BML Project Proposal

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1. Project Title

Bayesian Posterior-Guided Domain Shrinking for Efficient Gaussian Process Optimization

2. Problem Statement

Bayesian Optimization using Gaussian Processes faces computational challenges where classical acquisition functions like GP-UCB [2] require expensive optimization at each iteration. The REDS algorithm [1] addresses this through random exploration with domain shrinking, achieving order-optimal regret ($\tilde{O}(\sqrt{T\gamma_T})$ in noisy settings) with computational efficiency. However, REDS employs deterministic confidence bounds (UCB/LCB thresholds) for shrinking decisions, which do not fully leverage the probabilistic structure of Gaussian Process posteriors.

Existing methods present a trade-off: classical approaches like GP-UCB [2] and Thompson Sampling [3] are fully Bayesian but computationally expensive, while efficient methods like REDS use deterministic shrinking rules that ignore posterior distributions. No existing work combines random exploration's efficiency with Bayesian posterior sampling for domain shrinking. This creates a gap where deterministic rules may prematurely eliminate promising regions, especially in noisy environments where uncertainty quantification is critical.

This project introduces a novel approach by replacing deterministic shrinking with Bayesian posterior-guided decisions, where the GP posterior distribution directly informs region retention. This maintains computational efficiency while incorporating principled uncertainty handling, making both problem formulation (GP priors) and solution methodology (posterior-based decisions) fully Bayesian.

3. Tentative Solution

This project will investigate *Bayesian Posterior-Guided Domain Shrinking (BPG-DS)* as a solution for efficient Gaussian Process optimization. BPG-DS unifies *random exploration* and *Bayesian posterior sampling for domain shrinking* within a single framework.

BPG-DS introduces posterior sampling to guide structured domain reduction through operations of the form:

$$\mathcal{X}_{r+1} = \{x \in \mathcal{X}_r \mid p_{posterior}(x) \geq p_{thresh}\},$$

where $p_{posterior}(x)$ represents the posterior probability that x is near-optimal, computed via function samples from $\mathcal{GP}(\mu_r, k_r)$. The algorithm operates in epochs:

- **Random Exploration:** Sample N_r points uniformly from $\mathcal{X}_r$, observe $y_i = f(x_i) + \epsilon_i$.
- **GP Update:** Update posterior $\mathcal{GP}(\mu_r(x), \sigma_r^2(x))$ with observations.
- **Posterior Sampling:** Draw K samples $\{f^{(k)}\}_{k=1}^{K} \sim \mathcal{GP}(\mu_r, k_r)$ via Cholesky decomposition.
- **Bayesian Shrinking:** Retain x where fraction of samples indicating near-optimality exceeds p_{thresh}.

A key feature is its *posterior-based* pruning rule, which makes shrinking decisions based on samples from the GP posterior rather than deterministic bounds. This theoretically grounded approach eliminates heuristic thresholds but requires empirical validation for consistency across problems.

In this project, I will explore:

1. Comparative performance of BPG-DS versus existing methods (GP-UCB, REDS, Thompson Sampling).
2. Trade-offs between number of posterior samples K and shrinking confidence p_{thresh}.
3. Robustness and interpretability of the posterior-based criterion under varying noise levels.
4. Practical implementation on synthetic benchmarks (Branin, Hartmann) and real hyperparameter tuning tasks.

Implementation, experimentation, and analysis will guide refinement of BPG-DS, balancing theoretical soundness with empirical performance using standard libraries (scikit-learn/GPy, NumPy).

4. Significance / Impact

This project contributes a novel integration of Bayesian posterior sampling into domain shrinking, addressing the gap between expensive full Bayesian methods and efficient non-Bayesian approaches. By maintaining random exploration's simplicity while incorporating posterior-based decisions, BPG-DS offers computational tractability with theoretical rigor.

Practically, posterior sampling naturally weights decisions by uncertainty, potentially reducing premature region elimination and improving sample efficiency in noisy settings. Systematic evaluation against established baselines across benchmarks will provide comprehensive validation. The method uses standard GP libraries requiring only Cholesky decomposition for sampling, making it accessible for practitioners in hyperparameter tuning, experimental design, and adaptive sampling where uncertainty quantification is essential.

References

[1] Sudeep Salgia, Sattar Vakili, and Qing Zhao, *Random Exploration in Bayesian Optimization: Order-Optimal Regret and Computational Efficiency*, Proceedings of the 41st International Conference on Machine Learning (ICML), PMLR 235, 2024.

[2] Niranjan Srinivas, Andreas Krause, Sham Kakade, and Matthias Seeger, *Gaussian Process Optimization in the Bandit Setting: No Regret and Experimental Design*, Proceedings of the 27th International Conference on Machine Learning (ICML), 2010.

[3] Kirthevasan Kandasamy, Akshay Krishnamurthy, Jeff Schneider, and Barnabás Póczos, *Parallelised Bayesian Optimisation via Thompson Sampling*, Proceedings of the 21st International Conference on Artificial Intelligence and Statistics (AISTATS), PMLR 84, 2018.