LILO: BAYESIAN OPTIMIZATION WITH INTERACTIVE NATURAL LANGUAGE FEEDBACK

Katarzyna Kobalczyk*
DAMTP, University of Cambridge
knk25@cam.ac.uk

Zhiyuan Jerry Lin, Benjamin Letham, Zhuokai Zhao, Maximilian Balandat, Eytan Bakshy Meta

{zylin, bletham, zhuokai, balandat, ebakshy}@meta.com

ABSTRACT

For many real-world applications, feedback is essential in translating complex, nuanced, or subjective goals into quantifiable optimization objectives. We propose a language-in-the-loop framework that uses a large language model (LLM) to convert unstructured feedback in the form of natural language into scalar utilities to conduct BO over a numeric search space. Unlike preferential BO, which only accepts restricted feedback formats and requires customized models for each domain-specific problem, our approach leverages LLMs to turn varied types of textual feedback into consistent utility signals and to easily include flexible user priors without manual kernel design. At the same time, our method maintains the sample efficiency and principled uncertainty quantification of BO. We show that this hybrid method not only provides a more natural interface to the decision maker but also outperforms conventional BO baselines and LLM-only optimizers, particularly in feedback-limited regimes.

1 Introduction

Bayesian optimization (BO) is a powerful strategy for optimizing expensive-to-evaluate black-box objectives (Brochu et al., 2010; Shahriari et al., 2015; Frazier, 2018). Real BO deployments, however, frequently optimize for complex tradeoffs over many outcomes, where the objective is not clearly specified, and optimization must be guided by feedback from a decision maker (DM) rather than by direct access to ground-truth utility values. Existing preference BO methods address this by learning from comparisons or ratings (González et al., 2017; Chu & Ghahramani, 2005; Lin et al., 2022; Feng et al., 2024), yet they typically require narrow feedback formats, custom likelihoods models, and careful kernel or hyper-prior engineering for the surrogate model. In contrast, black box optimization approaches driven by large language models (LLMs) end-to-end offer a more flexible interface: they can translate rich natural language input and bring in domain knowledge (Liu et al., 2024; Yang et al., 2023; Brown et al., 2020). But BO, such approaches usually lack calibrated uncertainty estimates, principled exploration–exploitation tradeoffs, and reliable convergence guarantees.

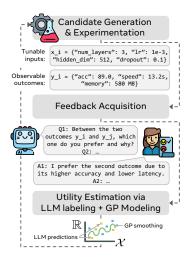


Figure 1: Core steps of LILO.

In this paper, we introduce *Language-in-the-loop Optimization* (LILO), a framework designed to combine the complementary strengths of BO and LLMs while avoiding their respective weaknesses. Rather than letting the LLM directly control the optimization, we place it in a supporting role: the LLM interprets free-form feedback and prior knowledge expressed in natural language, and translates them into structured signals for Gaussian process (GP) utility surrogates. This design

^{*}Work done while the author was an intern at Meta.

leverages LLMs' strengths at understanding language and contextual reasoning, while addressing the instability, poor sample efficiency, and weak generalization that arise when relying on LLMs' raw in-context learning (ICL) abilities (Brown et al., 2020; Zhao et al., 2024; Yin et al., 2024). By mapping natural language feedback into quantitative utilities that GPs can model, LILO preserves BO's calibrated uncertainty and acquisition mechanisms. Beyond showing that such a hybrid is feasible, we provide a systematic study of the design choices that make it effective and practical. The result is a principled, empirically validated framework that combines the expressivity of LLMs with the reliability of BO. In summary, our main contributions are as follows:

- 1. We propose LILO, a novel BO approach for settings that require eliciting utility information from a DM. LILO leverages natural language feedback, which can be more information-rich than pairwise comparisons or scalar ratings commonly used in other methods.
- 2. We show how to translate such natural language feedback into quantitative latent utilities that can be used effectively by a surrogate and acquisition function, systematically exploring the design choices required to render this approach both effective and practical.
- 3. We demonstrate the improved performance and sample efficiency of LILO compared to existing baselines on a variety of synthetic and real-world environments, outperforming both classic GP-based and LLM-based Bayesian optimization methods.
- 4. We show that the LLM is able to not merely serve as a "utility translator", but also successfully leverage its domain knowledge acquired during pre-training, enhancing the optimization.

1.1 PROBLEM DEFINITION

We consider the problem of optimizing the outputs of a black-box system with respect to preferences of a DM . Let $\mathcal{X} \subset \mathbb{R}^d$ denote the search space of controllable parameters, and let each $y \in \mathcal{Y} \subset \mathbb{R}^k$ define the outcomes of an experiment obtained through an expensive-to-evaluate function y = f(x), where $f: \mathcal{X} \to \mathcal{Y}$ maps parameters to outcomes in the outcome space \mathcal{Y} .

A DM associates with each observed outcome y a latent utility value $u = g(y) = (g \circ f)(x) \in \mathbb{R}$, where $g: \mathcal{Y} \to \mathbb{R}$ is an unknown utility function that reflects the DM's preferences. In practice, the DM is often unable to directly specify the closed form of the utility function, so the exact scalar utility value is not directly observable. Instead, the DM can provide feedback, e.g., based on pairwise comparisons (Lin et al., 2022) or, in this work, natural language, to inform about the shape of the utility function g. Our goal is to identify parameters $x \in \mathcal{X}$ that maximize satisfaction of the DM, i.e., to solve the composite optimization problem defined as:

$$x^* := \arg\max_{x \in \mathcal{X}} \ g(f(x)).$$

For example, as illustrated in Figure 1, in hyperparameter tuning for machine learning models, x would be the collection of hyperparameters such as batch size or the learning rate and y would be the model's evaluation metrics such as accuracy, training time, and memory usage. Given a specific set of outcomes y, the utility u reflects the DM's overall satisfaction about the observed outcomes y.

Note that this is a highly flexible setup that can accommodate a wide variety of problems. When there is no intermediate outcome that can be observed and the preference is directly defined over the parameter space \mathcal{X} , it is equivalent to letting y=f(x)=x, reducing this problem to the classic preferential BO (PBO) problem (González et al., 2017; Astudillo et al., 2023). When the y is high-dimensional (e.g., image or text) or involves hard-to-quantify outcomes (e.g., the decision maker's subjective feelings), the proposed method is still applicable by modeling the composite structure $(g \circ f)(x)$ directly instead of f and g separately and skipping explicit modeling of g completely.

2 Background & Related Works

Preferential Bayesian Optimization. Classic BO methods (Shahriari et al., 2015; Frazier, 2018) combine a probabilistic surrogate model – typically a GP – with an acquisition function that balances exploration and exploitation. *Preference learning* extends this idea to settings where explicit numerical objectives are unavailable and instead only preferential feedback (e.g. in form of pairwise or comparative judgments) can be obtained from a decision maker. The seminal work of Chu & Ghahramani (2005) introduced GP preference learning with a probit likelihood to model noisy pairwise data. González et al. (2017) formalized preferential BO, providing algorithms and guarantees for optimization from pairwise comparisons. Lin et al. (2022) extended this idea with *Bayesian*

optimization with preference exploration, where DMs provide feedback on hypothetical outcomes of experiments in order to best learn the DM's utility function. This decision-theoretic policy, Expected Utility of the Best (EUBO), had been extended to the best-out-of-k selection in Astudillo et al. (2023). Connections to dueling and multi-dueling bandits, made for instance by Sui et al. (2017), highlight links between kernelized BO and bandit feedback. Together, these methods demonstrate principled approaches to preference-guided optimization, but rely on rigidly structured feedback (pairwise or best-of-k comparisons), limiting their ability to exploit natural language feedback that is both more expressive and natural for human decision makers.

Optimization with LLMs. Modern LLMs have been shown to be effective optimizers when used with in-context demonstrations (Yang et al., 2023). Agarwal et al. (2025) explore dynamically updating LLM prompts with past solutions including uncertainty estimates. Other works (Ramos et al., 2023; Cai et al., 2025) explore the synergy of LLMs and BO based on GP surrogates. Liu et al. (2024) investigate using LLMs for warm starting BO, surrogate hints, and proposal generation. Kristiadi et al. (2024) treat LLMs as a fixed feature extractors and train standard BO surrogates on the embeddings. Austin et al. (2024) use a LLM to conduct preference elicitation within a BO loop to perform optimization over a discrete set of candidates based on binary feedback and maintain an explicit parametric posterior of each individual candidate point. While these studies show promising results, some of their designs may present challenges for scalability, data requirements, or coherent integration between LLM and BO components, as the roles of the LLM and surrogates are often used in parallel rather than in an inter-dependent manner within a unified framework.

In black-box optimization beyond BO, Alamdari et al. (2024) use LLMs to generate synthetic prior feedback to cold-start bandits. Ye et al. (2025) propose LOLA, integrating LLM predictions with UCB bandits for online content experiments. Kobalczyk et al. (2025) improve the LLM's abilities to ask good clarifying questions by leveraging concepts of Bayesian Experimental Design (BED) – shifting the conversation to maximize information gain in interaction with the decision maker.

LLM as Few-Shot Learners and Bayesian Predictors. The foundation of much of this work's natural language aspect lies in the ICL abilities of LLMs. The seminal GPT-3 paper (Brown et al., 2020) showed that LLMs can act as effective few-shot learners. Multiple subsequent works take a Bayesian view on ICL. Panwar et al. (2023) investigate conditions where transformers approximate Bayes-optimal predictors, while Falck et al. (2024) test the martingale property and find systematic deviations suggesting ICL is not strictly Bayesian. Müller et al. (2023) argue that ICL reflects approximate Bayesian posteriors learned during transformer pretraining. Requeima et al. (2024) propose extracting predictive distributions directly from LLMs, making the Bayesian link explicit through natural language conditioning. Zhu & Griffiths (2024) propose an iterated ICL mechanism to approximate the implicit Bayesian priors encoded in LLMs, offering a general-purpose interpretability tool that can inform how these models' beliefs might be leveraged or mitigated in the downstream optimization tasks such as BO or preference elicitation.

3 METHOD

3.1 LILO: LANGUAGE-IN-THE-LOOP OPTIMIZATION

The key idea behind LILO is to use an iterative preferential BO algorithm with an explicit GP-based utility model to steer the optimization in a principled fashion while harnessing the power of LLMs to extract preferences from the decision maker in the form of natural language feedback and agentically devise questions during such feedback elicitation. Figure 2 provides an overview of the optimization loop after initialization. We describe the core steps of LILO below. Algorithm 1 presents pseudocode, with subroutines described in Appendix A.1. The exact formats of the prompts used can be found in Appendix A.2.

