ADAPTIVE ACQUISITION SELECTION FOR BAYESIAN OPTIMIZATION WITH LARGE LANGUAGE MODELS

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ABSTRACT

Bayesian Optimization critically depends on the choice of acquisition function, but no single strategy is universally optimal; the best choice is non-stationary and problem-dependent. Existing adaptive portfolio methods often base their decisions on past function values while ignoring richer information like remaining budget or surrogate model characteristics. To address this, we introduce LMABO, a novel framework that casts a pre-trained Large Language Model (LLM) as a zero-shot, online strategist for the BO process. At each iteration, LMABO uses a structured state representation to prompt the LLM to select the most suitable acquisition function from a diverse portfolio. In an evaluation across 50 benchmark problems, LMABO demonstrates a significant performance improvement over strong static, adaptive portfolio, and other LLM-based baselines. We show that the LLM's behavior is a comprehensive strategy that adapts to real-time progress, proving its advantage stems from its ability to process and synthesize the complete optimization state into an effective, adaptive policy.

1 INTRODUCTION

Bayesian Optimization (BO) is a preeminent methodology for the global optimization of expensive-to-evaluate, black-box functions, a pervasive challenge across science and engineering (Shahriari et al., 2015). Its framework uses a surrogate model (often a Gaussian Process (GP)) to approximate the objective function and an acquisition function (AF) to intelligently select the next point to evaluate, balancing the trade-off between exploration and exploitation. A core challenge in BO is the selection of the AF. It is well-established that no single, fixed AF offers optimal performance across all problems (Hoffman et al., 2011); the best strategy is highly contingent on the characteristics of the objective function and can even change dynamically throughout a single optimization run. This has spurred the development of adaptive strategies that move beyond static AF selection to dynamically choose different AFs from a portfolio every iteration (Hoffman et al., 2011).

Existing adaptive portfolio methods, however, suffer from a critical limitation: their decisions are guided almost exclusively by a narrow view of the optimization process, typically relying on the history of observed function values. Portfolio-based strategies (Hoffman et al., 2011; Vasconcelos et al., 2019; 2022) operate on a reward signal derived from the past performance of each AF, utilizing only the function evaluations and the surrogate model's output. These methods largely ignore a wealth of other critical state information, such as the remaining optimization budget, the distance between evaluated points, and insights about the function's complexity encoded in the surrogate model's own hyperparameters (e.g., GP lengthscales). The core challenge is that designing a principled, algorithmic approach that can effectively reason over such a diverse and complex set of strategic, tactical, and landscape-related information has proven immensely difficult.

This paper bridges this gap by leveraging a Large Language Model (LLM) as a dynamic optimization strategist. We are motivated by the fact that modern LLMs, trained on immense corpora of scientific literature and code, possess a rich, nuanced, and implicitly encoded understanding of optimization principles. Instead of hand-crafting a complex policy covering all state information, we tap into this pre-trained knowledge, as well as the reasoning capabilities of the LLM to guide the exploration-exploitation balance in an optimization process. We introduce a new formulation of adaptive BO: casting acquisition function selection as an in-context decision-making problem solved by a pre-trained LLM, supported by a novel state serialization design. At each iteration, the complete, multi-

faceted optimization state is serialized into a structured textual prompt. The LLM then analyzes this rich state and select the most appropriate AF from a diverse portfolio for the immediate next step.

Experiments show LMABO consistently outperforms the baselines across diverse optimization problems. Ablation studies confirm the LLM leverages all components of the state summary, with performance dropping when any part is removed. A behavior analysis reveals a comprehensive strategy: LMABO prefers exploration when progress has stagnated, heavily exploits with low remaining budget, and aggresively switches between AFs; during early stages of optimization, the LLM is sensitive to all information; during middle stages, the performance history and process status are influential and towards the end, sensitive to only incumbent values. This proves that LMABO's success stems from its ability to reason over a complete set of strategic and tactical information.

The contributions of this work can be summarized as follows:

- We recast BO's acquisition function selection as an in-context decision-making task with an LLM as a closed-loop strategist to select the most appropriate AF.
- We propose a structured representation of the BO state, shown via ablations to be essential for effective zero-shot decision-making.
- On 50 benchmarks, LMABO outperforms static, adaptive, and LLM-based baselines, with analysis revealing emergent, state-aware strategies beyond simple heuristics.

2 Background

Bayesian Optimization is a sample-efficient framework for optimizing expensive-to-evaluate black-box functions (Frazier, 2018). Formally, let $f : \mathcal{X} \to \mathbb{R}$ be an unknown objective function defined over $\mathcal{X} \subset \mathbb{R}^d$. BO constructs a probabilistic surrogate model, typically a Gaussian Process (Rasmussen & Williams, 2005), to approximate f and quantify uncertainty in unexplored regions. At each iteration, given the set of previously observed evaluations $\mathcal{D}_{t-1}$, BO selects the next query point $x_t \in \mathcal{X}$ by maximizing an *acquisition function* $\alpha(x; \mathcal{D}_{t-1})$, which balances *exploration* (sampling in uncertain regions) and *exploitation* (sampling near low predicted values (for minimization)). There are many well-studied and effective AFs, including Expected Improvement (EI) (Mockus, 1998), Thompson Sampling (TS) (Chowdhury & Gopalan, 2017), and Upper Confidence Bound (UCB) (Srinivas et al., 2010), and each of them has their own advantages and disadvantages. This sequential strategy allows BO to efficiently converge towards the global optimum with relatively few function evaluations. More details about AFs used in this paper are provided in Appendix A.

A **Gaussian Process** is a nonparametric prior over functions, defined such that any finite collection of function values follows a joint Gaussian distribution. A GP is fully specified by its mean function $m(x)$ and covariance kernel $k(x, x')$, where the kernel encodes assumptions about the smoothness and structure of the underlying function. An example of a kernel is the squared exponential kernel:

$$k(x, x') = \sigma_f^2 \exp\left(-\tfrac{1}{2} \sum_{i=1}^{d} \frac{(x_i - x_i')^2}{\ell_i^2} \right),$$

where ℓ_i are the *lengthscales*, controlling function variation along each input dimension, and σ_f^2 is the *outputscale*, determining the overall variance of the function values. A small lengthscale means the function varies rapidly with input changes, and a small outputscale keeps predictions close to the mean with little variation. These hyperparameters are typically learned by maximizing the marginal likelihood of observed data, enabling GPs to adapt their complexity to the underlying objective.

3 Related Works

Portfolio-Based Strategies These methods treated AF selection as a portfolio allocation problem. GP-Hedge (Hoffman et al., 2011) framed the task as a *multi-armed bandit* problem, selecting AFs by first computing a reward signal derived from their past performance then randomly sampling an AF according to a probability distribution weighted by these rewards. Subsequent methods like No-PASt-BO (Vasconcelos et al., 2019) and SETUP-BO (Vasconcelos et al., 2022) sought to improve upon this by introducing memory factors to discount distant evaluations, but they still rely

on the same fundamental reward mechanism. Shahriari et al. (2014) used an information-theoretic approach with Entropy Search Portfolio (ESP), which shifted the selection criterion to a forward-looking measure of utility: the expected reduction in uncertainty about the location of the global optimum. However, a key limitation unites these strategies: their decisions are guided by a narrow view of the optimization state, focusing primarily on function values and uncertainty while ignoring other critical information like the remaining budget or characteristics of the surrogate model itself.

Learning-Based Strategies MetaBO (Volpp et al., 2020) and FSAF (Hsieh et al., 2021) meta-learn a state-dependent policy, formalizing AF selection as a reinforcement learning problem. Though related, these are not applicable to our setting, as they are designed for a transfer learning scenario, where a policy is learned on a distribution of source tasks and adapted to a new target task.

LLM-Based Bayesian Optimization With the recent success of LLMs, efforts have emerged to incorporate them into the BO process, though their roles have varied significantly. FunBO (Aglietti et al., 2025) uses the LLM as an algorithm generator to discover new AFs with a few function evaluations, but it does not participate in the adaptive process of AF selection. Other recent methods have integrated LLMs more directly into the optimization loop, but not for adaptive control. For instance, LLMP (Requeima et al., 2024) focuses on enhancing the surrogate model with natural language priors, while LLAMBO (Liu et al., 2024) uses the LLM for muiltiple steps in the optimization process including generating initial samples, surrogate modeling, and proposing candidate points. Unlike previous approaches, our LMABO does not enhance components of BO or generate functions offline. Instead, it recasts the AF selection itself as a sequential decision-making task solvable by in-context reasoning, representing a new paradigm for adaptive BO.

