LILO: Bayesian Optimization with Natural Language Feedback

Anonymous Authors[1]

Abstract

Many real-world optimization problems are guided by complex, subjective preferences that are difficult to express as explicit closed-form objectives. In response, we introduce Language-in-the-Loop Optimization (LILO), a Bayesian optimization (BO) framework that employs a large language model (LLM) to translate free-form natural language feedback and prior knowledge from a decision maker into structured preference signals, going beyond the restrictive scalar or pairwise feedback formats typically assumed in preferential BO. The LLM-derived preferences are integrated by a Gaussian process proxy model, enabling principled acquisition-driven exploration with calibrated uncertainty. By placing the LLM in a supporting role rather than as the optimizer itself, LILO preserves the sample efficiency and stability of BO while providing a flexible and expressive feedback interface. Across synthetic and real-world benchmarks, LILO consistently outperforms both conventional preference-based BO methods and LLM-only optimizers, with particularly strong gains in feedback-limited regimes.

1. Introduction

Bayesian optimization (BO) is a powerful approach for optimizing expensive-to-evaluate black-box objectives (Brochu et al., 2010; Shahriari et al., 2015; Frazier, 2018). In many real deployments, however, the true objective we ultimately care about is not a directly measurable scalar: it reflects a decision maker's (DM's) preferences over complex tradeoffs among multiple outcomes. As a result, optimization must be guided by DM feedback rather than by repeated evaluations of a known utility function.

Existing preference-based BO methods learn from structured feedback such as pairwise comparisons or rankings (González et al., 2017; Chu & Ghahramani, 2005; Lin et al., 2022; Feng et al., 2024). While principled, these approaches assume narrow feedback formats or require problem-specific modeling choices (e.g., custom likelihoods, kernels, or priors) to capture preferences over high-dimensional outcomes. In contrast, large language models (LLMs) provide a flexible interface: they can interpret rich natural language feedback and leverage domain knowledge expressed in text (Brown et al., 2020; Yang et al., 2023; Liu et al., 2024). But when used end-to-end as optimizers, LLM-driven methods generally lack calibrated uncertainty, principled exploration–exploitation tradeoffs, and sample efficiency — properties central to BO.

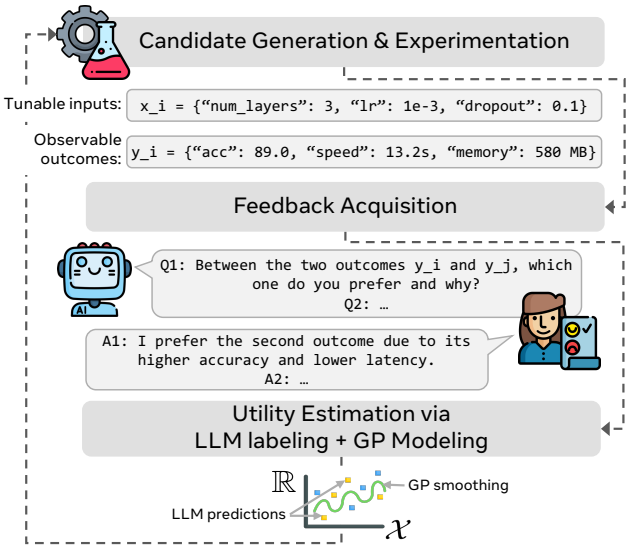

Figure 1. **LILO at a glance.** At each BO trial, a surrogate model is used to select a batch of candidate points to evaluate their outcomes. The DM provides free-form feedback messages, and an LLM agent translates the accumulated language into labeled pairwise preferences among observed outcomes (equivalently, among their corresponding inputs), which are used to update the pairwise GP surrogate for the next acquisition step.

We introduce ***L**anguage-**i**n-the-**l**oop **O**ptimization* (LILO), a framework that combines the expressivity of language feedback with the reliability of BO. LILO places the LLM in a *supporting* role: it translates free-form feedback and textual priors into structured preference information, which is integrated by a Gaussian process (GP) proxy model. After each round of experimentation, LILO uses accumulated natural language feedback to infer pairwise preferences between

[1]Anonymous Institution, Anonymous City, Anonymous Region, Anonymous Country. Correspondence to: Anonymous Author <anon.email@domain.com>.