Our BO procedure consists of T sequential trials indexed by $n \in \{1, 2, ..., T\}$. We define by $D_n^{\text{exp}} = \{(x_i, y_i)\}$ the accumulated *experimental dataset* consisting of input-output pairs observed up to trial n. Additionally, $D_n^{\text{pf}} = \{(q_j, a_j)\}$ denotes the *preference feedback dataset* that contains a history of the DM's natural language feedback in the form of answers a_j to LLM-generated queries q_j . From these datasets, in each trial, we fit two proxy GP models (for details see below):

- $M_{n-1}^x: \mathcal{X} \to \mathcal{P}(\mathbb{R})$, approximating the composite function $g \circ f: \mathcal{X} \to \mathbb{R}$,
- $M_{n-1}^{\mathcal{Y}}: \mathcal{Y} \to \mathcal{P}(\mathbb{R})$, approximating the DM's utility function $g: \mathcal{Y} \to \mathbb{R}$.

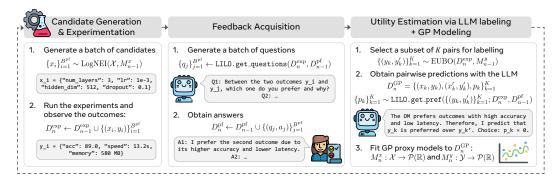


Figure 2: Overview of LILO: Configurations to be evaluated on the black box function are generated with a BO acquisition function leveraging the GP utility model. After observing associated outcomes, the LLM generates a set of questions for the decision maker based on all previously observed outcomes and user feedback. Responses are added to the LLM's conversation history, based on which the LLM is asked to provide preferential feedback on a set of pairwise comparisons. This feedback is then used to update the GP utility model, after which the iteration continues.

Algorithm 1: LILO: Language-in-the-loop Optimization

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 \begin{aligned} & \text{Require: Max number of iterations } T \text{, experiment batch size } B^{\text{exp}} \text{, feedback batch size } B^{\text{pf}} \text{. Optional:} \\ & Prior \text{ knowledge prompt } P_{\text{prior}} \\ & D_0^{\text{exp}} \leftarrow \varnothing; \\ & \{q_j\}_{j=1}^{B^{\text{pf}}} \leftarrow \text{LILO.get\_init\_questions}(); \\ & \{a_j\} \leftarrow \text{DM.get\_answers}(\{q_j\}_{j=1}^{B^{\text{pf}}}); \\ & D_0^{\text{pf}} \leftarrow \{(q_i, a_i)\}_{i=1}^{B^{\text{pf}}}; \\ & \text{for } n = 1 \text{ to T do} \\ & & \text{if } n = 1 \text{ then} \\ & & & \text{if } P_{prior} \neq \varnothing \text{ then} \\ & & & & & \text{lese} \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & & \\ & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\
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The entry point. Before entering the main optimization loop, the algorithm begins by eliciting the DM's high-level optimization goals. At this stage, no experimental outcomes exist $(D_0^{\text{exp}} = \emptyset)$, so the LILO agent generates B^{pf} general questions for the DM. After obtaining the DM's answers, the preference feedback dataset is instantiated as $D_0^{\text{pf}} = \{(q_j, a_j)\}_{j=1}^{B^{\text{pf}}}$.

Next, LILO proceeds to the main optimization loop, in which each trial consists of three stages: 1) Candidate Generation & Experimentation, 2) Feedback Acquisition, and 3) Utility Estimation via LLM Labeling + GP Modeling.

Candidate Generation & Experimentation. At n=1, when no proxy model has been fit yet, we generate the first batch of candidates uniformly at random. For n>1, using the current input-space model M_{n-1}^x , we optimize an acquisition function over the search space $\mathcal X$ to select a batch of $B^{\rm exp}$ candidate inputs $\{x_i\}_{i=1}^{B^{\rm exp}}$. Our acquisition function of choice is (Log) Noisy Expected Improvement (Ament et al., 2023), which is well-suited here because M_{n-1}^x is trained on noisy, LLM-derived

utility estimates rather than evaluations of the true utility function. Each selected input x_i is then evaluated on the (black-box) function f, producing outcomes $y_i = f(x_i)$. With this, the experimental dataset becomes $D_n^{\text{exp}} = D_{n-1}^{\text{exp}} \cup \{(x_i, y_i)\}_{i=1}^{B^{\text{exp}}}$.

Example Conversation of LILO with the DM agent

- $\mbox{-}\mbox{ DM:}$ My goal is to keep all metrics within my thermal comfort preferences.
- LILO: Can you provide more specific thresholds for each metric that you consider to be within your thermal comfort preferences?
- DM: To be honest, I prefer it when the air doesn't feel drafty at my neck, and I don't feel too much warmth coming from the ceiling. I also like it when there's not a big difference in temperature between my head and ankles. As for the floor, I find it comfortable when it's around 22-24 degrees Celsius. If it's too cold or too hot, my feet feel uncomfortable, and that affects my overall comfort.
- LILO: How do you prioritize these metrics relative to one another? For example, is minimizing PPD more important to you than minimizing DR, or are they equally important?
- DM: For me, it's really important that I don't feel drafty or too warm from the ceiling. If I had to choose, I'd say minimizing those feelings is a bit more important than the other factors. But, at the same time, I also value not having a big temperature difference between my head and ankles. It's all about finding a balance, I suppose. If one thing is off, it can really affect how I feel overall. [...]

Example 1: Example fragments of feedback elicitation conversation of LILO with the DM in one of the test problem (Thermal Comfort Type A). LILO is able to elicit and incorporate such qualitative feedback about optimization effectively as shown in our experiments in Section 4.

Feedback Acquisition. After obtaining new experimental outcomes, the LILO agent generates $B^{\rm pf}$ questions for the domain expert to answer. These queries can include both: high-level questions regarding overall optimization goals, and questions about specific outcomes observed (which ones are preferred, how to improve them, etc.). The prompt for question generation contains all experimental outcomes and human feedback messages obtained. The LLM produces a set of $B^{\rm pf}$ questions q_j , and the DM provides corresponding answers a_j . The preference feedback dataset becomes $D_n^{\rm pf} = D_{n-1}^{\rm pf} \cup \{(q_j, a_j)\}_{j=1}^{B^{\rm pf}}$.

Utility Estimation via LLM Labeling + GP Modeling. To convert the natural language feedback of the DM into a usable optimization signal, we construct a dataset of K pairwise preferences between outcomes in $D_n^{\rm exp}$. The LILO agent is tasked with labeling these comparisons based on the DM's preference feedback in $D_n^{\rm pf}$. We first select K informative outcome pairs $\{(y_k,y_k')\}$ – using the Expected Utility of Best Option (EUBO) acquisition function (Astudillo et al., 2023), which we approximate based on M_{n-1}^y . For each pair (y_k,y_k') , the LLM determines which outcome is more aligned with the DM's preferences, producing a label $p_k \in \{0,1\}$ indicating whether or not y_k is preferred over y_k' . This results in a dataset $D_n^{\rm GP} = \{((x_k,y_k),(x_k',y_k'),p_k)\}_{k=1}^K$, which we use to re-fit the pairwise GP (Chu & Ghahramani, 2005) proxy utility models: The input-space utility model $M_n^x: \mathcal{X} \to \mathcal{P}(\mathbb{R})$ and the outcome-space utility model $M_n^y: \mathcal{Y} \to \mathcal{P}(\mathbb{R})$. These updated models will be used in the next trial to guide candidate selection and further question generation.

3.2 Incorporating Prior Knowledge with LILO

In addition to providing feedback on observed outcomes, decision makers with domain expertise often possess strong prior beliefs about the optimization problem at hand. These priors may include expectations about optimal parameters x, or insights into how specific parameters influence outcomes y—that is, information about the underlying mapping f. Conventional BO approaches, however, make it challenging to incorporate such priors, as this typically requires interpreting the decision maker's knowledge by a human and manually encoding it into the model (e.g., through spe-

cialized kernels, custom mean functions, or carefully designed priors over the surrogate model's parameters). This process can be both time-consuming and error-prone, particularly when the expert's knowledge is qualitative and difficult to formalize mathematically. A natural language interface offers a more intuitive way for decision makers to express their prior knowledge.

In scenarios where such prior information is available, we introduce a modification to LILO that enables warm-starting the optimization process. Inspired by Liu et al. (2024), who demonstrate that LLMs can serve as effective candidate samplers when contextual knowledge is present, we propose replacing the uniform sampling at n=1 with LLM-based sampling. Specifically, given $D_0^{\rm pf}$ and additional prior information represented in textual form as $P_{\rm prior}$, we generate $B^{\rm pf}$ candidate points x_i via LLM prompting (see Prompt 6, Appendix A.2). Incorporation of prior knowledge is optional in LILO; in our experiments in Section 4.3.3 we demonstrate how leveraging a good prior can significantly enhance optimization performance.

4 EXPERIMENTS

4.1 BENCHMARKING SETUP

Test problems. We evaluate LILO on synthetic and real-world outcome functions f, subject to various utility functions g. In all our test problems we let \mathcal{X} be a hypercube inside \mathbb{R}^d and $\mathcal{Y} \subseteq \mathbb{R}^k$. Our main benchmark considers four outcome functions (one fully synthetic, and three simulating real-world outcomes):

- DTLZ2 (Deb et al. (2002), d=4, k=8) is a synthetic outcome function commonly used as a benchmark for multi-objective optimization algorithms.
- Vehicle Safety (Tanabe & Ishibuchi (2020), d = 5, k = 3), a simulator of a vehicle's mass and two safety-defining outcomes. The inputs are the thickness of the frontal structure of a car, which affect the vehicle's mass and safety.
- Car Cab Design (Liao et al. (2008), d = 7, k = 9), a simulator of a side-impact car crash test. The inputs measure the thickness of a car's structure, which influence the vehicle's mass, the physical impact on the passenger, and the physical impact on the car.
- Thermal Comfort (Fanger (1970); ISO7730 (2005), d = 8, k = 5) models perceptible thermal conditions and human dissatisfaction levels based on a set of environmental parameters that need to be optimized.

We consider several utility functions on the outcomes of these test problems:

- piecewise linear, modeling diminishing returns when outcomes reach their desired thresholds.
- beta products, describing bounded monotonic utilities that smoothly vary between increasing and decreasing marginal gains with respect to their inputs.
- L1 distance, measuring the L1 distance of outcomes from a pre-defined optimum point.
- For the Thermal Comfort problem, we consider two personas with different preferences: *Type A*) an office worker with light clothing and a moderate tolerance for different conditions; *Type B*) a summer athlete, wearing light sport kit, with a low tolerance for adverse conditions.

All test problems and outcome/utility combinations are described in detail in Appendix B. All utility functions are designed to take values in [0,1].