4 METHODOLOGY

4.1 LANGUAGE MODEL-ASSISTED ADAPTIVE BAYESIAN OPTIMIZATION (LMABO)

Our proposed method LMABO uses a pre-trained LLM to dynamically select the most appropriate acquisition function at each iteration of the BO process. The framework operates as a closed-loop system, where the LLM is prompted at each iteration with a rich representation of the optimization state to infer the most effective AF for evaluation. The entire process is detailed in Algorithm 1.

Algorithm 1 The LMABO Framework

Require: Objective function $f(\mathbf{x})$; Initial dataset $\mathcal{D}_0 = \{(\mathbf{x}_0, y_0), \dots\}$; Optimization budget T; Portfolio of acquisition functions $\mathcal{A} = \{\alpha_1, \alpha_2, \dots, \alpha_K\}$; Large Language Model Ψ.

Construct an initial prompt P_0 that defines the LLM's role as a BO expert and provides the set of available acquisition functions $\mathcal{A}$. ▷ See Appendix C
Send P_0 to Ψ to establish context. ▷ See Sec. 4.2
for $t = 1, 2, \dots, T$ **do**
    Fit a Gaussian Process model $\mathcal{GP}_{t-1}$.
    Generate state summary S_t from $\mathcal{GP}_{t-1}$ and optimization history. ▷ See Sec. 4.3
    Construct the update prompt P_t from S_t.
    Obtain the next acquisition function $\alpha_t \leftarrow \Psi(P_t)$. ▷ See Sec. 4.2
    Optimize α_t to find the next point to evaluate: $x_t \leftarrow \arg\max_x \alpha_t(x)$.
    Evaluate the true objective function: $y_t = f(x_t) + \eta_t$ with noise η_t.
    $\mathcal{D}_t \leftarrow \mathcal{D}_{t-1} \cup \{(x_t, y_t)\}$.
end for
return The point x^* corresponding to the best function value in $\mathcal{D}_T$.

4.2 THE LLM AS A ZERO-SHOT STRATEGIST

A core tenet of our LMABO framework is to leverage the reasoning capabilities of a large, pre-trained LLM in a zero-shot setting. This approach requires no task-specific fine-tuning to the LLM's weights. Instead, the model's strategic behavior is guided entirely through in-context learning, conditioned on an initial prompt, P_0, that structures the entire decision-making task. The initial

prompt, P_0, is a static instruction set that establishes the context for the entire optimization run. It is composed of several key components designed to elicit an expert-like decision-making process:

1. **Role-playing Instruction:** The prompt begins by providing the LLM with an instruction to act as an "expert in Bayesian Optimization". This contextual framing is used to condition the model, leveraging the patterns it learned during pre-training to emulate the decision-making process that a human expert might follow when presented with similar data.
2. **Available Actions:** We explicitly define the portfolio of available acquisition functions, $\mathcal{A}$. Each function is listed with its abbreviation (e.g., EI, UCB) and full name. We refrain from giving a description for each AF to avoid biased interpretations and instead rely on the LLM's encoded knowledge. Note that we default to UCB if the LLM's output is invalid.
3. **State Information Schema:** The prompt describes the structure of the state summaries, S_t, that it will receive at each subsequent step, explaining what each piece of information (e.g., GP lengthscales, current performance) represents.
4. **Output Formatting Constraint:** Finally, the prompt specifies a strict output format ("Acquisition abbreviation: Justification") to ensure responses can be reliably parsed.

P_0 is sent once at the beginning of the optimization to set the stage. At each iteration t, the update prompt P_t is formed by appending the new state summary, S_t (see the next section), to the established context of P_0. The full text for P_0 is provided in Appendix C for reproducibility.

4.3 Optimization State Representation

A key component of our LMABO framework is the translation of the high-dimensional, numerical state of the BO process into a concise, human-readable textual summary, S_t. This summary is designed to provide the LLM with a comprehensive, multi-faceted view of the optimization landscape and progress. The state summary S_t at each iteration t is composed of the following elements:

- **Process Status:** To contextualize the current step within the overall process, we provide the number of **evaluations performed** so far (N), the **remaining budget** (N_{rem}), and the problem **dimensionality** (D). The remaining budget, in particular, is critical for balancing the long-term need for exploration against the short-term need for exploitation.
- **Performance History:** To provide context on the optimization's progress, we include several performance indicators. These are the **incumbent objective value** (f_{min}), the observed **function value range**, and the **shortest distance** from the last evaluated point to any previous point (as an indicator of the last evaluation's exploration tendency).
- **GP Model Characteristics:** To inform the LLM about the current understanding of the function landscape, we provide key hyperparameters from the fitted surrogate model $\mathcal{GP}_{t-1}$. This includes the kernel's **outputscale** and summary statistics of the **lengthscales** (minimum, maximum, mean, and standard deviation).

These components are formatted into a structured string that becomes the core of the prompt P_t sent to the LLM at each iteration. See examples of these state summaries in Appendix C. The design of S_t balances compactness with completeness, enabling the LLM to leverage domain-specific signals (budget, GP hyperparameters, exploration metrics) without requiring training. Our ablation results (Table 2) demonstrate that omitting any of these elements significantly degrades performance, underscoring the importance of the representation.

5 Experiments

5.1 Experiment Setup

Baselines We employ a comprehensive set of 19 baselines spanning three categories:

- **Static Acquisition Functions:** These are standard and popular BO methods that use a single, fixed AF throughout the process. We include all 12 AFs that constitute the portfolio from which LMABO can select (see Appendix A for details).

- **Adaptive Acquisition Functions:** These methods adapt their AF based on the optimization state, including GP-Hedge (Hoffman et al., 2011), No-PASt-BO (Vasconcelos et al., 2019), SETUP-BO (Vasconcelos et al., 2022), and ESP (Shahriari et al., 2014).
- **LLM-based Methods:** State-of-the-art baselines that incorporate LLMs into the BO process, including LLAMBO (Liu et al., 2024) and LLMP (Requeima et al., 2024).

Benchmark Problems The evaluation is performed on a broad set of 50 problems to test for robustness and general applicability. These includes 30 synthetic benchmark functions from the COCO platform (Hansen et al., 2021) and the BoTorch library (Balandat et al., 2020). In addition, we use 20 real-world hyperparameter optimization problems from Bayesmark (Uber, 2020). This benchmark evaluates the practical applicability of LMABO on a common and important task in machine learning. Details of these benchmark problems are provided in Appendix B.

Implementation Details We implement LMABO with Gemini-2.5 Flash. For surrogate modeling of GP-based methods, we use a GP with a Matérn 5/2 kernel, and the implementations are built using standard modules from the BoTorch library. Each optimization run is initialized with $2D + 1$ points, where D is the dimensionality of the problem. The optimization budget is set to 50 iterations for problems with fewer than 10 dimensions and 100 iterations for problems with 10 or more dimensions. More implementation details are provided in Appendix B.

Evaluation Each experiment is repeated 10 times with different random seeds. For each method on each problem, we averaged the **Areas Under the Simple Regret Curves** (AUCs) over all 10 repetitions. We then compute **Relative Performance** (RP): for each problem, the method with the lowest (best) total AUC receives an RP of 1.0, and all other methods are assigned an RP equal to their total AUC divided by the best total AUC for that problem. This ensures aggregation across problems is not affected by different absolute scales of AUCs. A **rank** of each method on each problem is determined by sorting all methods by their total AUC (lower is better), assigning rank 1 to the best. Note that the ranking includes 19 baselines, 6 ablation variants, and 4 adaptive portfolio variants, resulting in a maximum rank of 29. RP and rank help provide a clear and concise summary of comparative performance across all methods and problems instead of plotting all regret curves for 29 methods on 50 problems. Experimental results will undergo a rigorous statistical analysis to ensure the validity of our findings. Details about the statistical tests are provided in Appendix B.3.

