mathbf{x})$ takes up a constant fraction of the volume of D , where the constant depends on both the stability parameter ϵ and the dimension p . A small caveat is that because the definition of \mathcal{R}_{bad} insists that the *every* point in the region \mathcal{R}_j is within distance ϵ of $\mathbf{x}_{m,\min}$, the left-hand side of (59) may be slightly below the relevant ratio of volumes above. However, since Theorem 2 assumes that $\frac{\epsilon}{B}$ is sufficiently small, the choices of M in (45) and (46) ensure that M is sufficiently large for this “quantization” effect to be negligible.

- For the second term in (58), we claim that

$$\frac{1}{M} \sum_{m=1}^M \sqrt{\sum_{j=1}^M \mathbb{E}_0[N_j] \bar{D}_m^j} \leq C_2 \frac{\eta}{\sigma} \sqrt{\frac{T}{M}} \quad (60)$$

for some $C_2 > 0$. To see this, we write

$$\begin{aligned} & \frac{1}{M} \sum_{m=1}^M \sqrt{\sum_{j=1}^M \mathbb{E}_0[N_j] \bar{D}_m^j} \\ &= O\left(\frac{1}{\sigma}\right) \cdot \frac{1}{M} \sum_{m=1}^M \sqrt{\sum_{j=1}^M \mathbb{E}_0[N_j] (\bar{v}_m^j)^2} \end{aligned} \quad (61)$$

$$\leq O\left(\frac{1}{\sigma}\right) \cdot \sqrt{\frac{1}{M} \sum_{m=1}^M \sum_{j=1}^M \mathbb{E}_0[N_j] (\bar{v}_m^j)^2} \quad (62)$$

$$= O\left(\frac{1}{\sigma}\right) \cdot \sqrt{\frac{1}{M} \sum_{j=1}^M \mathbb{E}_0[N_j] \left(\sum_{m=1}^M (\bar{v}_m^j)^2\right)} \quad (63)$$

$$= O\left(\frac{\eta}{\sqrt{M}\sigma}\right) \cdot \sqrt{\sum_{j=1}^M \mathbb{E}_0[N_j]} \quad (64)$$

$$= O\left(\frac{\sqrt{T}\eta}{\sqrt{M}\sigma}\right), \quad (65)$$

where (61) follows since the divergence $D(P_0(\cdot|\mathbf{x})\|P_m(\cdot|\mathbf{x}))$ associated with a point \mathbf{x} having value $v(\mathbf{x})$ is $\frac{v(\mathbf{x})^2}{2\sigma^2}$ (cf., (54)), (62) follows from Jensen’s inequality, (64) follows from Lemma 5, and (65) follows from $\sum_j N_j = T$.

Substituting (59) and (60) into (58), we obtain

$$\mathbb{E}[r_\epsilon(\mathbf{x}^{(T)})] \geq \eta \left(C_1 - C_2 \frac{\eta}{\sigma} \sqrt{\frac{T}{M}} \right), \quad (66)$$

which implies that the regret is lower bounded by $\Omega(\eta)$ unless $T = \Omega\left(\frac{M\sigma^2}{\eta^2}\right)$. Substituting M from (45) and (46), we deduce that the conditions on T in the theorem statement are necessary to achieve average regret $\mathbb{E}[r_\epsilon(\mathbf{x}^{(T)})] = O(\eta)$ with a sufficiently small implied constant.