Baselines. We compare LILO against the following baselines (full details for all baselines are provided in Appendix B): \blacktriangleright true utility BO: a GP-based BO that directly observes ground-truth utilities $u_i = g(y_i)$ for each outcome y_i . Since utilities are never directly accessible in practice, this baseline serves as an oracle "gold standard". \blacktriangleright preferential BO: a setup with binary pairwise comparison feedback instead of natural language feedback. Pairwise comparisons between two outcomes y, y' are derived from the ground-truth utility differences g(y) - g(y'). Similarly to true utility BO, this can be seen as a "gold standard" baseline, as in practice, pairwise comparison feedback is noisy due to inconsistencies in human decision-making. \blacktriangleright LLM (2-step): an ablation of our method in which the GP model and acquisition function are replaced by LLM-based candidate generation. Specifically, in each iteration, the LLM first estimates utilities for previously observed outcomes D_n^{exp} (via pairwise comparisons) and then selects the next candidate batch through in-context learning. The prompt for candidate generation contains the dataset D_n^{exp} with the utility estimates based on the M_n^y model and the history of conversation with the DM from D_n^{pf} . This baseline resembles the LLAMBO method of Liu et al. (2024). The key difference lies in the fact that in the original setup

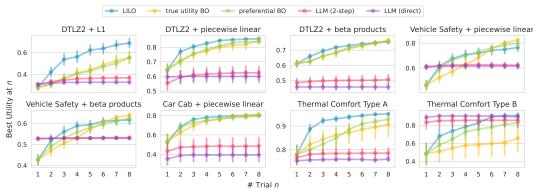


Figure 3: Maximum value of the ground-truth utility achieved after n iterations. Error bars are 95% confidence intervals of the mean max value across 30 replications.

of LLAMBO, the ground-truth utilities of individual candidates x are directly observable. Here, they must be estimated based on the natural language feedback. \blacktriangleright LLM (direct): a fully end-to-end LLM approach, where new candidates are proposed directly based on the observed $(D_n^{\rm pf}, D_n^{\rm exp})$ omitting the intermediate utility estimation step.

Simulation environment. We run the BO loop for T=8 iterations, setting $B^{\rm exp}=d$ (the dimension of the search space). For the main experiments we use a feedback batch size of $B^{\rm pf}=2$ (see Appendix C.2 for an ablation across varying values of $B^{\rm pf}$). The true utility BO baseline receives true utility observations for $B^{\rm pf}$ outcomes selected from $D_n^{\rm exp}$. The preferential BO baseline receives pairwise comparison feedback for $B^{\rm pf}$ outcome pairs selected from $D_n^{\rm exp}$. In both methods, we use the EUBO acquisition function to select the data points on which the quantitative feedback is provided (see Appendix C.4 for an ablation on the choice of the feedback acquisition function). For methods involving natural language feedback, answers to questions posed by the LLM agent are simulated with another LLM containing a textual description of the ground-truth utility function in the prompt (see Appendix B.3 for details). In the main paper, both the DM and LILO agents are instantiated with the Llama-3.3-70b-instruct language model. Results for other choices of LLM models are presented in Appendix C.1.

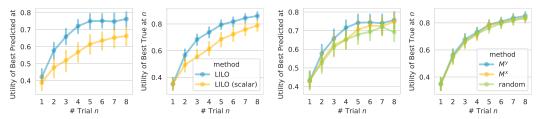
4.2 KEY RESULTS

We first present the results on a set of 8 environments, where no prior knowledge about the problem is provided ($P_{prior} = \varnothing$), except for the variable names in the Vehicle Safety, Car Cab Design, and Thermal Comfort environments. For fairness of comparison with the quantitative baselines, we use LILO with random initialization, as initialization leveraging the LLM's world knowledge may give a significant performance boost as we later show in Section 4.3.3

Figure 3 shows the maximum ground-truth utility achieved after n trials of experimentation and feedback collection, that is, $\max_{x\in D_n^{\exp}}g(f(x))$. We observe that LILO consistently outperforms the baselines, especially early on during the optimization. In some environments, where outcomes correspond to semantically meaningful quantities, the two LLM baselines show good zero-shot performance, but in general, they fail to improve meaningfully over the course of the optimization. This observation aligns with the in-context learning literature on its diminishing return over number of examples provided (Brown et al., 2020; Zhao et al., 2024; Yin et al., 2024). Remarkably, LILO also substantially outperforms the true utility and preferential BO baselines – this is due to the fact that natural language feedback can convey much richer information about the overall DM's preferences than only localized, point-specific feedback. The DM may provide auxiliary feedback not only on the performance of specific outcomes, but also on the overall shape of their underlying utility function (e.g., the directionality of the utility function with respect to different metrics, their relative importance, etc.). See Example 1 and Appendix D for example conversations from the benchmark. With increasing number of experimental trials, the advantage of natural language feedback diminishes and scalar or pairwise utility feedback baselines catch up.

4.3 Additional Studies

In this section, we present additional studies providing insights into the key elements of LILO.



- (a) Performance of LILO with pairwise vs. scalar util- (b) Comparison of methods for LLM pairwise preference labeling.

Figure 4: Comparison of LILO variants. Average results over three DTLZ2 environments (30 replications per environment, values min-max standardized within an environment before aggregation).

4.3.1 Pairwise comparisons vs. direct utility estimation.

The default utility estimation step in LILO relies on LLM-generated pairwise comparisons. As an alternative, we consider directly prompting the LLM to output scalar utility values. In this variant, instead of labeling pairwise preferences, the LLM produces scalar predictions $\hat{u}_i \in [0,1]$ for each $(x_i, y_i) \in D_n^{\text{exp}}$, resulting in a dataset $D_n^{\text{GP}} = \{(x_i, y_i, \hat{u}_i)\}$. This dataset is then used to fit proxy models M_n^x and M_n^y as standard GPs. All other parts of the pipeline remain unchanged. The prompt used for this method and the modified algorithm are presented in Appendix A.

Results. To compare the two approaches, we conducted an ablation study on the three DTLZ2 environments with varying utility functions. Figure 4a reports average results over 30 replications per environment. The right pane shows the maximum ground-truth utility achieved until the n-th iteration. On the left, we report the ground-truth utility of the best candidate according to the proxy model M_n^y , i.e. $g(\hat{x}_n^*)$, where $\hat{x}_n^* = \arg\max_{x \in D_n^{\exp}} M_n^y(f(x))$. In practice, it may be preferable or even necessary to use the utility model to do this "best point selection"; especially with many observations, it will be impractical for the DM to compare a large slate of options at once – in fact, they may not be able to do this well due to mental overload. The results demonstrate that pairwise comparisons provide more reliable utility estimates than direct scalar predictions, **leading to improved optimization performance.** This observation for LLMs mirrors findings in human preference elicitation, where pairwise comparisons have been shown to yield more consistent and accurate judgments than absolute scalar ratings (Phelps et al., 2015; Hoeijmakers et al., 2024).

4.3.2 THE CHOICE OF PAIRS FOR LLM LABELING.

During the utility estimation step of LILO, we prompt the agent to label a subset of K pairwise comparisons between outcomes from D_n^{exp} , $\{(y_k, y_k')\}_{k=1}^K$. This set of outcomes is selected by comparisons between outcomes from D_n^{exp} , $\{(y_k, y_k')\}_{k=1}^K$. This set of outcomes is selected by comparisons between outcomes from D_n^{exp} , $\{(y_k, y_k')\}_{k=1}^K$. puting the value of the EUBO acquisition functions with respect to the M_{n-1}^y model, and selecting the top K pairs with the highest EUBO values. In our experiments, we use K = 64. In this section, we ablate this step by comparing it against random pair selection, and against a method that uses the M_{n-1}^x instead of the M_{n-1}^y model. For the latter, the EUBO is computed on pairs of inputs (x_k, x_k') and the top K pairs of corresponding outcomes (y_k, y'_k) are passed to the LLM for labeling.

Results. Figure 4b shows the results obtained on the three DTLZ2 environments. We observe that the use of the M_{n-1}^y model for pair selection with respect to EUBO improves the predictive performance of the outcome-space proxy in identifying the best candidate (left pane). This improvement, however, does not directly translate to significant differences in terms of the optimization performance measured with respect to the ground-truth utility function (right pane). Thus, if the outcome space \mathcal{Y} is high dimensional (e.g., text or image), and the mapping $\mathcal{Y} \to \mathbb{R}$ hard to model, fitting the outcome space GP models may be omitted and we may simply select points for labeling using M_{n-1}^x or even randomly, simplifying the pipeline.

4.3.3 Incorporating prior knowledge.

As described in Section 3.2, LILO can also incorporate domain priors to boost optimization performance. In the following, we demonstrate this empirically, considering three types of prior messages P_{prior} : \triangleright point: A message providing a sample candidate with high expected utility: "Based on my experience, the following inputs should bring good results: $\{x\}$ ". The promising candidate is generated by sampling uniformly at random N candidates, computing their ground-truth utilities, and randomly sampling a single point from the top q% of data points. \triangleright area: A message providing expected bounds of good candidates: "Based on my experience, inputs within these ranges should bring good results: {bounds}". The bounds are computed by sampling uniformly at random N candidates, computing their ground-truth utilities, and taking the 0.25 and 0.75 quantiles of the top q% of data points, as the lower and upper bounds, respectively. \blacktriangleright domain: A message contextualizing the input parameters and the outputs. This is applicable only to semantically-meaningful environments: Vehicle Safety, Car Cab Design and Thermal Comfort. Exact forms of these messages are provided in Appendix B.4. For the DTLZ2 outcome function, we apply the point and area priors. For point knowledge we use q=10 and for area knowledge we use q=5 with N=5000 in both cases. For Vehicle Safety, Car Cab Design and Thermal Comfort we apply the domain priors.

Results. Figure 5 presents a comparison of LILO's performance with and without prior knowledge integrated into the optimization pipeline. As expected, incorporating prior knowledge through LLM-based initialization substantially improves the starting point, resulting in better overall optimization performance. For a more detailed breakdown of the results, see Appendix C.3. We also note that point and area knowledge types depend on the accuracy of externally provided information about $(g \circ f)$ and, in principle, could be incorporated into conventional BO pipelines using model-based approaches. However, LILO's success with domain priors relies on the contextual understanding provided by the LLM's pre-training, which would be challenging to replicate with standard model-based methods. This ability to incorporate various types of prior knowledge in a unified fashion further underscores LILO's flexibility.

4.3.4 ADDITIONAL EXPERIMENTAL RESULTS

Beyond the results described above, we further conduct a series of additional experiments on the robustness of LILO, such as the choice of LLM models (Appendix C.1) or the choice of the batch size of the feedback queries (Appendix C.2).

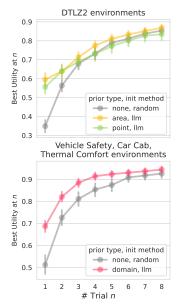


Figure 5: LILO with and without prior knowledge.

5 DISCUSSION AND CONCLUSION

We presented LILO, a novel algorithm for language-in-the-loop optimization that enables decision makers to perform interactive black-box optimization by communicating their preferences through rich, natural language feedback. This addresses a key challenge in settings where optimization objectives are not explicitly available, but where classic preference learning approaches (e.g. using pairwise feedback) are not sample-efficient enough. LILO demonstrates compelling performance in our benchmarks, and has been successfully applied in multiple real-world optimization campaigns involving complex tradeoffs between multiple metrics in online A/B testing at Meta.

