Minimum Regret Search for Single- and Multi-Task Optimization
Supplementary Material

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1. Synthetic Single-Task Benchmark with Model Mismatch

We present results for an identical setup as reported in Section 5.1, with the only difference being that the test functions have been sampled from a GP with rational quadratic kernel with length scale $l = 0.1$ and scale mixture $\alpha = 1.0$. The kernel used in the GP surrogate model is not modified, i.e., an RBF kernel with length scale $l = 0.1$ is used. Thus, since different kind of kernel govern test functions and surrogate model, we have model mismatch as would be the common case on real-world problems. Figure 1 summarizes the results of the experiment. Interestingly, in contrast to the experiment without model mismatch, for this setup there are also considerable differences in the mean simple regret between MRS and ES: while ES performs slightly better initially, it is outperformed by MRS for $N > 60$. We suspect that this is because ES tends to explore more locally than MRS once $p^\star$ has mostly settled onto one region of the search space. More local exploration, however, can be detrimental in the case of model-mismatch since the surrogate model is more likely to underestimate the function value in regions which have not been sampled. Thus a more homogeneous sampling of the search space as done by the more global exploration of MRS is beneficial. As a second observation, in contrast to a no-model-mismatch scenario, $\text{MRS}^{\text{point}}$ performs considerably worse than MRS when there is model-mismatch. This emphasizes the importance of accounting for uncertainty, particularly when there is model mis-specification.

According to the median simple regret, the difference between MRS, $\text{MRS}^{\text{point}}$, ES, and EI is less pronounced in Figure 1. Moreover, the histograms of the regret distribution exhibit less outliers (regardless of the method). We suspect that this stems from properties of the test functions that are sampled from a GP with rational quadratic rather than from the model-mismatch. However, a conclusive answer on this would require further experiments.

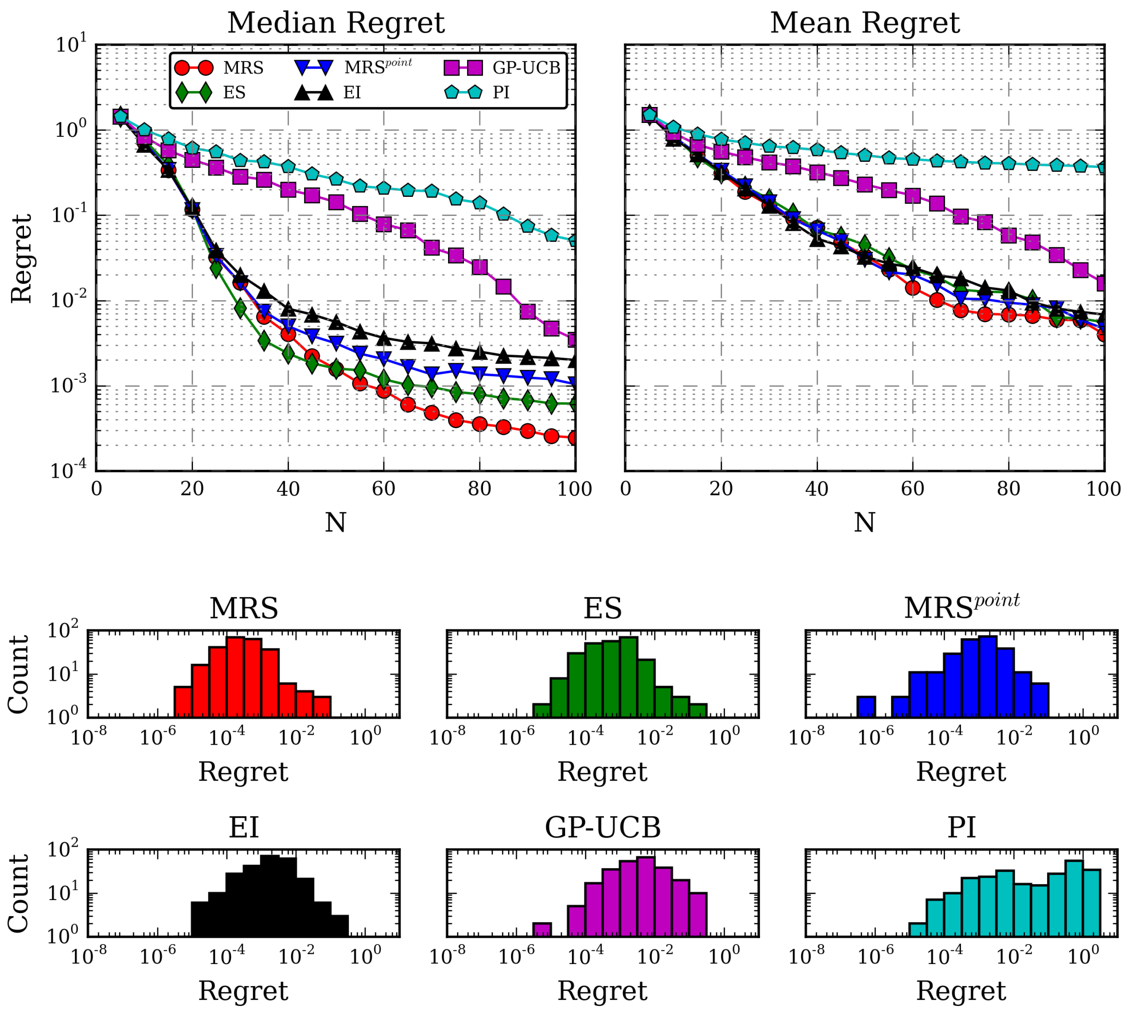

Figure 1. (Top) Median and mean simple regret over 250 repetitions for different acquisition functions. Shown is the simple regret of the recommendation $\tilde{\mathbf{x}}_N$ after N trials, i.e., the point which maximizes the GP posterior mean. (Bottom) Histogram of the simple regret after performing $N = 100$ trials for different acquisition functions (note the log-scales).