5.2 Main Results

The results, summarized in Table 1, demonstrate that LMABO achieves a substantial performance improvement over all baseline categories. Averaged across problems, LMABO's total AUC is 9.3% lower than the best static AF, 55% lower than the best LLM-based method, and 16.1% lower than the best adaptive portfolio method; consequently, LMABO ranks among the top four methods on average. LMABO's relatively low variation (CV = 0.368) indicates high consistency across different seeds. A typical LMABO run with 50 iterations uses about 6000 tokens (≈\$0.01); both this expense and the LLM call latency of roughly 1 second per iteration are negligible relative to the cost of evaluating expensive black-box functions (which often takes minutes or hours per evaluation) and are justified by the resulting performance gains.

Static AFs are inherently unreliable. While strong heuristics like EI or LogEI are among the best in this class with relatively low RPs and ranks, their performance is brittle; on some problems, their rank drops to as low as 20th, highlighting the risk of a fixed strategy. In addition, adaptive portfolio methods, though achieving competitive results, frequently exhibit higher variability and are less robust across the heterogeneous problem suite. These approaches depend on heuristics for weighting past acquisition performance and thus can be slow to adapt when the task-specific landscape changes or when surrogate uncertainty dynamics differ across problems. Given the same AF portfolio, LMABO mitigates this shortcoming by considering other important factors including the process status, performance history and surrogate model characteristics, which enables faster, more consistent adaptation and yields significantly better average performance. LLM-based methods, while occasionally ranking among the top performers (e.g., LLAMBO is in the top three on 12 out of 50 problems), generally exhibit inconsistent results and often fall behind other approaches. This highlights that simply incorporating an LLM is not sufficient; effective navigation of the

Table 1: **Overall performance comparison of LMABO against all baselines across 50 optimization problems**. P-values from Friedman tests in the last row indicate statistically significant differences among methods for both RP and rank. The third and fifth columns show p-values of post-hoc pairwise comparisons between LMABO and each method, which confirms that the differences in performance between LMABO and all methods are significant. Exploitative AFs are marked in blue and explorative AFs are marked in magenta (see Appendix A for details).

Method	Mean RP↓ (Interquartile Range)	P-value (RP)	Mean Rank↓ (Min - Max)	P-value (Rank)	Mean CV of AUC
Static Acquisition Functions					
PI	1.498 (1.079–1.475)	2.740e-03	11.84 (1–27)	7.600e-05	0.451
LogPI	1.367 (1.089–1.449)	4.082e-03	10.68 (1–28)	1.674e-04	0.475
EI	1.316 (1.109–1.502)	2.632e-04	9.56 (1–25)	9.648e-06	0.438
LogEI	1.336 (1.142–1.480)	6.091e-06	10.00 (1–26)	1.353e-06	0.425
PosMean	1.382 (1.078–1.403)	4.655e-03	10.94 (1–28)	1.674e-04	0.454
PosSTD	6.943 (2.206–5.508)	2.505e-08	26.48 (3–29)	2.320e-08	0.479
UCB	1.733 (1.222–2.016)	1.963e-07	17.58 (1–28)	9.710e-08	0.373
TS	2.046 (1.286–1.872)	8.609e-08	18.64 (1–28)	4.781e-08	0.355
KG	1.636 (1.233–1.741)	4.766e-08	17.66 (3–27)	3.594e-08	0.400
PES	2.914 (1.561–3.235)	2.116e-08	23.94 (7–29)	2.032e-08	0.378
MES	2.779 (1.163–1.664)	3.629e-07	14.98 (1–28)	1.112e-07	0.399
JES	1.595 (1.279–1.694)	3.126e-08	18.08 (1–27)	3.131e-08	0.388
LLM-based Methods					
LLAMBO	2.646 (1.135–2.366)	1.165e-04	17.70 (1–29)	1.042e-06	0.428
LLMP	2.755 (1.514–2.490)	2.718e-08	23.28 (1–29)	2.529e-08	0.326
Adaptive Portfolio Methods					
GP-Hedge	1.422 (1.206–1.517)	1.239e-07	12.42 (1–25)	1.112e-07	0.418
No-PASt-BO	1.505 (1.186–1.722)	9.572e-08	14.06 (1–28)	1.112e-07	0.370
SETUP-BO	1.536 (1.155–1.688)	8.609e-08	13.88 (1–28)	6.129e-08	0.420
ESP	1.601 (1.273–1.674)	3.126e-08	16.82 (1–29)	3.742e-08	0.419
LMABO	**1.193** (1.050–1.247)	–	**4.04** (1–13)	–	0.367
P-values of Friedman Tests		3.846e-71		3.846e-71	

exploration-exploitation trade-off is crucial for robust BO. LMABO addresses this by explicitly framing AF selection as a decision-making task in which the LLM can make informed, context-aware decisions to balance the trade-off effectively.

5.3 Ablation Studies

Our ablation studies confirm that each component of the LMABO framework is crucial for achieving its superior performance, with statistically significant degradation in performance compared to the full model once a component is removed, as shown in Table 2. However, these studies also demonstrate the robustness of our core framework, as the ablated versions still achieve respectable results, often performing on par with or better than many established baselines.

LMABO's performance is inherently coupled with the underlying LLM. With a small open-source model in our LMABO-8B experiment, we observed a noticeable performance drop, though LMABO-8B still achieves competitive results. LMABO-30B, using a larger model with improved thinking capabilities, recovers much of this drop, approaching that of the full LMABO with Gemini-2.5 Flash and outperforming all baselines. This demonstrates that LMABO's effectiveness is not tied to a specific LLM, but rather benefits from the general reasoning capabilities of strong LLMs.

Removing the remaining budget leads to the smallest performance drop, which means that this information is the least critical of the three ablated inputs. GP model characteristics and shortest distance information are equivalently impactful on the effectiveness of the LMABO. The large drop in LMABO-AB4 demonstrates that instructing the LLM to avoid AFs that failed to improve the

Table 2: **Ablation study on the components of LMABO**. We analyze the contribution of LMABO's key components by comparing the full model to five ablated versions. LMABO-AB1, LMABO-AB2, and LMABO-AB3 remove the remaining budget, GP model characteristics, and shortest distance information, respectively. LMABO-AB4 removes the instruction to avoid AFs that did not yield improvement over the incumbent solution. LMABO-8B/30B uses open-source LLMs (Qwen3-8B and Qwen3-30B-A3B-Thinking-2507 (Team, 2025)). The Mean RP and Mean Rank are calculated using the same global ranking of all baseline and ablation methods as in Table 1.

Method	Mean RP↓ (Interquartile Range)	P-value (RP)	Mean Rank↓ (Min - Max)	P-value (Rank)	CV of (AUC)
Ablation Methods					
LMABO-AB1	1.381 (1.159–1.538)	2.940e-07	11.46 (2–25)	1.376e-07	0.393
LMABO-AB2	1.474 (1.213–1.625)	3.126e-08	14.60 (3–25)	2.500e-08	0.403
LMABO-AB3	1.479 (1.226–1.614)	1.519e-07	14.36 (1–24)	4.781e-08	0.397
LMABO-AB4	1.892 (1.406–1.914)	2.304e-08	20.76 (3–28)	2.246e-08	0.429
LMABO-8B	1.458 (1.184–1.628)	1.617e-07	13.80 (1–25)	1.112e-07	0.386
LMABO-30B	1.275 (1.101–1.338)	2.632e-04	7.76 (2–18)	6.414e-05	0.388
LMABO	1.193 (1.050–1.247)	–	4.04 (1–13)	–	0.367

incumbent is essential. Without this guidance, we find that the LLM repeatedly selects ineffective AFs, leading to significantly worse optimization performance.

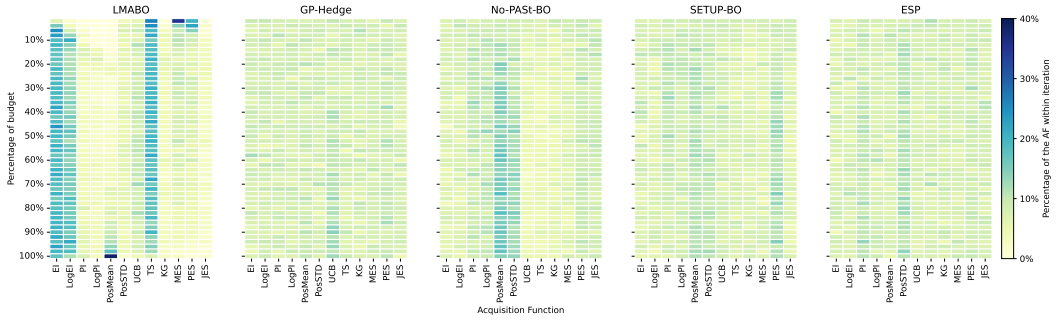
6 Analysis

To understand LMABO's strategy, we performed an in-depth analysis of its AF selection behavior, which reveals a multi-faceted strategy with clear preferences, following distinct temporal patterns, and, most importantly, adapting its behavior in response to the real-time optimization state.