The reason of LILO's superior performance is multi-faceted. Natural language feedback is far more information-rich than other common forms of preference elicitation such as pairwise comparison as demonstrated by the experimental results where LILO achieves very competitive optimization results with just a few feedback queries. On the other hand, LLM-based optimization methods are fit to handle natural language feedback through ICL yet, their performance can plateau rather quickly. This phenomenon is observed throughout our experimentation where LLM-based methods' optimization traces start relatively high in the first iteration and then stop progressing meaningfully throughout the rest of the experiment. LILO is able to overcome such stagnation by keeping the valid probabilistic modeling and principled acquisition mechanism of BO while leveraging LLMs for its human-friendly natural language interface, agentic feedback acquisition, and domain knowledge (from both the DM as well as the LLM).

While our results are strong, several promising directions remain. The fidelity of the LLM estimator is ultimately limited by the model's ability to interpret nuanced feedback. Our benchmarks in Appendix C.1 show robustness across models, with even moderately sized ones yielding meaningful gains. Future work could explore how scaling, fine-tuning, or architectural advances further enhance optimization quality. Hybrid approaches that combine unstructured natural language with structured quantitative feedback are another possibility to mitigate the limits of ICL in the utility estimation step of LILO.

Moreover, LLM-based estimators may occasionally encode preferences or priors too strongly, risking subtle bias toward the model's own world knowledge rather than the intended optimization target. In our experiments, we found this effect to be manageable by ablating over a variety of utility functions and test problem combinations. Yet, future work could explore calibration strategies or adaptive weighting schemes that better balance the advantages of informative model priors with fidelity of the provided feedback.

Although we validated LILO extensively using both synthetic and real optimization problems, understanding its behavior across a broader range of tasks and feedback sources remains an exciting area. Evaluating performance with different natural language agents, including but not limited to human decision makers, can shed light on the robustness and generalization of the proposed method.

Looking forward, these directions open opportunities for advancing language-in-the-loop optimization toward even more adaptive, trustworthy, and broadly applicable optimization systems across diverse domains.

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A DETAILS ON THE METHOD

A.1 PSEUDO CODE

Algorithm 2 presents a pseudo code of LILO. The fit_proxy_models subroutine is presented in Algorithm 3.

The algorithm for LILO with scalar utility estimation is identical to LILO with pairwise preference labeling except for the fit_proxy_models subroutine, which is replaced with point-wise utility estimation as a scalar value in [0,1]. The exact procedure is presented in Algorithms 4. Prompts used in the LILO.xxx subroutines are presented in section A.2.

Algorithm 2: LILO: Language-in-the-Loop Optimization

```
Input: Max number of iterations T, experiment batch size B^{\text{exp}}, feedback batch size B^{\text{pf}}.
          Optional: Prior knowledge prompt P_{\text{prior}}
D_0^{\text{exp}} \leftarrow \bar{\varnothing};
# Ask the DM about their optimization goals
\{q_j\}_{j=1}^{B^{pf}} \leftarrow \text{LILO.get\_init\_questions}();
\{a_j\} \leftarrow \text{DM.get\_answers}(\{q_i\}_{i=1}^{B^{\text{pf}}});
D_0^{\text{pf}} \leftarrow \{(q_i, a_i)\}_{i=1}^{B^{\text{pf}}};
for n=1 to T do
     # Sample a batch of candidates;
     if n = 1 then
          if P_{prior} \neq \emptyset then
            \{x_i\}_{i=1}^{B^{\exp}} \sim \text{LILO.sample\_init\_candidates}(D_0^{\operatorname{pf}}, P_{\operatorname{prior}});
           \{x_i\}_{i=1}^{B^{\text{exp}}} \sim \text{Uniform}(\mathcal{X});
     else
      \{x_i\}_{i=1}^{B^{\exp}} \sim \text{LogNEI}(\mathcal{X}; M_{n-1}^x);
     # Run experiments and update the experimental dataset
     D_n^{\text{exp}} \leftarrow D_{n-1}^{\text{exp}} \cup \{(x_i, y_i) : y_i = \hat{f}(x_i)\}_{i=1}^{B^{\text{exp}}};
     # Generate a batch of questions
     \{q_j\}_{j=1}^{B^{\mathrm{pf}}} \leftarrow \texttt{LILO.get\_questions} \big(D_n^{\mathrm{exp}}, D_{n-1}^{\mathrm{pf}}, \{y_i\}_{i=1}^{2B^{\mathrm{pf}}}\big);
      # Obtain human answers
     \{a_j\}_{j=1}^{B^{\mathrm{pf}}} \leftarrow \mathtt{DM.get\_answers}\big(\{q_j\}_{j=1}^{B^{\mathrm{pf}}}\big);
     # Update the preference feedback dataset
     D_n^{\mathrm{pf}} \leftarrow D_{n-1}^{\mathrm{pf}} \cup \{(q_j, a_j)\}_{j=1}^{B^{\mathrm{pf}}};
     # Fit proxy models
     M_n^x, M_n^y \leftarrow \text{fit\_proxy\_models}(D_n^{\text{exp}}, D_n^{\text{pf}}, M_{n-1}^y);
```

A.2 LILO PROMPTS

In all prompts, experiment_data is a markdown-formatted table of outcomes from D_n^{exp} . human_feedback is the series of questions and answer stored in D_n^{pf} .

In prompt 2 for question generation, selected_outcome_indices is the set of $2B^{\rm pf}$ indices of selected outcomes with the feedback acquisition function (EUBO).

In prompts 3, 4, human_feedback_summary is a summary of human_feedback self-generated by LILO using the prompt presented in 5. We empirically found that including this self-summarization step brings slight improvements to the resulting estimates of the LLM.

In prompt 3, pair_str is a markdown-formatted table with two rows indexed by option_0 and option_1.

Algorithm 3: LILO fit_proxy_models subroutine

```
Input: Experimental dataset D^{\text{exp}}, Feedback dataset D^{\text{pf}}, optional preference model M^y,
           number of pairs for labeling K = 64.
# Generate all possible combinations of outcome pairs
N \leftarrow |D^{\text{exp}}|
 \{(y_i,y_i')\}_{i=1}^{\frac{N(N-1)}{2}} \leftarrow \texttt{get\_outcome\_pair\_combinations}(D^{\texttt{exp}})  if M^y = None \ \textbf{then}
  _{-} \{(y_{k},y_{k}')\}_{k=1}^{K} \leftarrow \texttt{random\_sample}(\{(y_{i},y_{i}')\}_{i=1}^{\frac{N(N-1)}{2}}, \texttt{size} = K)
else
     for i=1 to \frac{N(N-1)}{2} do
      v_i \leftarrow \text{EUBO}((y_i, y_i'))
     \texttt{indices} \leftarrow \texttt{argsort}(\{v_i\}_{i=1}^{\frac{N(N-1)}{2}})[-K:] \; / / \; \texttt{Get indices of top} \; \; K \; \; \texttt{EUBO}
   [ \{(y_k, y_k')\}_{k=1}^K \leftarrow \{(y_i, y_i') : i \in \texttt{indices} \} ]
# Label the selected pairs with LILO
for k = 1 to K do
 p_k \leftarrow \texttt{LILO.get\_pairwise\_pref}(y_k, y_k', D^{\mathsf{exp}}, D^{\mathsf{pf}})
D^{GP,y} \leftarrow \{(y_k,y_k',p_k)\}_{k=1}^K D^{GP,x} \leftarrow \{(x_k,x_k',p_k)\}_{k=1}^K \ // \ x_k,x_k' \text{ are the inputs corresponding to}
M^y \leftarrow \text{fit\_pairwise\_gp}(D^{GP,y})
M^x \leftarrow \text{fit\_pairwise\_gp}(D^{GP,x})
return M^x, M^y
```

Algorithm 4: LILO (scalar) fit_proxy_models subroutine

```
\begin{array}{l} \textbf{Input: Experimental dataset } D^{\text{exp}}, \textbf{Feebdback dataset } D^{\text{pf}}. \\ N \leftarrow |D^{\text{exp}}| \\ \{\hat{u}_i\}_{i=1}^N \leftarrow \texttt{LILO.estimate\_utilities}(\{y_i\}_{i=1}^N; D^{\text{exp}}, D^{\text{pf}}) \\ D^{GP,y} \leftarrow \{(y_i, \hat{u}_i)\}_{i=1}^N \\ D^{GP,x} \leftarrow \{(x_i, \hat{u}_i)\}_{i=1}^N \\ x_i' \texttt{ s are the inputs corresponding to } y_i' \texttt{ s } \\ M^y \leftarrow \texttt{fit\_simple\_gp}(D^{GP,y}) \\ M^x \leftarrow \texttt{fit\_simple\_gp}(D^{GP,x}) \\ \textbf{return } M^x, M^y \\ \end{array}
```

A.3 IMPLEMENTATION DETAILS

In our implementation of the algorithm we rely on the BoTorch Python library (Balandat et al., 2020) to implement the subroutines of GP model fitting, acquisition function evaluation and candidate generation. Specifically, proxy GP models are instances of PairwiseGP or SingleTaskGP classes, with their default settings.

When querying the LLM to provide pairwise labels or scalar utility estimates, we use multiple LLM samples for more reliable estimates. In our simulations, the number of LLM calls per each labeling instance is set to 5. We use all LLM predictions (with replicates) to fit the GP proxy models enabling the proxy models to capture the predictive uncertainty of the LLM in its decision.

```
You are an expert in determining whether a human decision maker (DM)
is going to be satisfied with a set of experimental outcomes y = \{
y_names).
## Human feedback messages:
We have also received the following messages from the DM:
{human_feedback}
## Your task:
Given the above your task is to predict the probability of the
decision maker being satisfied with the experimental outcomes.
In order to better understand the decision maker's utility function
you want to ask them about their optimization goals.
Provide a list of questions you would ask the decision maker to better
understand their internal utility model.
Return your final answer a a json file with the following format
containing exactly {n_questions} most important questions:
'''json
{ {
    "q1" : <question1>,
    "q{n_questions}" : <question{n_questions}>
} }
```

Prompt 1: The prompt used for question generation in the LILO.get_init_questions subroutine.

```
You are an expert in determining w whether a human decision maker (DM)
is going to be satisfied with a set of experimental outcomes y = \{
y_names } .
## Experimental outcomes:
So far, we have obtained the following experimental outcomes:
{experiment_data}
## Human feedback messages:
We have also received the following messages from the DM:
{human_feedback}
## Your task:
Given the above your task is to predict pairwise preferences between
experimental outcomes.
In order to better understand the decision maker's utility function
you want to ask them about their optimization goals or for feedback
regarding specific experimental outcomes.
Here are some points it may be useful to ask the decision maker about
{selected_outcome_indices}.
First, analyse the decision maker's goals and feedback messages to
understand their overall preferences.
Then, provide a list of questions you would ask the decision maker to
better understand their internal utility model.
Your questions can be either general or referring to specific outcomes
. For instance, you may ask the decision maker:
- questions clairfying the optimzation objective,
- to rank two (or more) outcomes,
- how to improve certain outcomes,
- for a likert-scale rating regarding a specific outcome,
- etc.
When referring to specific outcomes, always state the arm_index
involved.
Your questions should help you predict pairwise preferences between
any two experimental outcomes from the set of experimental outcomes
provided above.
Return your final answer a a json file with the following format
containing exactly {n_questions} most important questions:
'''json
{ {
    "q1" : <question1>,
    "q{n_questions}" : <question{n_questions}>
} }
```

