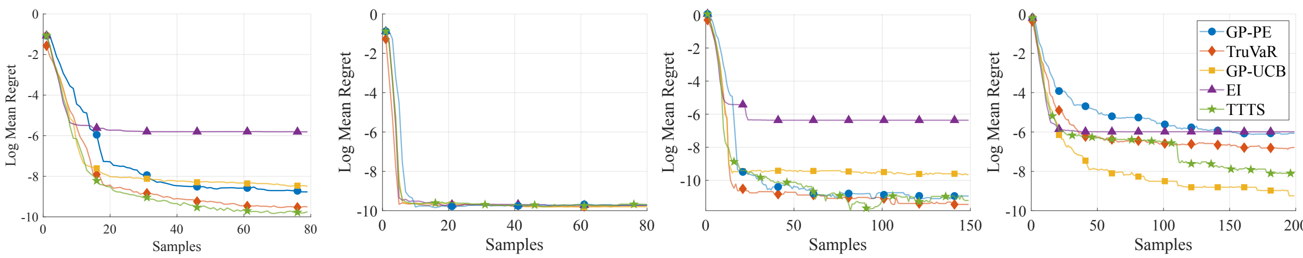
Algorithm 1 Gaussian Process Pure Exploration (GP-PE)

Input: $\mathcal{D}_N, N > 1, \mu, k, \sigma_n^2, T < N$
$M_0 \leftarrow \mathcal{D}_N; A_0 \leftarrow \emptyset;$
for $t = 1, 2, \ldots, T$ **do**
  $\mathbf{x}_t = \arg\max_{\mathbf{x} \in \mathcal{D}_N} \min_{\mathbf{x}_i \in A_{t-1}} \|\mathbf{x} - \mathbf{x}_i\|;$
  Sample $y_t = f(\mathbf{x}_t) + \varepsilon_t;$
  $A_t \leftarrow A_{t-1} \cup \{\mathbf{x}_t\};$
end for
Compute $l_T, M_T;$
Return $\mathbf{x}_{T+1} = \arg\max_{\mathbf{x} \in M_T} \mu_{A_T}(\mathbf{x});$



(a) Rational quadratic (b) Sq. exponential ($l = 0.4$) (c) Sq. exponential ($l = 0.1$) (d) Matérn $3/2$

Figure 1. Fig. 1a, 1b, 1c, 1d shows the log of the regret averaged over 100 trials achieved with GP-PE, TruVaR (Bogunovic et al., 2016), GP-UCB (Srinivas et al., 2012), EI (Shahriari et al., 2015), and top-two Thompson sampling (TTTS) (Russo, 2016) algorithms when applied to functions sampled from rational quadratic, squared exponential, and Matérn 3/2 kernels. The performance of GP-PE is indicated by the blue line. On average, GP-PE performs well in minimizing simple regret for functions with low variation as evidenced by Fig. 1a, 1b, and 1c.

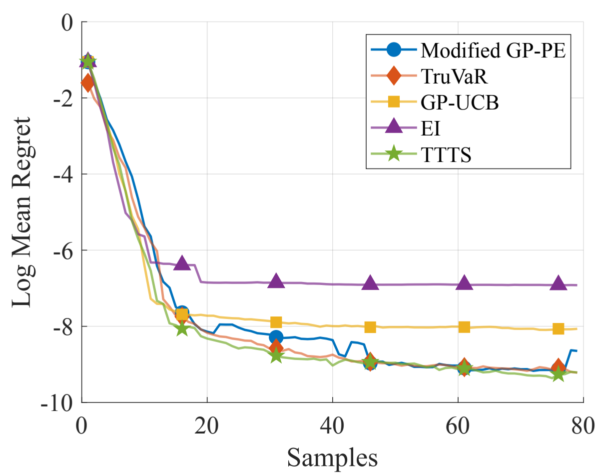


Figure 2. The log of the simple regret is plotted over 80 function evaluations selected with modified GP-PE, TruVaR (Bogunovic et al., 2016), GP-UCB (Srinivas et al., 2012), EI (Shahriari et al., 2015), and TTTS (Russo, 2016) algorithms applied to 100 functions sampled from the rational quadratic kernel. On average, modified GP-PE now decreases the simple regret more rapidly (shown by the blue line) when compared to the unmodified version of the algorithm (see Fig. 1a).

References

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