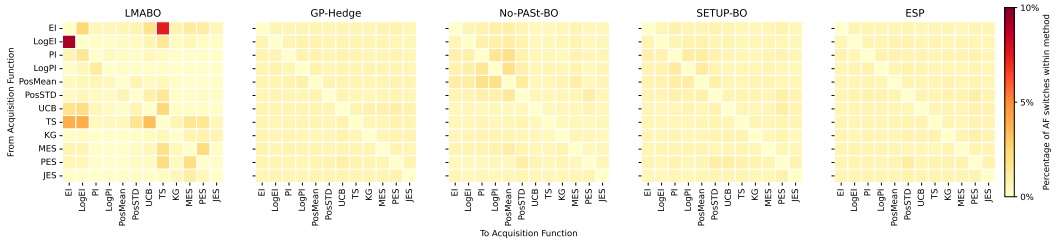
Overall Preferences In Figure 1a, we observe that LMABO exhibits a clear preference for certain AFs (e.g. EI, LogEI, and TS). EI's usage often increases slightly at the beginning as a response to early improvements, while TS's usage decreases gradually near the end as the need for exploration diminishes. PosMean is heavily used near the end for LMABO as a last effort to find improvements. Another surprising observation is the high usage of MES and PES in the first few iterations, but this seems to align with the initial goal of quickly reducing uncertainty about the global optimum. However, the strong performance of LMABO also involves other factors, as discussed later. On other adaptive portfolio methods, there is no clear preference for any AF, and the selection is more uniformly distributed. The only exception is No-PASt-BO with an increasing preference for PosMean as the budget runs out. From this figure, a first insight is that LMABO's success partly stems from a well-calibrated preference for strong AFs, rather than a uniform exploration of all options, as well as a dynamic adjustment of these preferences over time.

On a separate note, the adaptive portfolio baselines can be at a disadvantage without knowing the strengths of EI and LogEI. We conducted an additional experiment where these methods operate on only a curated subset comprising of EI, LogEI, and TS - the three most frequently selected AFs by LMABO. We indeed observe a performance improvement for these methods except for GP-Hedge (detailed results in Appendix E), but the curated versions are still strictly outperformed by LMABO.

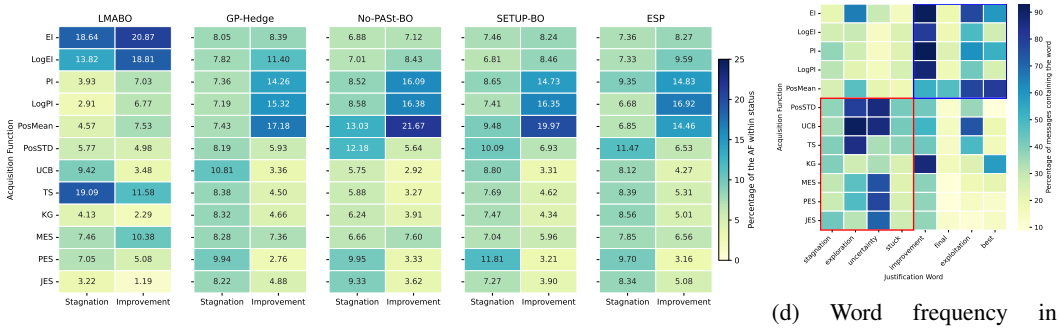
Switching the AF in Response to the Optimization State In Figure 1b, a notable difference is observed between LMABO and the adaptive portfolio baselines in terms of AF switching. LMABO is the only method to perform a high number of switches between the group of explorative AFs (i.e. the first five AFs) and exploitative AFs (i.e. the remaining seven AFs) throughout the optimization process, as seen in the bottom left and top right of the figures. The dynamic adjustment mentioned earlier is more evident here, as LMABO frequently switches between exploration and exploitation. Figure 1c shows increased usage of exploitative AFs during improvement phases for all methods, which aligns with the goal of refining the search around promising areas. However, combined with the findings from Figure 1b, the adaptive portfolio baselines seem to demonstrate a passive, one-directional learning by using more exploitative functions after success, but their sparse switching



(a) AF selection frequency over the optimization process



(b) AF switch frequency



(c) AF selection frequency by improvement/stagnation status. "Stagnation" is defined as no improvement in the incumbent, and "Improvement" is defined as any change in the incumbent.

(d) Word frequency in justifications. Red box is the explorative group. Blue box is the exploitative group.

Figure 1: LMABO's acquisition function selection behavior across all problems.

patterns reveal a "sticky" policy that is slow to abandon a strategy, even when it is failing. This is likely because of their reliance on past successes to guide future choices, which can lead to overcommitment to a single AF. In contrast, LMABO employs an active, bi-directional strategy, not only learning to exploit on improvement but also decisively switching back to exploratory functions to escape stagnation. This demonstrates that LMABO's core advantage lies not just in identifying a good heuristic, but in its superior, more agile policy for knowing when that heuristic is no longer effective and a different approach is required.

The Failure of Simple Meta-strategies In Figure 1, it can be observed that LMABO uses EI and TS more often than other options in the exploitative and explorative groups, respectively, and also frequently switches between the two. To further validate that LMABO's success is not simply because of switching between EI and TS, we compare it against two straightforward meta-strategies: (1) alternating between EI and TS every k iterations and (2) explore first (with TS), then exploit (with EI). In Figure 2, these simple heuristics demonstrate inconsistent, problem-dependent performance, failing to offer a robust advantage over the static baselines across the diverse set of problems. In contrast, LMABO achieves a consistently faster convergence in all showcased scenarios. These results demonstrate that LMABO's behavior cannot be reduced to a simple scripted heuristic.

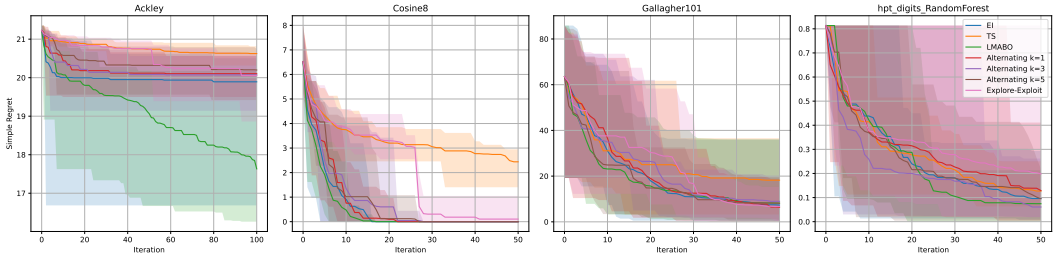


Figure 2: Comparison of LMABO to simple meta-strategies: (1) Alternating pattern between EI and TS every k iterations, and (2) explore first, then exploit. EI and TS are included for reference. LogEI and UCB are also popular options in the exploitative and explorative groups, respectively, but we chose EI and TS as they are the most frequently selected by LMABO in their respective categories.

Linking AF Selection to Justification To verify a consistent link between the LLM's AF choices and its justifications, we analyzed keywords appeared in the justifications across different AFs. In Figure 1d, explorative AFs are strongly associated with terms like "exploration" or "stagnation", and exploitative AFs are strongly associated with terms like "exploitation" or "improvement". This confirms that the LLM's selections are consistent with its justification, and that it is possible to use these justfication to understand the decision of the LLM.