Prompt 2: The prompt used for question generation in the LILO.get_questions subroutine.

```
You are an expert in determining whether a human decision maker (DM)
is going to be satisfied with a set of experimental outcomes y = \{
y_names } .
## All experimental outcomes:
{experiment_data}
## Human feedback messages:
We have also received the following messages from the DM:
{human_feedback}
{human_feedback_summary}
## Your task:
Given a pair of outcomes--option_0 and option_1, your goal is to
decide which one is more preferable according to the DM's preferences.
{pair_str}
Provide your prediction as a json file with the following format:
'''json
{ {
    "reasoning": "Your reasoning about the DM's preferences and
option_0 vs. option_1. Do not insert new lines in your reasoning.",
    "answer" : 0 or 1
}}
where in "answer" you should return 0 if option_0 is preferred, or 1
if option_1 is preferred.
Return just the json file (with the header '''json), nothing else.
```

Prompt 3: The prompt used for pairwise comparison labeling used in the LILO.get_pairwise_pref subroutine.

```
You are an expert in determining whether a human decision maker (DM)
is going to be satisfied with a set of experimental outcomes y = \{
y_names } .
## Experimental outcomes:
So far, we have obtained the following experimental outcomes:
{experiment_data}
## Human feedback messages:
We have also received the following messages from the DM:
{human_feedback}
{human_feedback_summary}
## Your task:
Given the above your task is to predict the probability of the
decision maker being satisfied with the experimental outcomes.
First, analyse the human feedback messages to understand the DM's
preferences.
Then, provide your predictions for all y's in the set of all
experimental outcomes above.
Return your final answer as a jsonl file with the following format:
'''jsonl
{ {
    "arm index": "{idx0}",
    "reasoning": <reasoning>,
    "p_accept": <probability>
} }
{ {
    "arm_index": "{idx1}",
    "reasoning": <reasoning>,
    "p_accept": <probability>
} }
{ {
    "arm_index": "{idxn}",
    "reasoning": <reasoning>,
    "p_accept": <probability>
}}
Where <reasoning> should be a short reasoning for your prediction and
oprobability> should be your best estimate for the probability between
\ensuremath{\text{0}} and \ensuremath{\text{1}} that the DM will be satisfied with the corresponding outcome.
Provide your predictions for ALL y's in the set of experimental
outcomes above. That is, for EACH outcome from {idx0}. to {idxn}.
Do not generate any Python code. Just return your predictions as plain
 text.
```

Prompt 4: The prompt used for scalar utility estimation used in the LILO.estimate_utilities subroutine.

```
You are an expert in determining whether a human decision maker (DM)
is going to be satisfied with a set of experimental outcomes y = \{
y_names}.
## Experimental outcomes:
So far, we have obtained the following experimental outcomes:
{experiment_data}
## Human feedback messages:
We have also received the following messages from the DM:
{human_feedback}
## Your task:
Given the above your task is to summarize the human feedback messages
into a clear description of the DM's optimization goals.
Make your summary as quantitative as possible so that it can be easily
used for utility estimation.
After analysis the human feedback messages, return your final answer
as a json file with the following format:
'''json
{ {
    "summary": <summary>
} }
Remember about the '''json header!
```

Prompt 5: The prompt used for generating the human_feedback_summary by LILO for pairwise comparisons or scalar utility estimation.

```
You are performing optimization of a utility function u(x) = g(y) = g(x)
f(x)), where x is a vector of parameters: x = \{x_names\} and y = f(x) = x_names
{y_names} is a vector of outcomes.
Each dimensions of x is in the range [0, 1].
Your goal is to find the parameters x that maximize the utility.
## Prior knowledge:
You have obtained the following prior knowledge about the experiment:
{prior_knowledge}
## Human feedback messages:
You have also received the following messages from the DM:
{human_feedback}
## Your task:
Given the above your task is the generate a set of {n\_candidates}
candidate parameters x for the next round of experimentation.
First, analyse the information above, then return your final answer as
a json file with the following format:
'''json
{ {
    "0": <candidate0>,
    "1": <candidate1>,
    "{n}": <candidate{n}>,
} }
Where each <candidatei> is a list of the candidate parameter values in
Do not write a python code for candidate generation. Just return the
required json.
Do not add any comments to your json. Remember about the '''json
header.
```

Prompt 6: The prompt used for candidate generation by LILO at n=1 when prior knowledge is available (LILO.sample_init_candidates subroutine).

B SIMULATION SETUP

We evaluate LILO and the baselines on synthetic and real-world outcome functions as well as several utility functions. In all our test problems we have $\mathcal{X} = \mathbb{R}^d$ and $\mathcal{Y} = \mathbb{R}^k$. The main benchmark considers three outcome functions: DTLZ2 (d=4,k=8, Deb et al. (2002)), $Vehicle\ Safety\ (d=5,k=3)$, Tanabe & Ishibuchi (2020)), and $Car\ Cab\ Design\ (d=7,k=9)$, Liao et al. (2008)). These test problems are matched with several utility functions: piecewise linear, beta products, and the L1 distance. All outcome and utility functions are described in detail in this section.

In our simulations, we run the BO loop for T=8 iterations, setting $B^{\rm exp}=d$ (the dimension of the search space). At n=1 we hard-code the first message of the DM agent to seed the conversations. These messages are utility-dependent and presented in section B.2.

B.1 OUTCOME FUNCTIONS

DTLZ2 The DTLZ2 function was introduced by Deb et al. (2002), allowing for arbitrary input dimension d and output dimension k subject to d > k. $\mathcal{X} = [0, 1]^d$. For a DLTZ2 function f with a k-dimensional output and d-dimensional input, we have:

$$m := d - k + 1$$

$$h(x) := \sum_{i=m}^{d-1} (x_i - 0.5)^2$$

$$f_j(x) = -(1 + h(x)) \left(\prod_{i=1}^{k-j-1} \cos\left(\frac{\pi}{2}x_i\right) \right) \mathbb{1}_{j>1} \sin\left(\frac{\pi}{2}x_{k-j-1}\right)$$

In our experiments we use d = 8 and k = 4.

Vehicle Safety This a test problem for optimizing vehicle crash-worthiness with d=5 and k=3. $\mathcal{X}=[1,3]^5$. We refer the readers to Tanabe & Ishibuchi (2020) for details on function definition. We normalize each component of y=f(x) to lie between 0 and 1 based on empirical bound on the outcome space \mathcal{Y} .

Car Cab Design We refer the readers to Liao et al. (2008) for details. Note that in the original problem, there are stochastic components which we replace with deterministic components fixed at their original mean values in order to obtain a deterministic ground-truth outcome function. We normalize each component of y = f(x) to lie between 0 and 1 based on empirical bound on the outcome space \mathcal{Y} .

Thermal Comfort The problem setting follows the ISO 7730 and ASHRAE 55 models, which predict human thermal sensation and dissatisfaction based on six core factors: air temperature, mean radiant temperature, humidity, air speed, clothing insulation, and metabolic rate (Fanger, 1970; ISO7730, 2005; ASHRAE55, 2020). From these, outcome measures such as Predicted Percentage Dissatisfied (PPD), draft risk (DR), vertical air temperature difference, radiant temperature asymmetry, and floor surface temperature are derived, each with threshold values associated with acceptable comfort. The goal of the optimization agent is to find environmental parameters that minimize discomfort and keep all outcomes within desirable ranges, reflecting realistic expectations of the occupant rather than arbitrary synthetic functions. This setting is widely used in thermal comfort research and can be visualized via the CBE Thermal Comfort Tool (Tartarini et al., 2020). In our implementation, the outcome function has two fixed, non-optimizable parameters: clothing insulation (clo $\in [0.3, 1.2]$) and metabolic rate (met $\in [1.0, 2.0]$) which differ for the two versions of the environments considered in this paper, as detailed in the next section.

B.2 Utility Functions

L1 distance We consider a utility function which is the L1 distance from a pre-specified point y_{opt} . This choice of the utility function mimics the scenario where the DM wishes to keep the outcomes close to a specific desirable state.

For DTLZ2, we set $y_{\text{opt}} = [0.8, 1.0, 0.7, 1.25]$.

The message seeding the conversation takes the following form:

Goal message (L1 distance)

My goal is to bring all the outcome metrics as close to $\{\text{opt_y}\}$ as possible.

Beta products Prior work on preference learning has utilized the Beta CDF to form utility functions. The Beta CDF provides a convenient, bounded monotonic transform that smoothly varies between increasing and decreasing marginal gains with respect to their inputs. Our utility function takes the following form:

$$g(y; \alpha, \beta) = \prod_{i=1}^{k} \text{BetaCDF}(y_i; \alpha_i, \beta_i)$$

For the DTLZ2 outcome function we set:

$$\alpha = [0.5, 2.0, 2.0, 2.0]$$

$$\beta = [0.5, 1.0, 2.0, 5.0]$$

For the Vehicle Safety outcome function we set:

$$\alpha = [0.5, 1.0, 1.5]$$
$$\beta = [1, 2, 3]$$

For this utility function, the message seeding the conversation takes the following form:

Goal message (beta products)

My goal is to bring all the outcome metrics as close to 1 as possible. Results are strongest only when every metric is high - if any metric is low, it significantly reduces the overall performance.

Piecewise linear Analogously to Lin et al. (2022) we also consider a piecewise linear utility function. Its shape corresponds to diminishing marginal returns on outcomes and sharp declines in utility when desired thresholds are note met. For a k-dimensional input vector y, this utility function is defined as:

$$g(y; \beta_1, \beta_2, t) = \sum_{i=1}^{k} h_i(y_i),$$

where

$$h_i(y_i) = \begin{cases} \beta_{1,i} y_i + (\beta_{1,i} - \beta_{2,i}) t_i & \text{if } y_i < t_i \\ \beta_{2,i} y_i & \text{if } y_i \ge t_i \end{cases}.$$

For the DTLZ2 problem, we set

$$\beta_1 = [4.0, 3.0, 2.0, 1.0]$$

$$\beta_2 = [0.4, 0.3, 0.2, 0.1]$$

$$t = [1.0, 0.8, 0.5, 0.5]$$

For the Vehicle Safety problem, we set

$$\beta_1 = [2, 6, 8]$$

$$\beta_2 = [1, 2, 2]$$

$$t = [0.5, 0.8, 0.8]$$

For the Car Cab Design problem, we set

$$\begin{split} \beta_1 &= [7.0, 6.75, 6.5, 6.25, 6.0, 5.75, 5.5, 5.25, 5.0, 4.75, 4.5] \\ \beta_2 &= [0.5, 0.4, 0.375, 0.35, 0.325, 0.3, 0.275, 0.25, 0.225, 0.2, 0.175] \\ t &= [0.64, 0.68, 0.96, 0.88, 1.06, 0.65, 0.84, 0.86, 0.58, 0.7, 0.53] \end{split}$$

Here, thresholds t_i correspond to the 0.75 quintiles of the outcome values y_i . The seeding message takes the following form:

Goal message (piecewise linear)

My goal is to achieve the following thresholds in each outcome $\{t\}$. Improvements over the thresholds are always good, but less important than bringing the outcomes to their threshold values. The further away an outcome is from its threshold, the higher is its negative impact on the overall performance.