B.2.3 From average to high-probability regret

Recall that we are considering functions whose values lie in the range $[-2\eta, 2\eta]$, implying that $r_\epsilon(\mathbf{x}^{(T)}) \leq 4\eta$. Letting T_η be the lower bound on T derived above for achieving average regret

$O(\eta)$ (i.e., we have $\mathbb{E}[r_\epsilon^{(T_\eta)}] = \Omega(\eta)$), it follows from the reverse Markov inequality (i.e., Markov’s inequality applied to the random variable $4\eta - r_\epsilon^{(T_\eta)}$) that

$$\mathbb{P}[r_\epsilon(\mathbf{x}^{(T_\eta)}) \geq c\eta] \geq \frac{\Omega(\eta) - c\eta}{4\eta - c\eta} \quad (67)$$

for any $c > 0$ sufficiently small for the numerator and denominator to be positive. The right-hand side is lower bounded by a constant for any such c , implying that the probability of achieving ϵ -regret at most $c\eta$ cannot be arbitrarily close to one. By renaming $c\eta$ as η' , it follows that in order to achieve some target ϵ -stable regret η' with probability sufficiently close to one, a lower bound of the same form as the average regret bound holds. In other words, the conditions on T in the theorem statement remain necessary also for the high-probability regret.

We emphasize that Theorem 2 concerns the high-probability regret when “high probability” means *sufficiently close to one* as a function of ϵ , p , and the kernel parameters (but still constant with respect to T and η). We do not claim a lower bound under any particular *given* success probability (e.g., η -optimality with probability at least $\frac{3}{4}$).

C Details on Variations from Section 4

We claim that the STABLEOPT variations and theoretical results outlined in Section 4 are in fact special cases of Algorithm 1 and Theorem 1, despite being seemingly quite different. The idea behind this claim is that Algorithm 1 and Theorem 1 allow for the “distance” function $d(\cdot, \cdot)$ to be completely arbitrary, so we may choose it in rather creative/unconventional ways.

In more detail, we have the following:

- For the unknown parameter setting $\max_{\mathbf{x} \in D} \min_{\boldsymbol{\theta} \in \Theta} f(\mathbf{x}, \boldsymbol{\theta})$, we replace \mathbf{x} in the original setting by the concatenated input $(\mathbf{x}, \boldsymbol{\theta})$, and set

$$d((\mathbf{x}, \boldsymbol{\theta}), (\mathbf{x}', \boldsymbol{\theta}')) = \|\mathbf{x} - \mathbf{x}'\|_2. \quad (68)$$

If we then set $\epsilon = 0$, we find that the input \mathbf{x} experiences no perturbation, whereas $\boldsymbol{\theta}$ may be perturbed arbitrarily, thereby reducing (7) to $\max_{\mathbf{x} \in D} \min_{\boldsymbol{\theta} \in \Theta} f(\mathbf{x}, \boldsymbol{\theta})$ as desired.

- For the robust estimation setting, we again use the concatenated input $(\mathbf{x}, \boldsymbol{\theta})$. To avoid overloading notation, we let $d_0(\boldsymbol{\theta}, \boldsymbol{\theta}')$ denote the distance function (applied to $\boldsymbol{\theta}$ alone) adopted for this case in Section 4. We set

$$d((\mathbf{x}, \boldsymbol{\theta}), (\mathbf{x}', \boldsymbol{\theta}')) = \begin{cases} d_0(\boldsymbol{\theta}, \boldsymbol{\theta}') & \mathbf{x} = \mathbf{x}' \\ \infty & \mathbf{x} \neq \mathbf{x}' \end{cases}. \quad (69)$$

Due to the second case, the input \mathbf{x} experiences no perturbation, since doing so would violate the distance constraint of ϵ . We are then left with $\mathbf{x} = \mathbf{x}'$ and $d_0(\boldsymbol{\theta}, \boldsymbol{\theta}') \leq \epsilon$, as required.

- For the grouped setting $\max_{G \in \mathcal{G}} \min_{\mathbf{x} \in G} f(\mathbf{x})$, we adopt the function

$$d(\mathbf{x}, \mathbf{x}') = \mathbf{1}\{\mathbf{x} \text{ and } \mathbf{x}' \text{ are in different groups}\}, \quad (70)$$

and set $\epsilon = 0$. Considering the formulation in (7), we find that any two inputs \mathbf{x} and \mathbf{x}' yield the same ϵ -stable objective function, and hence, reporting a point \mathbf{x} is equivalent to reporting its group G . As a result, (7) reduces to the desired formulation $\max_{G \in \mathcal{G}} \min_{\mathbf{x} \in G} f(\mathbf{x})$.