Information Sensitivity Analysis To assess the sensitivity of LMABO to the information provided in the prompt, we conducted a sensitivity analysis by perturbing the values fed to the LLM in the state representation across early, middle and late stages. Due to space constraints, we summarize the key findings here (detailed results are in Appendix G). During the early stage, the LLM is highly reactive to all information changes, including the process status, performance history, and GP model characteristics. During the middle stage, performance history and process status are most influential. In the late stage, the LLM is less sensitive to perturbations and is mostly changing its decision in response to new incumbent values where it exhibits a strong preference for exploitative AFs. While perturbing the values presents inherent limitations (e.g. the perturbed values may be unrealistic or inconsistent with other state variables), the results still provide valuable insights into the LLM's decision-making process. Overall, we find that LMABO is highly sensitive to tactical variables like performance history with evident signs of stagnation/improvement and process status, while correctly showing robustness to changes in secondary GP parameters that do not alter the overall strategic context. This demonstrates that the LLM is synthesizing the state summary to weigh the relative importance of different inputs, a key feature of its effective, state-aware policy.

7 Conclusion

We introduced LMABO, a novel framework that successfully utilizes a pre-trained LLM as a zero-shot, online strategist for selecting acquisition functions in Bayesian Optimization. By prompting the LLM with a comprehensive, real-time summary of the optimization state, LMABO dynamically controls the exploration-exploitation trade-off. Our extensive experiments on 50 benchmarks show that this approach significantly outperforms strong static, adaptive, and other LLM-based baselines. Ablation studies and analysis of the LLM's behavior confirm its success stems from a well-rounded state-aware strategy that adapts well to the optimization's progress.

This paper focused on standard BO with Gaussian Processes, and future work could adapt LMABO to other surrogate models and optimization settings. For instance, in constrained BO, the LLM could be leveraged to dynamically balance objective improvement against constraint satisfaction. Overall, LMABO opens new avenues for integrating LLMs into adaptive optimization frameworks, leveraging their reasoning capabilities for decision-making in complex tasks.

Reproducibility Statement

We submitted the code as a supplementary material. The code includes the implementation of our method, baselines, and scripts to reproduce the main experiments. We also provide details of the experimental setup and datasets used in the experiments in the appendix. Upon acceptance, we will make the code publicly available.

LLM Usage

Large Language Models were used for correcting grammar and improving writing clarity along with updating the related works. We used Gemini Pro and ChatGPT for these purposes.

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A List of Acquisition Functions

The acquisition function $\alpha(x; \mathcal{D})$ guides the selection of query points in BO by quantifying the utility of evaluating f at x. By maximizing $\alpha(x; \mathcal{D})$ over the search space, we identify points that balance exploration (sampling where uncertainty is high) and exploitation (sampling where the surrogate predicts low function values). Details of the AFs used in our experiments are as follows:

- Probability of Improvement (PI) (Kushner, 1964):

$$\alpha_{\mathrm{PI}}(x) = \Phi\left(\frac{\mu(x) - \tau}{\sigma(x)}\right),$$

where Φ is the standard normal CDF, $\mu(x)$ and $\sigma(x)$ are the posterior mean and standard deviation, and τ is a target (e.g., the incumbent solution). PI selects points with high probability of improving upon τ.

- Expected Improvement (EI) (Mockus, 1998):

$$\alpha_{\mathrm{EI}}(x) = (\mu(x) - \tau)\,\Phi(z) + \sigma(x)\,\phi(z), \quad z = \frac{\mu(x) - \tau}{\sigma(x)},$$

  where ϕ is the standard normal PDF. EI measures the expected magnitude of improvement.

- Log Probability of Improvement (LogPI) (Balandat et al., 2020) and Log Expected Improvement (LogEI) (Ament et al., 2023): These are numerically stable variants of PI and EI, respectively, that operate in the log domain to handle vanishing values and gradients.

- Upper Confidence Bound (UCB) (Srinivas et al., 2010):

$$\alpha_{\mathrm{UCB}}(x) = \mu(x) + \kappa\,\sigma(x),$$

  where $\kappa > 0$ controls the exploration weight. UCB explicitly balances exploitation (mean) and exploration (uncertainty).

- Thompson Sampling (TS) (Chowdhury & Gopalan, 2017): Draws a sample $\tilde{f} \sim p(f \mid \mathcal{D})$ and selects x maximizing $\tilde{f}(x)$. TS provides a randomized exploration strategy consistent with the posterior.

- Posterior Mean (PosMean) and Posterior Standard Deviation (PosStd): Using $\alpha_{\mathrm{mean}}(x) = \mu(x)$ yields pure exploitation, while $\alpha_{\mathrm{std}}(x) = \sigma(x)$ performs pure exploration.

- Knowledge Gradient (KG) (Wu & Frazier, 2016): This look-ahead function quantifies the expected increase in the maximum value of the function that results from collecting a new observation at a candidate point x.

- Information-theoretic AFs:
  - Predictive Entropy Search (PES) (Hernández-Lobato et al., 2014): Selects points that maximize the expected reduction in entropy of the distribution over the location of the global optimum.
  - Max-value Entropy Search (MES) (Wang & Jegelka, 2017): Focuses on reducing uncertainty about the maximum function value rather than its location.
  - Joint Entropy Search (JES) (Tu et al., 2022): A recent AF that generalizes PES and MES by considering the joint entropy of both the location and value of the optimum.

We use the implementations of these AFs from the BoTorch library (Balandat et al., 2020) in our experiments. For KG, PES, MES, and JES, we use their available batch implementations with a batch size of 1. We consider PosSTD, UCB, TS, KG, PES, MES, and JES to be in the exploratory category, while the exploitative AFs include PosMean, PI, LogPI, EI, and LogEI.

B Experimental Details

B.1 List of Benchmarks

We evaluate LMABO on a diverse suite of 50 benchmark problems, including synthetic functions and real-world hyperparameter optimization tasks. The synthetic benchmarks are isted in Table 3, with 15 functions from the COCO suite (Hansen et al., 2021) and 15 from BoTorch (Balandat et al., 2020). For hyperparameter optimization tasks, we follow the practice of Liu et al. (2024) and use datasets and ML models available on Bayesmark (Uber, 2020) to form 20 dataset-model pairs. The datasets include Breast, Digits, Wines and Diabetes, and the ML models include Decision Tree, Random Forest, SVM, AdaBoost, and MLPSGD. The dimensionality of these search spaces ranges from 2 to 8. We use the empirical optimum found by all methods (as the true optima are unknown for many problems) to compute the simple regret at each iteration. See Appendix D.1 of Liu et al. (2024) for full details about the hyperparameter optimization tasks.

Table 3: COCO and BoTorch synthetic benchmark functions used in our experiments.

COCO benchmarks (15)		BoTorch synthetic benchmarks (15)	
Name	Dimensionality	Name	Dimensionality
BucheRastrigin	5	Ackley	50
LinearSlope	5	Beale	2
AttractiveSector	5	Bukin	2
StepEllipsoid	5	Cosine8	8
Discus	5	DixonPrice	15
BentCigar	5	DropWave	2
SharpRidge	5	EggHolder	2
DifferentPowers	5	Griewank	9
Weierstrass	5	Hartmann	6
SchaffersIllCond	5	HolderTable	2
CompositeGriewankRosenbrock	10	Levy	13
Gallagher21	5	Michalewicz	10
Gallagher101	5	StyblinskiTang	21
Katsuura	5	Shekel	4
LunacekBiRastrigin	5	SixHumpCamel	2

B.2 Implementation Details

We follow the standard practice to optimize the GP hyperparameters by maximizing the log marginal likelihood at each iteration. We use the default implementation of GP regression in BoTorch (Balandat et al., 2020) which has hyperparameter priors from (Hvarfner et al., 2024) to enhance performance on high-dimensional tasks. All acquisition functions are optimized using multi-start LBFGS-B, except for TS and PES. For both TS and PES, we use discrete optimization over a finite set of randomly sampled candidates due to the high computational cost of evaluating the acquisition functions. This practice of AF optimization applies to running experiments with all static acquisition functions, all adaptive portfolio baselines, and LMABO.

For all experiments, both Gemini-2.5 Flash and Qwen3-8B were queried with a temperature of 0.0. Again, for invalid or failed LLM responses, we fall back to UCB. The fallback rate is extremely small at only about 0.11% of all queries (i.e. out of 10,000 queries, only 11 of them do not follow the "Acquistion abbreviation: justfication" format). This indicates that LLM failures are rare and have minimal impact on overall optimization performance. All adaptive portfolio baselines, such as GP-Hedge, were implemented using their standard configurations as described in their respective publications, except that the portfolio of acquisition functions was expanded to include all 12 AFs listed in Appendix A.