Thermal Comfort Our utility maps the outcome vector $Y = [PPD, DR, dT_{vert}, dT_{pr}, T_{floor}]$ to a scalar $U \in [0,1]$ via per–outcome desirabilities that enforce being "within range", with using the Derringer-Suich desirability functions. For the four "smaller is better" outcomes (PPD, DR, dT_{vert} , dT_{pr}) we use a one–sided acceptable band with a comfort threshold L and an unacceptable threshold H and define

$$d_{\text{small}}(y; L, H, s) = \begin{cases} 1, & y \le L, \\ \left(\frac{H - y}{H - L}\right)^s, & L < y < H, \\ 0, & y \ge H, \end{cases}$$

so values at or below L are fully desirable, values beyond H are unacceptable, and values in between taper smoothly with shape $s \geq 1$. For floor temperature T_{floor} we target a comfort band [l, h] and tolerate a wider band $[l_{\min}, h_{\max}]$ by

$$d_{\mathrm{band}}(t; l, h, l_{\mathrm{min}}, h_{\mathrm{max}}, s) = \begin{cases} 1, & l \leq t \leq h, \\ \left(\frac{t - l_{\mathrm{min}}}{l - l_{\mathrm{min}}}\right)^{s}, & l_{\mathrm{min}} < t < l, \\ \left(\frac{h_{\mathrm{max}} - t}{h_{\mathrm{max}} - h}\right)^{s}, & h < t < h_{\mathrm{max}}, \\ 0, & t \leq l_{\mathrm{min}} \text{ or } t \geq h_{\mathrm{max}}. \end{cases}$$

The overall utility is the geometric mean of the five desirabilities,

$$U(Y) = \left(d_{\text{small}}(\text{PPD}) \cdot d_{\text{small}}(\text{DR}) \cdot d_{\text{small}}(dT_{\text{vert}}) \cdot d_{\text{small}}(dT_{\text{pr}}) \cdot d_{\text{band}}(T_{\text{floor}})\right)^{1/5},$$

We consider two versions of this utility functions with varying comfortable ranges of the outcome metrics

Type A. These settings are meant to simulate preferences of an office worker in light clothing and a moderate tolerance for different conditions.

$$\begin{split} l_{\rm PPD} &= 0.0, \; h_{\rm PPD} = 30.0, \\ l_{\rm DR} &= 10.0, \; h_{\rm DR} = 35.0, \\ l_{\rm dT_{\rm vert}} &= 3.0, \; h_{\rm dT_{\rm vert}} = 9.0, \\ l_{\rm dT_{\rm pr}} &= 5.0, \; h_{\rm dT_{\rm pr}} = 22.0, \\ l_{\rm min,T_{\rm floor}} &= 16.0, \; l_{\rm T_{\rm floor}} = 19.0, \; h_{\rm T_{\rm floor}} = 26.0, \; h_{\rm min,T_{\rm floor}} = 30.0. \end{split}$$

In Thermal Comfort Type A the clothing and metabolic rate parameters of the outcome function are set to clo = 0.61 and met = 1.0, respectively.

Type B. These settings are meant to simulate preferences of a summer athlete wearing light sport kit, with a lower tolerance for adverse conditions.

$$\begin{split} l_{\rm PPD} &= 0.0, \ h_{\rm PPD} = 24.0, \\ l_{\rm DR} &= 30.0, \ h_{\rm DR} = 45.0, \\ l_{\rm dT_{\rm vert}} &= 2.5, \ h_{\rm dT_{\rm vert}} = 6.0, \\ l_{\rm dT_{\rm pr}} &= 4.0, \ h_{\rm dT_{\rm pr}} = 12.0, \\ l_{\rm min,T_{\rm floor}} &= 19.0, \ l_{\rm T_{\rm floor}} = 20.0, \ h_{\rm T_{\rm floor}} = 23.0, \ h_{\rm min,T_{\rm floor}} = 25.0. \end{split}$$

In Thermal Comfort Type B the clothing and metabolic rate parameters of the outcome function are set to clo = 0.3 and met = 2.0, respectively.

The seeding message takes the following form:

Goal message (Thermal Comfort

My goal is to keep all metrics within my thermal comfort preferences.

B.3 LLM-based simulation of the human preference feedback

Evaluating black box optimization algorithm rigorously is challenging due to the replications required to discern performance in the presence of the inherent variance of the evaluation of the optimization traces. This is exacerbated in our setting where the algorithm is based on feedback from human decision makers. To be able to evaluate LILO rigorously, we therefore simulate the human preference feedback with another LLM.

For all our experiments we use Llama-3.3-70b-instruct as the language model for the human feedback simulator. A high-level representation of the prompt used to generate the answers is presented in prompt 7. utility_func_desc is a textual description of the specific utility function. outcomes_markdown is a markdown-formatted table of outcomes $y_i \in D^{\text{exp}}$ and their corresponding pre-computed ground-truth utilities $g(y_i)$. questions_str are the questions $\{q_j\}_{j=1}^{B^{\text{pf}}}$ generated by LILO. Finally utility_constraints contain additional utility-specific instructions for the LLM to generate human-like feedback and to not reveal explicitly the exact functional form of the utility, ensuring the generated answers sound natural.

B.4 Prior Knowledge Messages P_{PRIOR}

Below we present the prior messages P_{prior} used in our experiments from section 4.3.3.

DTLZ2 (point knowledge)

- Based on my experience, the following inputs should bring good results: {promising_point}.

DTLZ2 (area knowledge)

- Based on my experience, inputs within these ranges should bring good results {bounds}:

Vehicle Safety (domain knowledge)

- y_1 measures the reduction in vehicle's mass, y_2 measures the reduction in integration of acceleration between two time points, y_3 measures the reduction in toe board intrusion in the offset-frontal crash.
- The parameters x measure the thickness of five reinforced members around the frontal structure of a car, which can significantly affect the crash safety.

Car Cab Design (domain knowledge)

- ${\-}$ A car is subjected to a side-impact crash test. The outcome variables y measure the following:
- The effect of the side-impact on a dummy is measured in terms of head injury, load in abdomen, pubic symphysis force, viscous criterion (V \star C), and rib deflections at the upper, middle and lower rib locations.
- The effect on the car are considered in terms of the vehicle's weight, the velocity of the B-Pillar at the middle point and the velocity of the front door at the B-Pillar.
- The parameters x describe some design aspects of the car. An increase in dimension of the car parameters may improve safety, but with a burden of an increased weight of the car. These parameters are and their ranges are:

```
x1: Thickness of B-Pillar inner [0.5, 1.5]
```

- x2: Thickness of B-Pillar reinforcement [0.45, 1.35]
- x3: Thickness of floor side inner [0.5, 1.5]
- x4: Thickness of cross members [0.5, 1.5]
- x5: Thickness of door beam [0.875, 2.625]
- x6: Thickness of door beltline reinforcement [0.4, 1.2]
- x7: Thickness of roof rail [0.4, 1.2]
- NOTE: The presented values of outcomes y represent the reduction in mass, forces, velocities etc. So the goal is to increase y_1, \ldots, y_{11} , corresponding to lowering the vehicle's weight and minimizing the impact on the dummy and the car.

B.5 BASELINES

B.5.1 QUANTITATIVE BASELINES

The quantitative baseline methods follow an analogous procedure to LILO, where the Q&A natural language feedback is replace with either scalar values of the utilities associated with a batch of outcomes (true utility BO) or pairwise comparisons between outcomes based on their ground-truth utilities (preferential BO). This feedback is obtained on $B^{\rm pf}$ outcomes y_i or paired outcomes (y_i, y_i') sampled with the EUBO acquisition function. To extend predictions to the entire data set $D_n^{\rm exp}$, we fit a simple / pairwise GP model $M_n^y: \mathcal{Y} \to \mathcal{P}(\mathbb{R})$. Subsequently a proxy model $M_n^x: \mathcal{X} \to \mathcal{P}(\mathbb{R})$ is fit to the predictions of M_n^y .

We present the exact implementation of these methods in algorithms 5 and 6.

B.5.2 LLM 2-STEP AND DIRECT

We also implement two versions of an LLM-based approach to candidate generation for optimization.

LLM (2-step) follows the same algorithm 2 as LILO with the following two exceptions:

- In the candidate generation step, instead of using the LogNEI acquisition function, we prompt the LLM to generate a set of candidates using prompt 8.
- We omit the sentence Here are some points it may be useful to ask the decision maker about ..., letting the LLM ask for arbitrary points from D_n^{exp} .