Preliminary work. Under review by the International Conference on Machine Learning (ICML). Do not distribute.

observed outcomes, fit a pairwise GP surrogate, and apply standard BO acquisition functions to propose the next batch of candidates. This design preserves BO's calibrated uncertainty and acquisition-driven exploration, while enabling a natural, information-dense feedback channel.

Beyond introducing this hybrid design, we study the key choices that make LILO effective in practice, including (i) translating natural language into optimization-relevant utility signals, (ii) performing LLM-based preference labeling under a budget, and (iii) incorporating textual prior knowledge to warm-start the search. Across synthetic and real-world benchmarks, LILO consistently outperforms both LLM-based optimizers and BO baselines relying on quantitative feedback, particularly in early optimization stages. In summary, our main contributions are:

1. We propose LILO, a Bayesian optimization framework that elicits utility information via free-form natural language feedback, enabling a more expressive interface than standard pairwise or scalar feedback.
2. We introduce a utility estimation mechanism based on scalable LLM-based preference labeling and GP modeling, enabling calibrated uncertainty and acquisition-driven exploration under noisy, indirect feedback.
3. We demonstrate that LILO outperforms conventional BO baselines and LLM-only black-box optimization methods across synthetic and real-world problems.
4. We show that LILO can incorporate textual prior knowledge to warm-start optimization by leveraging the LLM's pretrained domain knowledge.

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 tunable parameters, and let each $y \in \mathcal{Y} \subset \mathbb{R}^k$ define the outcomes of an experiment obtained through an expensive-to-evaluate, black-box function $f : \mathcal{X} \to \mathcal{Y}, x \mapsto y = f(x)$.

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, like 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 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, 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 $\mathcal{X}$, the setting 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).

2. 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 paradigm to settings where numerical utilities are unavailable and only relative judgments can be obtained from a DM. Early work by Chu & Ghahramani (2005) introduced GP-based preference learning with a probit likelihood for noisy pairwise comparisons, while González et al. (2017) formalized preferential BO and established convergence guarantees. Subsequent extensions explored other querying strategies, including eliciting preferences over hypothetical outcomes (Lin et al., 2022) and best-of-k or multi-dueling formulations (Sui et al., 2017; Astudillo et al., 2023). Together, these methods provide a principled foundation for preference-guided optimization, but they rely on rigidly structured feedback. In practice, however, DMs may want to express their preferences in natural language, conveying high-level goals, tradeoffs, and qualitative constraints that are difficult to capture through conventional feedback formats. In contrast to these works, LILO leverages free-form natural language feedback as its primary interface, while retaining a GP surrogate and acquisition-driven optimization over continuous search spaces.

Optimization with LLMs. Recent work revealed that LLM could be excellent few-shot learners and Bayesian predictors (Brown et al., 2020; Panwar et al., 2023; Falck et al., 2024; Requeima et al., 2024; Zhu & Griffiths, 2024). Researchers then explored using LLMs as black-box optimizers hinging on their in-context learning abilities (Yang et al., 2023). Several studies investigate the use of LLMs for warm-starting, candidate proposal or proxy modeling itself (Liu et al., 2024). Other works explore the synergy of LLMs and BO based on GP surrogates either by employing LLMs to guide exploration (Ramos et al., 2023; Cai et al., 2025; Agarwal et al., 2025) or use them as fixed feature extractors for BO surrogates (Kristiadi et al., 2024). Other approaches

assume a discrete set of candidate options represented by predefined feature vectors and use LLMs to elicit preferences over this finite domain (Austin et al., 2024; Handa et al., 2024). While these methods demonstrate that LLMs can be useful in black-box optimization, they often treat the LLM and the surrogate model as parallel or loosely coupled components, or rely on assumptions (e.g., discrete candidate sets or domain featurization) that limit scalability to complex search spaces. In contrast, LILO integrates the LLM and the BO surrogate in an interdependent manner: the LLM's role is to interpret language feedback and generate structured preference labels, which are then absorbed by a GP proxy model governing exploration and exploitation.