B.3 Statistical Tests

Results in Tables 1, 2 and 5 follow a standardized statistical analysis to ensure the significance of the results. This statistical analysis is conducted separately for both mean RPs and ranks (across 10 repetitions) of 29 methods on 50 benchmarks. Firstly, to assess the significance of performance differences between the methods, we first apply the Friedman test (a non-parametric test for data that is not normally distributed) on the matrix of mean RPs (or ranks). The null hypothesis of the Friedman test is that all methods perform equally, while the alternative hypothesis is that at least one method performs differently. If the Friedman test indicates significant differences, we follow up with post-hoc pairwise comparisons using the Wilcoxon signed-rank test with Holm-Bonferroni correction to control for multiple comparisons, specifically comparing each baseline method against LMABO. The null hypothesis for each pairwise comparison is that there is no difference in performance between LMABO and a baseline, while the alternative hypothesis is that the performances of LMABO and the baseline differ. We set a significance level of 0.05 for all statistical tests.

C PROMPTS

Figure 1 shows the complete, unabridged initial prompt (P_0) used to instruct the LLM in our experiments. This prompt was developed through a very brief iterative process of 6-7 trials. The refinements were not aimed at tuning for performance on a specific benchmark, but rather to ensure accurate formatting of the LLM's responses and to encourage a full consideration of all information in the optimization state representation. Examples of follow up prompts during the optimization process are shown in Table 7. For KG, PES, MES, and JES, we denote them by qKG, qPES, qMES, and qJES, respectively, in the initial prompt to align with the naming conventions in BoTorch (Balandat et al., 2020). In constructing the initial prompt, we observed the following phenomena during preliminary experiments that informed the final design:

- A full history of past function values and AF choices was not necessary for each input prompt, as the LLM seems capable of inferring relevant optimization history from previous input prompts.
- Specific examples of AF choices (e.g. "UCB: brief justification") in the prompt could bias the LLM towards a particular choice, so we replaced them with placeholders. Before this change, we found that Qwen3-8B often mimicked the exemplar choices if specific AFs were mentioned as examples, and only stopped doing so when the examples were replaced with placeholders.
- The LLM sometimes ignored certain details, such as the number of remaining iterations, so we added an assurance in the prompt to consider all provided context.

D RUNTIME COMPARISON

Table 4 shows the average runtime, in minutes, for 50 iterations of the methods across all tested benchmarks. LMABO only incurs a moderate overhead compared to static AFs due to the LLM query at each iteration, but it is significantly faster than adaptive portfolio methods that require optimizing multiple AFs at each iteration. Since the curated versions of adaptive portfolio methods only optimize 3 AFs instead of 12, they are much faster than their full versions while achieving better performance (as shown in Table 5), suggesting that a smaller, well-chosen portfolio can be beneficial for these methods. Among LLM-based methods, LLAMBO is comprable in speed to LMABO, while LLMP is much slower due to inferring with an open-source model locally. This higher runtime is also observed on LMABO-8B and LMABO-30B, the ablated versions of LMABO that use an open-source model.

Table 4: Average runtime for 50 iterations of all methods across all benchmarks (in minutes).

Method	Runtime	Method	Runtime
PosSTD	2.20	GP-Hedge	109.18
PosMean	2.06	GP-Hedge-Curated	12.01
PI	2.62	No-PASt-BO	113.67
LogPI	2.09	No-PASt-BO-Curated	14.94
EI	2.14	SETUP-BO	104.42
LogEI	2.15	SETUP-BO-Curated	7.24
UCB	2.07	ESP	50.61
TS	4.62	ESP-Curated	6.01
KG	12.88	LMABO	7.42
PES	8.93	LMABO-AB1	6.69
MES	3.73	LMABO-AB2	8.17
JES	5.45	LMABO-AB3	7.79
LLAMBO	9.21	LMABO-AB4	6.46
LLMP	29.35	LMABO-8B/30B	17.85

Table 5: **Comparing adaptive portfolio methods between using a large portfolio (of 12 AFs) and a curated portfolio (of 3 AFs)**. The curated methods are denoted with a "-Curated" suffix.

Method	Mean RP↓ (Interquartile Range)	P-value (RP)	Mean Rank↓ (Min - Max)	P-value (Rank)	CV of (AUC)
GP-Hedge	1.422 (1.206–1.517)	1.239e-07	12.42 (1–25)	1.112e-07	0.418
GP-Hedge-Curated	1.487 (1.233–1.670)	3.126e-08	15.06 (2–28)	5.444e-08	0.372
No-PASt-BO	1.505 (1.186–1.722)	9.572e-08	14.06 (1–28)	1.112e-07	0.370
No-PASt-BO-Curated	1.469 (1.218–1.579)	7.656e-08	14.38 (1–24)	7.235e-08	0.409
SETUP-BO	1.536 (1.155–1.688)	8.609e-08	13.88 (1–28)	6.129e-08	0.420
SETUP-BO-Curated	1.503 (1.243–1.556)	3.126e-08	14.76 (1–26)	4.781e-08	0.374
ESP	1.601 (1.273–1.674)	3.126e-08	16.82 (1–29)	3.742e-08	0.419
ESP-Curated	1.506 (1.240–1.537)	9.572e-08	15.06 (2–26)	1.112e-07	0.422

Table 6: Responses to the initial prompt P_0.

Problem	Response
Cosine8	Yes, I understand the context. I am ready to receive the first summary of the Bayesian Optimization process.
Weierstrass	Okay, I understand. I am ready to receive the summary of the Bayesian Optimization process and recommend the next acquisition function. I will strictly follow the specified output format.
hpt_wine_MLPSGD	Yes, I understand the task and the available acquisition functions. I am ready to receive the first summary of the Bayesian Optimization process.

E Curated Set for Adaptive Portfolio Baselines

In this experiment, the adaptive portfolio baselines (i.e. GP-Hedge, No-PASt-BO, SETUP-BO, and ESP) are restricted to a curated subset of acquisition functions: EI, LogEI, and TS. The curated methods also participated in the calculation of relative performance, rank, and statistical tests mentioned in Section 5. No-PASt-BO, SETUP-BO, and ESP show a performance improvement when using the curated set, while GP-Hedge shows a degradation.

F LLM Response Examples

F.1 Responses to the Initial Prompt

Table 6 shows the responses of Gemini-2.5 Flash to the initial prompt across some different optimization problems. The responses confirm the LLM's understanding of the task and readiness to proceed with the optimization process.

F.2 Responses During Optimization

Table 7 shows example responses from Gemini-2.5 Flash at different stages of an optimization run of the Weierstrass function. As seen on the table, the LLM adapts its acquisition function choices based on all provided context, including the number of remaining iterations, the current best objective value, the model's lengthscales, and the shortest distance between points. Contrary to the popular choice of TS in early iterations in other cases, the first response opts for EI when it observes a wide range of function values. The second and fourth responses both select LogEI after a new best value is found, showing the LLM's ability to recognize when an improvement-focused acquisition is appropriate. Although both EI and LogEI are suitable in these contexts (as well as other exploitative AFs like PI), the LLM's choice of LogEI is influenced by the wide range of function values and the modest gain compared to the range (which were from -6.576 to -9.980 for the second response and from -10.148 to -11.302 for the fourth response). This is helpful when the values of EI may become very small, as LogEI is more numerically stable. The third response chooses TS to escape

a stagnation phase in response to failed improvements and over-exploration signs (demonstrated by the smaller shortest distance). Finally, with only one iteration left, the LLM selects EI to maximize the chance of a final improvement.

G Information Sensitivity Analysis

Tables 8, 9, 10, and 11 show the results of our information sensitivity analysis at early, middle, and late stages of optimization, respectively. For these experiments, we perturb each element of the state representation S_t individually while keeping all other elements fixed to their original values at iteration T in an optimization run. Input prompts from previous iterations were not modified, so the LLM's memory of the optimization history remains intact.