LLM (direct) Omits the step of utility estimation and generates the candidates directly based on the raw human feedback and observed inputs and outcomes from D_n^{exp} . The prompt used is presented in prompt 9

```
DM's answer generation
Suppose you are a decision maker evaluating the results of a multi-
objective optimization problem.
You are given a set of multi-dimensional outcomes y = \{y_names\}
{utility_func_desc}
You have observed the following outcomes with their corresponding
utility values and contributions to the overall utility.
## Outcomes:
{outcomes_markdown}
The utility values are on a scale [0, 1], where (1 - very satisfied,
0.5 - neutral, 0 - very dissatisfied).
Based on the above information, provide answers to the following
questions:
## Questions:
{questions_str}
Return your final answer as a json file with the following format:
'''json
{ {
    "q1" : <answer to q1>,
    "q{n_questions}" : <answer to q{n_questions}>
} }
Before providing your final answers, analyze the shape of the utility
function in light of the questions posed.
In your final answers, you cannot reveal the explicit formula of the
utility function.
The form and the values of the utility functions is a "latent" feature
of the human expert, thus you should not refer to it explicitly or
even mention its existence.
{utility_constraints}
State your answers in the first person (you are the decision maker).
Avoid vacuous statements.
```

Prompt 7: The prompt used for answer generation in the DM.get_answers subroutine.

```
You are performing optimization of a utility function u(x) = g(y) = g(y)
f(x)), where x is a vector of parameters: x = \{x_n = x\} and y = f(x) = x
 {y_names} is a vector of outcomes.
Each dimensions of x is in the range [0, 1].
Your goal is to find the parameters x that maximize the utility.
## Experimental Outcomes
So far, you have also observed the following inputs x and their
estimated utilities:
{experiment_data}
## Human feedback messages:
We have also received the following messages from the DM:
{human_feedback}
## Your task:
Given the above your task is the generate a set of {n_candidates}
candidate parameters x for the next round of experimentation.
Your candidates should maximize the expected improvement over the
current best candidate x^* = \{x_star\} with utility u(x^*) = \{u_star\}.
First, analyse the information above, then return your final answer as
a json file with the following format:
'''json
{ {
    "0": <candidate0>,
    "1": <candidatel>,
    "{n}": <candidate{n}>,
} }
Where each <candidatei> is a list of the candidate parameter values in
[0, 1].
Do not write a python code for candidate generation. Just return the
required json.
Do not add any comments to your json. Remember about the '''json
header.
```

Prompt 8: The prompt used for candidate generation by the LLM (2-step) baseline. In the above, experiment_data is a markdown formatted table of outcomes y_i and their estimate utilities via the LLM-based proxy model $M_{n-1}^y(y_i)$. x_star and u_star are determined based on the estimated utilities (not ground truth $g(y_i)$'s as these are latent, non-observable quantities).

```
Candidate Generation, LLM (direct)
You are performing optimization of a utility function u(x) = q(y) = q(y)
f(x)), where x is a vector of parameters: x = \{x\_names\} and y = f(x) = x
 {y_names} is a vector of outcomes.
Each dimensions of x is in the range [0, 1].
Your goal is to find the parameters x that maximize the utility.
{experiment_data}
## Human feedback messages:
We have also received the following messages from the DM:
{human_feedback}
## Your task:
Given the above your task is the generate a set of {n_candidates}
candidate parameters x for the next round of experimentation.
First, analyze the human feedback messages to understand the DM's
preferences.
Then, generate a set of {n_candidates} candidate parameters x, trading
-off exploration and exploitation.
Return your final answer as a json file with the following format:
'''json
{ {
    "0": <candidate0>,
    "1": <candidate1>,
    "{n}": <candidate{n}>,
} }
Where each <candidatei> is a list of the candidate parameter values: {
x_names, each in [0, 1].
Do not write a python code for candidate generation. Just return the
required json.
Do not add any comments to your json.
```

Prompt 9: The prompt used for candidate generation in the LLM (direct) baseline. experiment_data is a markdown-formatted table of inputs and outcomes. human_feedback is the set of questions and answers from $D_{n-1}^{\rm pf}$.

Algorithm 5: True utility BO

```
Input: Max number of iterations T, Experiment batch size B^{\text{exp}}, Feedback batch size B^{\text{pf}}.
D_0^{\text{exp}} \leftarrow \varnothingD_0^{\text{pf}} \leftarrow \varnothing
for n = 1 to T do
      # Sample a batch of candidates
      if n = 1 then
        [x_i]_{i=1}^{B^{\text{exp}}} \sim \text{Uniform}(\mathcal{X})
       else
         \lfloor \{x_i\}_{i=1}^{B^{\exp}} \sim \text{LogEI}(\mathcal{X}; M_{n-1}^x) 
      ^{\#} Run the experiments and update the experimental dataset D_n^{\exp} \leftarrow D_{n-1}^{\exp} \cup \{(x_i,y_i): y_i = f(x_i)\}_{i=1}^{B^{\exp}} ^{\#} Sample a batch of outcomes for feedback
      if n = 1 then
        \lfloor \{y_i\}_{i=1}^{B^{\mathrm{pf}}} \sim \mathrm{random\_sample}(D^{exp})
       else
         | \{y_i\}_{i=1}^{B^{pf}} \sim \text{EUBO}(D_n^{exp}, M_{n-1}^y) 
       # Update the preference feedback dataset
      D_n^{\mathrm{pf}} \leftarrow D_{n-1}^{\mathrm{pf}} \cup \{(y_j, u_j) : u_j = g(y_j)\}_{j=1}^{B^{\mathrm{pf}}} # Fit a Y->U GP
       M_n^y \leftarrow \text{fit\_simple\_gp}(D_n^{\text{pf}})
      # Label all experimental datapoints D_n^{\mathrm{GP}} \leftarrow \{(x_i,y_i,\hat{u}_i): (x_i,y_i) \in D_n^{\mathrm{exp}}\} \ / \ \hat{u}_i{'}{'} s are the mean predictions with respect to M_n^y: \mathcal{Y} \rightarrow \mathcal{P}(\mathbb{R})
       # Fit the proxy model
     D_n^{\text{GP},x} \leftarrow \{(x_i, \hat{u}_i) : (x_i, y_i, \hat{u}_i) \in D_n^{\text{GP}}\}
M_n^x \leftarrow \text{fit\_simple\_gp}(D_n^{GP,x})
```

Algorithm 6: Preferential BO

```
Input: Max number of iterations T, Experiment batch size B^{\text{exp}}, Feedback batch size B^{\text{pf}}.
D_0^{\text{exp}} \leftarrow \varnothing, \\ D_0^{\text{pf}} \leftarrow \varnothing
for n = 1 to T do
     # Sample a batch of candidates
      if n=1 then
       [x_i]_{i=1}^{B^{\text{exp}}} \sim \text{Uniform}(\mathcal{X})
       ^{\#} Run the experiments and update the experimental dataset D_n^{\exp} \leftarrow D_{n-1}^{\exp} \cup \{(x_i,y_i): y_i = f(x_i)\}_{i=1}^{B^{\exp}} ^{\#} Sample a batch of paired outcomes for feedback
      if n = 1 then
       \lfloor \{(y_i,y_i')\}_{i=1}^{B^{\mathrm{pf}}} \sim \mathtt{random\_sample}(D^{exp})
      else
       \{(y_i, y_i')\}_{i=1}^{B^{pf}} \sim \text{EUBO}(D_n^{exp}, M_{n-1}^y)
      # Update the preference feedback dataset
      D_n^{\text{pf}} \leftarrow D_{n-1}^{\text{pf}} \cup \{(y_j, y_j', p_j) : p_j = \mathbb{1}\{g(y_j) > g(y_j')\}\}_{j=1}^{B^{\text{pf}}}
      # Fit a Y->U GP
      M_n^y \leftarrow \texttt{fit\_pairwise\_gp}(D_n^{\texttt{pf}})
      # Label all experimental datapoints
      D_n^{\mathrm{GP}} \leftarrow \left\{ (x_i, y_i, \hat{u}_i) : (x_i, y_i) \in D_n^{\mathrm{exp}} \right\} / / \ \hat{u}_i{'} \text{s are the mean predictions} with respect to M_n^y : \mathcal{Y} \rightarrow \mathcal{P}(\mathbb{R})
      # Fit the proxy model
     \begin{array}{l} D_n^{\text{GP},x} \leftarrow \{(x_i, \hat{u}_i) : (x_i, y_i, \hat{u}_i) \in D_n^{\text{GP}}\} \\ M_n^x \leftarrow \text{fit\_simple\_gp}(D_n^{GP,x}) \end{array}
```

C ADDITIONAL EXPERIMENTAL RESULTS

C.1 LLM ABLATION STUDY

We compare the performance of LILO depending on the choice of the LLM model. We compare the following models: Llama-3.3-70b-instruct, Llama-4-scout-17b-16e-instruct, and Qwen-3-14b. The LLM used to simulate human feedback remains set to Llama-3.3-70b-instruct across the comparisons.

We run the ablation study for the following 3 environments: the DTLZ2 outcome function, combined with the L1, beta products and piecewise linear utility functions. As in the main benchmark, we set $B^{\rm pf}=2$ and $B^{\rm exp}=d=8$.

Results. Table 1 presents the results. We observe that LILO performs similarly across all three LLMs, demonstrating that the success of our method is agnostic to the choice of a specific language model. We were unable to test the performance of LILO with smaller language models (e.g. LLama-3.1-8B or Qwen-3-8b) due to difficulties in ensuring that the LLM's outputs follow the required json structure, leading to parsing errors.

C.2 PREFERENCE FEEDBACK BATCH SIZE ABLATION

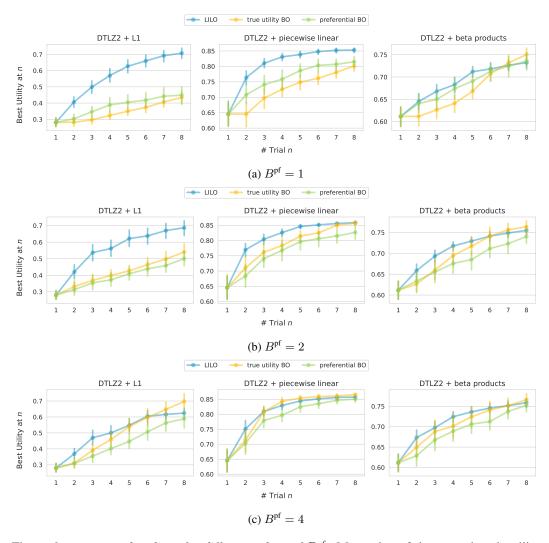


Figure 6: LILO vs. baselines for different values of B^{pf} . Max value of the ground-truth utility achieved after n iterations. Error bars are 95% confidence intervals of the mean max value across 30 simulation replications.

Table 1: LLM ablation study. Max value of the ground-truth utility achieved after n iterations. Error bars are 1 standard deviation of the mean across 30 simulation replications.