The variations of STABLEOPT described in (20)–(26), as well as the corresponding theoretical results outlined in Section 4 follow immediately by substituting the respective choices of $d(\cdot, \cdot)$ and ϵ above into Algorithm 1 and Theorem 1. It should be noted that in the first two examples, the definition of γ_t in (14) is modified to take the maximum over not only $\mathbf{x}_1, \dots, \mathbf{x}_t$, but also $\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_t$.

D Lake Data Experiment

We consider an application regarding environmental monitoring of inland waters, using a data set containing 2024 in situ measurements of chlorophyll concentration within a vertical transect plane, collected by an autonomous surface vessel in Lake Zürich. This data set was considered in previous

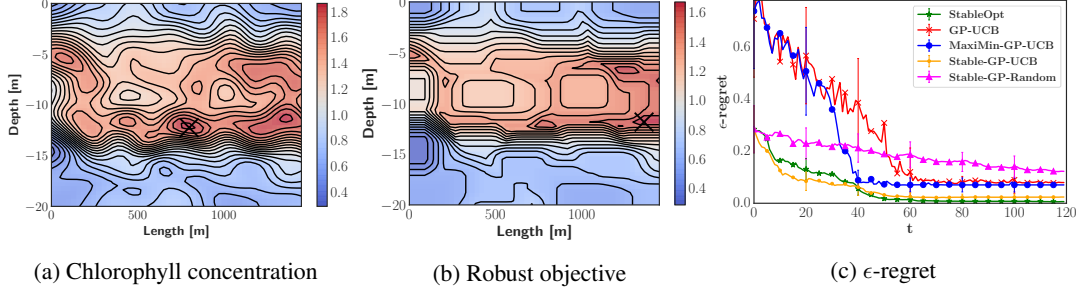


Figure 7: Experiment on the Zürich lake dataset; In the later rounds STABLEOPT is the only method that reports a near-optimal ϵ -stable point.

works such as [7, 15] to detect regions of high concentration. In these works, the goal was to locate all regions whose concentration exceeds a pre-defined threshold.

Here we consider a different goal: We seek to locate a region of a given size such that the concentration throughout the region is as high as possible (in the max-min sense). This is of interest in cases where high concentration only becomes relevant when it is spread across a sufficiently wide area. We consider rectangular regions with different pre-specified lengths in each dimension:

$$\Delta_{\epsilon_D, \epsilon_L}(\mathbf{x}) = \{\mathbf{x}' - \mathbf{x} : \mathbf{x}' \in D, |x_D - x'_D| \leq \epsilon_D \cap |x_L - x'_L| \leq \epsilon_L\}, \quad (71)$$

where $\mathbf{x} = (x_D, x_L)$ and $\mathbf{x}' = (x'_D, x'_L)$ indicate the depth and length, and we denote the corresponding stability parameters by (ϵ_D, ϵ_L) . This corresponds to $d(\cdot, \cdot)$ being a weighted ℓ_∞ -norm.

We evaluate each algorithm on a 50×50 grid of points, with the corresponding values coming from the GP posterior that was derived using the original data. We use the Matérn-5/2 ARD kernel, setting its hyperparameters by maximizing the likelihood on a second (smaller) available dataset. The parameters ϵ_D and ϵ_L are set to 1.0 and 100.0, respectively. The stability requirement changes the global maximum and its location, as can be observed in Figure 7. The number of sampling rounds is $T = 120$, and each algorithm is initialized with the same 10 random data points and corresponding observations. The performance is averaged over 100 different runs, where every run corresponds to a different random initialization. In this experiment, STABLE-GP-UCB achieves the smallest ϵ -regret in the early rounds, while in the later rounds STABLEOPT is the only method that reports a near-optimal ϵ -stable point.