While perturbing the values may present some noises in the results, we still observe some clear trends across all four tables. Firstly, information about the process status (e.g. number of points evaluated, remaining budget) and the performance history (e.g. incumbent objective value, function value range, shortest distance) have a significant impact on the LLM's acquisition function choices. Reducing the remaining budget or having a new incumbent objective value tends to shift the LLM's preference towards exploitative AFs. However, in Tables 8 and 9, we observe that a very small improvement in the incumbent objective value (e.g. from 1.24 to 1.244 in Table 8 and from -9.98 to -9.982 in Table 9) can lead to a switch back to an explorative AF. This suggests that the LLM is sensitive to the magnitude of improvement relative to the overall function value range. Secondly, information about the model state (e.g. lengthscales, outputscale) appears to have a more subtle influence on the LLM's choices. While perturbing these elements does lead to some changes in the selected AFs, the changes are less consistent and pronounced compared to the other state elements. This indicates that the LLM may prioritize information about the optimization progress and performance over the surrogate model's internal parameters when making decisions.

```
You are an expert in Bayesian Optimization, specifically tasked with recommending the most suitable acquisition function for the next iteration to minimize an objective function.

For context, we use a Gaussian Process as the surrogate model with a Matern 5/2 kernel with ARD.

I will provide you with a summary of the Bayesian Optimization process at each step. This summary will include the following information:
- **N:** The total number of points evaluated so far.
- **Remaining iterations:** The number of iterations left in the optimization process.
- **D:** The dimensionality of the search space (number of input parameters).
- **f_range:** The range of the objective function values observed so far.
- **f_min:** The current best (lowest) observed objective value.
- **Shortest distance**: The shortest distance from the last point to any other point, indicating whether it is exploiting too much.
- **Model lengthscales:** These are crucial hyperparameters of the Gaussian Process model's kernel.
They describe how the model perceives the smoothness and relevance of each input dimension to the objective function.
You will receive their range (min/max), mean, and standard deviation.
- **Model outputscale: ** It defines the overall magnitude or amplitude of the function's variation.

Available acquisition functions you can choose from, with brief descriptions of their primary uses:
1.  PI (Probability of Improvement)
2.  LogPI (Log Probability of Improvement)
3.  EI (Expected Improvement)
4.  LogEI (Log Expected Improvement)
5.  UCB (Upper Confidence Bound)
6.  PosMean (Posterior Mean):
7.  PosSTD (Posterior Standard Deviation)
8.  TS (Thompson Sampling)
9.  qKG (Knowledge Gradient)
10. qPES (Predictive Entropy Search)
11. qMES (Max-value Entropy Search)
12. qJES (Joint Entropy Search)

At each step:
- **Review the provided summary of the optimization process and consider the current state of the optimization.**
- **Select the acquisition function that you believe will be best for the optimization process.**
- **Avoid reusing acquisition functions that failed to improve the objective function in previous iterations.**

When responding, select the acquisition function you deem most appropriate.
Your justification should briefly explain why that function is suitable given the provided optimization summary, referencing relevant aspects like exploration/exploitation balance, remaining iterations, or model characteristics.
The response must strictly follow the format "Acquisition abbreviation: justification", similar to these examples:
- 'AF_ABBREVIATION: Your justification for choosing this specific function.'
- 'XXX: A brief reason explaining why XXX is the optimal choice now.'
Firstly, just give a brief confirmation that you understand the task and the available acquisition functions.
```

Listing 1: The unabridged initial prompt (P_0) provided to the LLM.

Input Prompt	Response
Current optimization state: - N: 11 - Remaining iterations: 50 - D: 5 - f_range: Range [-5.982, 83.765], Mean 26.466 (Std Dev 35.075) - f_min: -5.982 - Shortest distance: 0.455 - Lengthscales: Range [0.261, 59.707], Mean 27.581 (Std Dev 24.557) - Outputscale: 0.898	EI: Given the early stage (N=11, 50 iterations remaining) and the wide range of observed function values and varying lengthscales, there is still significant uncertainty and potential for discovering better regions. EI provides a robust balance between exploration (considering areas of high uncertainty) and exploitation (seeking expected improvement over the current best, f_min), making it an excellent choice for building a better global understanding of the objective function while still prioritizing improvement.
Current optimization state: - N: 21 - Remaining iterations: 40 - D: 5 - f_range: Range [-9.980, 106.046], Mean 23.896 (Std Dev 34.093) - f_min: -9.980 - Shortest distance: 0.427 - Lengthscales: Range [0.513, 399.250], Mean 154.676 (Std Dev 188.785) - Outputscale: 1.212	LogEI: Thompson Sampling successfully discovered a new f_min. With this new best observation and 40 iterations remaining, LogEI is a strong choice. It is effective for finding further significant improvements, especially when dealing with a potentially wide range of objective values (as indicated by f_range) or when the current best is challenging to beat. LogEI provides a more robust measure of improvement compared to standard EI, by focusing on the log of the improvement, which can help in navigating the complex landscape suggested by the varying lengthscales and ensure continued progress.
Current optimization state: - N: 40 - Remaining iterations: 21 - D: 5 - f_range: Range [-10.148, 132.117], Mean 15.999 (Std Dev 33.416) - f_min: -10.148 - Shortest distance: 0.204 - Lengthscales: Range [0.449, 3.865], Mean 1.786 (Std Dev 1.159) - Outputscale: 1.618	TS: Both JES and PES failed to improve f_min. The lengthscales have drastically shortened and become concentrated, indicating the model believes the function is very localized, yet this hasn't yielded improvements. The shortest distance is also very small (0.20), suggesting potential over-exploitation. With 21 iterations remaining, Thompson Sampling is the best choice to break this persistent stagnation and localized search. By sampling a new function from the posterior, TS can explore regions that the current model might be overlooking or prematurely discarding, offering a fresh, diverse exploration strategy to find new global optima.
Current optimization state: - N: 50 - Remaining iterations: 11 - D: 5 - f_range: Range [-11.302, 132.117], Mean 12.749 (Std Dev 30.799) - f_min: -11.302 - Shortest distance: 0.346 - Lengthscales: Range [0.494, 2.198], Mean 1.532 (Std Dev 0.611) - Outputscale: 2.069	LogEI: EI successfully improved f_min! With a new best value found and only 11 iterations remaining, it's crucial to build on this success with an improvement-focused acquisition function. LogEI is an excellent choice as it continues to seek expected improvement, but its logarithmic scaling makes it particularly robust to the magnitude of objective function values. This allows it to efficiently pinpoint further significant improvements or refine the search around the new f_min, ensuring we maximize the chances of finding an even better optimum in these final, critical iterations.
Current optimization state: - N: 60 - Remaining iterations: 1 - D: 5 - f_range: Range [-12.135, 132.117], Mean 11.070 (Std Dev 29.387) - f_min: -12.135 - Shortest distance: 0.503 - Lengthscales: Range [0.548, 2.468], Mean 1.615 (Std Dev 0.653) - Outputscale: 2.821	EI: With only 1 iteration remaining, the primary goal is to make the absolute best attempt to improve the current f_min. EI (Expected Improvement) is the most robust and direct improvement-focused acquisition function. It directly optimizes for the expected gain over the current best observed value, offering the most pragmatic strategy to find a final, better optimum, especially since it demonstrated success in finding the most recent f_min just a few iterations ago.

Table 7: Example responses from the LLM during an optimization run of the Weierstrass function. The left column includes the input prompts fed to the LLM. Each response includes the LLM's selected acquisition function along with its justification.

Table 8: **Information Sensitivity Analysis for Early Stage ($T = 5$).** We perturb the values of each element in the state representation S_t and observe the resulting changes in the output AF chosen by the LLM. The highlighted values indicate the original state element values at $T = 5$ in a Griewank optimization run. We show explorative AFs in blue and exploitative AFs in magenta for better tracking of AF changes between the two groups. The original input prompt and response are shown at the bottom of the table.