(a)	D	ΓLZ2	+	L1

method # trial	LILO (Llama-3.3-70b)	LILO (Llama-4-scout)	LILO (Qwen3-14B)	preferential BO	true utility BO
1 2 3 4 5	0.28 ± 0.01 0.42 ± 0.02 0.54 ± 0.03 0.56 ± 0.03 0.62 ± 0.02 0.64 ± 0.02	0.28 ± 0.01 0.43 ± 0.02 0.53 ± 0.02 0.59 ± 0.02 0.64 ± 0.02 0.67 ± 0.02	0.28 ± 0.01 0.42 ± 0.02 0.54 ± 0.03 0.59 ± 0.03 0.63 ± 0.03 0.66 ± 0.03	0.28 ± 0.01 0.31 ± 0.02 0.35 ± 0.02 0.37 ± 0.02 0.41 ± 0.02 0.44 ± 0.02	0.28 ± 0.01 0.33 ± 0.02 0.37 ± 0.02 0.4 ± 0.02 0.43 ± 0.02 0.46 ± 0.02
7 8	0.67 ± 0.02 0.67 ± 0.02 0.69 ± 0.02	0.07 ± 0.02 0.7 ± 0.02 0.71 ± 0.02	0.69 ± 0.02 0.71 ± 0.02	0.44 ± 0.02 0.46 ± 0.02 0.5 ± 0.02	0.5 ± 0.02 0.54 ± 0.03

(b) DTLZ2 + beta products

method	LILO (Llama-3.3-70b)	LILO (Llama-4-scout)	LILO (Qwen3-14B)	preferential BO	true utility BO
# trial					
1	0.61 ± 0.01	0.61 ± 0.01	0.61 ± 0.01	0.61 ± 0.01	0.61 ± 0.01
2	0.66 ± 0.01	0.67 ± 0.01	0.66 ± 0.01	0.63 ± 0.01	0.63 ± 0.01
3	0.69 ± 0.01	0.69 ± 0.01	0.69 ± 0.01	0.66 ± 0.01	0.66 ± 0.01
4	0.72 ± 0.01	0.71 ± 0.01	0.7 ± 0.01	0.68 ± 0.01	0.69 ± 0.01
5	0.73 ± 0.0	0.73 ± 0.01	0.71 ± 0.01	0.69 ± 0.01	0.72 ± 0.01
6	0.74 ± 0.01	0.74 ± 0.01	0.73 ± 0.01	0.71 ± 0.01	0.74 ± 0.01
7	0.75 ± 0.01	0.75 ± 0.01	0.73 ± 0.01	0.72 ± 0.01	0.76 ± 0.01
8	0.76 ± 0.01	0.75 ± 0.0	0.73 ± 0.01	0.74 ± 0.01	0.76 ± 0.01

(c) DTLZ2 + piecewise linear

method # trial	LILO (Llama-3.3-70b)	LILO (Llama-4-scout)	LILO (Qwen3-14B)	preferential BO	true utility BO
1	0.65 ± 0.02	0.65 ± 0.02	0.65 ± 0.02	0.65 ± 0.02	0.65 ± 0.02
2	0.77 ± 0.01	0.76 ± 0.01	0.76 ± 0.01	0.68 ± 0.02	0.71 ± 0.02
3	0.8 ± 0.01	0.82 ± 0.01	0.82 ± 0.01	0.74 ± 0.01	0.76 ± 0.02
4	0.83 ± 0.01	0.83 ± 0.01	0.84 ± 0.01	0.77 ± 0.02	0.78 ± 0.01
5	0.85 ± 0.0	0.84 ± 0.01	0.85 ± 0.0	0.8 ± 0.01	0.81 ± 0.01
6	0.85 ± 0.0	0.85 ± 0.01	0.85 ± 0.0	0.81 ± 0.01	0.83 ± 0.01
7	0.86 ± 0.0	0.85 ± 0.0	0.86 ± 0.0	0.81 ± 0.01	0.85 ± 0.01
8	0.86 ± 0.0	0.86 ± 0.0	0.86 ± 0.0	0.83 ± 0.01	0.86 ± 0.0

C.3 INCORPORATING PRIOR KNOWLEDGE

In Figure 7 we present an environment-by-environment view of the results from Section 4.3.3.

C.4 BASELINES - FEEDBACK ACQUISITION ABLATION

This section is aimed to justify the choice of feedback acquisition functions used by the quantitative baselines.

For true utility BO, we consider EUBO, Max Value Entropy Search, and a random acquisition function. For preferential BO, replicating the setup of Lin et al. (2022), we compare EUBO, BALD, and a random acquisition function.

Results. We compute the results for the following three environments: the DTLZ2 outcomes function combined with the L1 distance, beta products and piecewise linear utility functions. As in the main results, we let $B^{\rm exp}=d$ and $B^{\rm pf}=2$. Table 2 shows the results averaged across all three environments. Overall, the differences in performance are not substantial among alternatives. Across

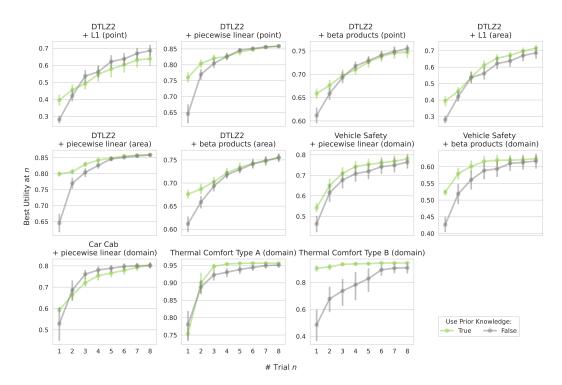


Figure 7: Performance of LILO with and without prior knowledge. Results across environments and knowledge types.

all methods, we observe a slight advantage of EUBO against the alternatives, hence we have chosen it as a default choice of the acquisition function for the baseline methods.

Table 2: The choice of feedback acquisition function. Values represent the average of the best ground-truth utility at iteration n. Averaged across three simulation environments and 30 replications per environment; min-max standardized within an environment before aggregation. Error bars represent 1 standard deviation of the mean.

(a) True Utility BO

Method # trial	EUBO	Max Value Entropy Search	random
1	0.45 ± 0.017	0.45 ± 0.017	0.45 ± 0.017
2	0.537 ± 0.017	0.528 ± 0.017	0.529 ± 0.017
3	0.61 ± 0.017	0.587 ± 0.017	0.603 ± 0.017
4	0.668 ± 0.017	0.652 ± 0.017	0.668 ± 0.017
5	0.723 ± 0.017	0.712 ± 0.017	0.721 ± 0.017
6	0.775 ± 0.016	0.762 ± 0.017	0.771 ± 0.016
7	0.812 ± 0.016	0.806 ± 0.017	0.802 ± 0.016
8	0.851 ± 0.015	0.84 ± 0.016	0.831 ± 0.016

(b) Preferential BO

Method # trial	EUBO	BALD	random
1	0.451 ± 0.017	0.451 ± 0.017	0.451 ± 0.017
2	0.563 ± 0.017	0.57 ± 0.017	0.568 ± 0.017
3	0.654 ± 0.016	0.633 ± 0.017	0.634 ± 0.017
4	0.713 ± 0.016	0.688 ± 0.016	0.688 ± 0.017
5	0.767 ± 0.014	0.742 ± 0.015	0.738 ± 0.016
6	0.805 ± 0.013	0.781 ± 0.014	0.775 ± 0.015
7	0.835 ± 0.012	0.817 ± 0.013	0.809 ± 0.014
8	0.864 ± 0.011	0.843 ± 0.012	0.84 ± 0.012

D EXAMPLE CONVERSATIONS FROM THE BENCHMARKS

We present example conversations of LILO with the DM agent to showcase what are the typical questions that our agent asks and what is the form of feedback that it receives. We would like to highlight how for the Thermal Comfort environment the simulated human responses are more qualitative rather than quantitative in nature.

Example conversation (DTLZ2 + piecewise linear) - DM: My goal is to achieve the following thresholds in each outcome: $y_1 >= 1.0$, $y_2 >= 0.8$, $y_3 >= 0.5$, $y_4 >= 0.5$. Improvements over the thresholds are always good, but less important than bringing the outcomes to their threshold values. The further away an outcome is from its threshold, the higher is its negative impact on the overall performance. - LILO: How do you prioritize improvements in outcomes that are already above their threshold values compared to those below their threshold values? - DM: I prioritize improvements in outcomes that are below their threshold values over those that are already above, as meeting these thresholds has a significant impact on my overall satisfaction. - LILO: Are there any interactions or trade-offs between outcomes that you consider when evaluating overall satisfaction (e.g., is underperforming in one outcome acceptable if others overperform)? - DM: Yes, I consider interactions and trade-offs between outcomes, taking into account their relative importance to my overall satisfaction, which is not solely determined by their threshold values but by the impact of their improvement on my satisfaction. - LILO: Considering outcomes \$1_0\$ and \$1_2\$, how do you trade off between \$y_1\$ being slightly above its threshold in \$1_0\$ and \$y_4\$ being significantly above its threshold in 1_2 , given that y_2 and \$y_3\$ are below their thresholds in both cases? Specifically, which outcome do you prefer and why? - DM: I prefer outcome \$1_0\$ because \$y_1\$ being slightly above its threshold of 1.0 takes precedence due to its higher importance. - LILO: Considering outcomes 2_0 and 2_1 , both have y_1 above its threshold, but \$y_2\$ is below its threshold in both cases. Given that y_4 in 2_0 is above its threshold and in 2_1 is significantly below, and \$y_3\$ is slightly above its threshold in both , which outcome do you prefer and why? - DM: I prefer outcome \$2_0\$ because it has \$y_4\$ above its threshold, contributing positively to my overall satisfaction, unlike \$2_1\$ where \$y_4\$ is significantly below its threshold.

Example 2: Example fragments of conversation of ${\tt LILO}$ with the DM on the DTLZ2 + piecewise linear environment.

Thermo + type A

- DM: My goal is to keep all metrics within my thermal comfort preferences.
- LILO: Can you provide more specific thresholds for each metric that you consider to be within your thermal comfort preferences?
- DM: To be honest, I prefer it when the air doesn't feel drafty at my neck, and I don't feel too much warmth coming from the ceiling. I also like it when there's not a big difference in temperature between my head and ankles. As for the floor, I find it comfortable when it's around 22-24 degrees Celsius. If it's too cold or too hot, my feet feel uncomfortable, and that affects my overall comfort.
- LILO: How do you prioritize these metrics relative to one another? For example, is minimizing PPD more important to you than minimizing DR, or are they equally important?
- DM: For me, it's really important that I don't feel drafty or too warm from the ceiling. If I had to choose, I'd say minimizing those feelings is a bit more important than the other factors. But, at the same time, I also value not having a big temperature difference between my head and ankles. It's all about finding a balance, I suppose. If one thing is off, it can really affect how I feel overall. LILO: Considering arm_index 1_0 (PPD: 25.67%, DR: 13.52%, dT_vert: 0.24K, dT_pr: 1.02K, T_floor: 18.47C) and arm_index 1_3 (PPD: 9.02%, DR: 3.27%, dT_vert: 4.14K, dT_pr: 17.08K, T_floor: 25.52C), which one do you prefer and why?
- DM: I prefer arm_index 1_3. I feel more comfortable with the conditions in 1_3 , even though the temperature difference between my head and ankles is a bit higher. The air feels calmer and less turbulent, which makes me feel more at ease. In 1_0, I feel a bit chilly, especially on the floor, which is slightly too cold for my liking. I wish it were a bit warmer, around 20-22C would be perfect. - LILO: On a scale of 1-5, how satisfied are you with $arm_index 1_5$ (PPD: 57.90%, DR: 0%, dT_vert: 0.50K, dT_pr: 19.41K, T_floor: 27.10C), and would you like to see improvements in any specific metrics? - DM: I'd rate my satisfaction with arm_index 1_5 as a 1 out of 5. I feel quite uncomfortable with these conditions. The air feels stale, and I feel a bit too warm from the ceiling, which is making me feel uneasy. Also, the floor temperature is a bit too high, I prefer it when it's around 20-24C. I'd like to see improvements in reducing the warmth from the ceiling and adjusting the floor temperature to a more comfortable range.

Example 3: Example fragments of conversation of LILO with the DM on the Thermal Comfort + Type A environment.