State element		Output AF given element value					
# points evaluated	Value	5	**9**	20	40	50	500
	AF	PES	LogEI	LogEI	PosSTD	PosSTD	PES
Remaining budget	Value	1	10	40	**46**	50	100
	AF	PosMean	LogEI	PES	LogEI	PES	PES
Incumbent objective value	Value	-100	-10	0	1	1.24	**1.244**
	AF	LogEI	EI	EI	EI	KG	LogEI
Maximum function value	Value	2	100	190	**194.081**	200	1000
	AF	LogEI	LogEI	UCB	LogEI	LogEI	PES
Mean of function value	Value	2	20	50	**56.326**	60	100
	AF	PosSTD	UCB	LogEI	LogEI	LogEI	LogEI
Std Dev of function value	Value	1	10	60	**63.145**	70	100
	AF	JES	PES	PES	LogEI	PES	PES
Shortest distance	Value	0.01	0.05	**0.06**	0.07	0.1	0.5
	AF	PES	LogEI	LogEI	LogEI	LogEI	MES
Minimum of lengthscales	Value	0.01	0.1	0.2	**0.231**	0.3	0.45
	AF	LogEI	PES	LogEI	LogEI	LogEI	PES
Maximum of lengthscales	Value	0.25	0.4	**0.452**	0.5	1.0	10.0
	AF	LogEI	EI	LogEI	PES	LogEI	EI
Mean of lengthscales	Value	0.24	0.3	**0.342**	0.4	0.45	
	AF	MES	LogEI	LogEI	LogEI	LogEI	
Std Dev of lengthscales	Value	0.01	0.1	**0.110**	0.2	1.0	10.0
	AF	PES	PES	LogEI	LogEI	LogEI	JES
Outputscale	Value	0.01	0.1	0.8	**0.865**	0.9	10.0
	AF	LogEI	LogEI	LogEI	LogEI	EI	KG

Original input prompt

Current optimization state:
- N: 9
- Remaining iterations: 46
- D: 2
- f_range: Range [1.244, 194.081], Mean 56.326 (Std Dev 63.145)
- f_min: 1.244
- Shortest distance: 0.060
- Lengthscales: Range [0.231, 0.452], Mean 0.342 (Std Dev 0.110)
- Outputscale: 0.865

Original response

LogEI: ‘f_min‘ has stalled for two iterations and the shortest distance is again very low (0.060), indicating potential over-exploitation or getting stuck in a flat region. LogEI is suitable here because it is less sensitive to the absolute magnitude of improvement and focuses on relative improvements, which helps to escape local minima or flat regions where small absolute improvements are still valuable, while also maintaining a strong exploration component given the many remaining iterations. We also need to avoid reusing EI which was used 2 iterations ago and did not improve f_min.

Table 9: **Information Sensitivity Analysis for Middle Stage ($T = 25$).** This table follows the same format as Table 8 but for $T = 25$ in a CompositeGriewankRosenbrock optimization run.

State element		Output AF given element value					
# points evaluated	Value	5	20	40	45	50	100
	AF	PI	PI	KG	TS	JES	LogPI
Remaining budget	Value	1	5	20	26	30	100
	AF	PI	LogEI	KG	TS	TS	LogPI
Incumbent objective value	Value	-1000	-200	-100	-92	-91.2	-91.176
	AF	PosMean	PI	LogPI	JES	JES	TS
Maximum function value	Value	1	20	200	208.249	210	1000
	AF	JES	TS	KG	TS	JES	UCB
Mean of function value	Value	-90	-50	-40.161	-40	0	200
	AF	PES	PES	TS	PES	TS	TS
Std Dev of function value	Value	1	10	50	55.658	60	100
	AF	JES	TS	TS	TS	JES	KG
Shortest distance	Value	0.01	0.1	0.7	0.714	0.8	1.0
	AF	UCB	TS	JES	TS	UCB	TS
Minimum of lengthscales	Value	0.01	0.1	0.9	0.989	1.0	10.0
	AF	JES	JES	JES	TS	KG	KG
Maximum of lengthscales	Value	30.0	100.0	200.0	208.249	210	1000.0
	AF	JES	PES	JES	TS	JES	TS
Mean of lengthscales	Value	1.0	10.0	20.0	29.547	30.0	200.0
	AF	JES	JES	JES	TS	PES	JES
Std Dev of lengthscales	Value	0.1	10.0	60.0	62.256	70.0	200.0
	AF	KG	TS	KG	TS	KG	JES
Outputscale	Value	0.1	3.0	3.731	4.0	10.0	100.0
	AF	UCB	PES	TS	KG	JES	PES

Original input prompt

Current optimization state:
- N: 45
- Remaining iterations: 26
- D: 10
- f_range: Range [-91.176, 208.249], Mean -40.161 (Std Dev 55.658)
- f_min: -91.176
- Shortest distance: 0.714
- Lengthscales: Range [0.989, 204.500], Mean 29.547 (Std Dev 62.256)
- Outputscale: 3.731

Original response

TS: ‘f_min‘ remains stagnant for four iterations, and ‘qMES‘ did not yield an improvement, despite the refined lengthscales. The lengthscales have slightly widened again, indicating some lingering uncertainty. With a significant number of remaining iterations and persistent stagnation, ‘TS‘ (Thompson Sampling) is a strong choice. It provides a robust, probabilistic, and fundamentally different exploration strategy by sampling from the GP posterior. This approach is excellent for escaping local optima and discovering genuinely new, high-potential regions, especially when other more deterministic or information-theoretic methods have struggled to find a better ‘f_min‘, and the model still has some uncertainty in its overall landscape understanding.

Table 10: **Information Sensitivity Analysis for Late Stage** ($T = 45$) **- Part 1.** This table follows the same format as Table 8 but for $T = 45$ in a hpt_breast_MLPSGD optimization run.

State element		Output AF given element value					
# points evaluated	Value	5	20	50	54	60	100
	AF	LogPI	JES	JES	JES	JES	JES
Remaining budget	Value	1	5	6	10	50	100
	AF	EI	KG	JES	JES	JES	JES
Incumbent objective value	Value	-100	-10	-1	-0.92	-0.917	-0.916
	AF	EI	EI	EI	EI	LogEI	JES
Maximum function value	Value	-0.7	-0.4	-0.360	-0.3	-0.1	0.0
	AF	JES	KG	JES	JES	JES	JES
Mean function value	Value	-0.9	-0.8	-0.738	-0.7	-0.4	
	AF	JES	JES	JES	KG	JES	
Std Dev function value	Value	0.01	0.1	0.152	0.2	0.5	1.0
	AF	JES	JES	JES	JES	JES	JES
Shortest distance	Value	0.01	0.1	0.4	0.459	0.5	1.0
	AF	JES	JES	JES	JES	KG	JES

Table 11: **Information Sensitivity Analysis for Late Stage ($T = 45$) - Part 2.** Continuation of Table 10.

State element		Output AF given element value					
Minimum of lengthscales	Value	0.001	0.004	0.01	0.1	1.0	10.0
	AF	JES	JES	KG	JES	JES	JES
Maximum of lengthscales	Value	1600	2000	4000	4234.465	5000	10000
	AF	JES	KG	JES	JES	JES	JES
Mean of lengthscales	Value	1.0	100.0	1500.0	1514.580	1600	4000
	AF	JES	JES	JES	JES	JES	KG
Std Dev of lengthscales	Value	10.0	100.0	1600.0	1683.459	1700.0	4000.0
	AF	JES	JES	JES	JES	JES	JES
Outputscale	Value	0.01	0.1	0.8	0.818	0.9	10.0
	AF	JES	JES	JES	JES	JES	JES

Original input prompt	**Original response**
Current optimization state: - N: 54 - Remaining iterations: 6 - D: 6 - f_range: Range [-0.916, -0.360], Mean -0.738 (Std Dev 0.152) - f_min: -0.916 - Shortest distance: 0.459 - Lengthscales: Range [0.004, 4234.465], Mean 1514.580 (Std Dev 1683.459) - Outputscale: 0.818	qJES: ‘f_min‘ remains unchanged, meaning qMES did not immediately lead to an improvement. The lengthscales are still extremely large and variable (Range [0.004, 4234.465], Mean 1514.580, Std Dev 1683.459), indicating persistent, profound uncertainty in the GP model’s understanding of the objective function. With only 6 iterations remaining (N=54), and ‘f_min‘ still stagnant despite various information-theoretic methods, a comprehensive information-gathering strategy is needed to make the best final decision. qJES (Joint Entropy Search) is an advanced acquisition function that directly aims to reduce the entropy of the *joint* posterior distribution of the optimal value *and* its location. In these very late stages with high model uncertainty, a holistic understanding of both the value and location of the optimum is crucial for making the final, most informed decision. qJES provides a more complete information gain than qPES or qMES alone, making it ideal for the limited remaining budget to resolve uncertainty about the true optimum. (qJES was used at N=32, and its strength in holistic uncertainty reduction makes it appropriate for this critical, late-stage, high-uncertainty scenario).