3. Background

In this section, we familiarize the reader with pairwise GP models and the EUBO acquisition function which play a key role in preferential BO and our framework.

Pairwise GP. A standard model for pairwise preference data follows the work of Chu & Ghahramani (2005), where a latent utility function $g : \mathcal{Y} \to \mathbb{R}$ is endowed with a GP prior. Given a pair of outcomes (y, y') and a binary label $s \in \{0, 1\}$ indicating whether y is preferred over y', preferences are assumed to arise from utility differences modeled with the probit likelihood:

$$\Pr(s = 1 \mid g) = \Phi\left(\frac{g(y) - g(y')}{\sqrt{2}\lambda}\right), \qquad (1)$$

where Φ is the standard normal CDF and the learned hyperparameter λ governs the noise of the preferential response. Because the probit likelihood is non-Gaussian, the posterior over latent utilities is intractable. The Laplace approximation is used to obtain a Gaussian approximation. This enables tractable prediction and acquisition optimization. Further details can be found in Chu & Ghahramani (2005).

In this work, we model the composite utility $u(x) = g(f(x))$ as a GP over $\mathcal{X}$; preferences are elicited over outcomes y but induce pairwise comparisons between the corresponding inputs x so that we are able to optimize and generate new candidates directly in the parameter space.

EUBO. In the setup of Lin et al. (2022), the goal is to learn the latent utility function g via obtaining pairwise preference feedback. The Expected Utility of Best Option (EUBO) acquisition function guides preference-exploration by selecting comparisons expected to yield the greatest increase in the utility of the best option. Concretely, consider a pair of outcomes $\{y_1, y_2\}$. EUBO is defined as:

$$\mathrm{EUBO}(y_1, y_2) = \mathbb{E}\big[\max\{g(y_1), g(y_2)\}\big]. \qquad (2)$$

Under a Gaussian posterior, the above expression can be computed analytically by standard results for a truncated normal differences. By selecting a pair of outcomes with the highest EUBO, one actively queries about top-utility options, accelerating convergence towards high-utility outcomes while minimizing the number of preference queries. (Astudillo et al., 2023) generalize EUBO to q outcomes.

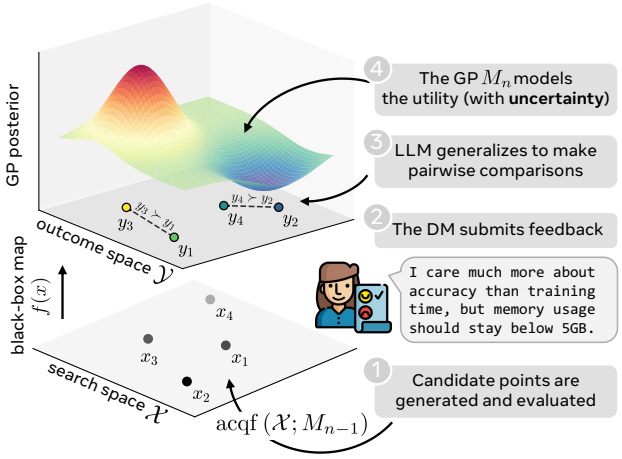

Figure 2. **A single natural-language message can constrain many preferences.** The DM's feedback expresses global tradeoffs and constraints on the latent utility $u(x) = g(f(x))$, inducing pairwise preferences among observed outcomes. LILO uses an LLM to convert the feedback history into pairwise labels, fits a pairwise GP proxy M_n to obtain a smooth posterior over utility u with uncertainty for the next acquisition.

4. Method

The key idea behind LILO is to adopt an iterative BO-style algorithm with an explicit GP-based utility model to steer the optimization in a principled fashion while utilizing LLMs to elicit free-form language feedback from the DM and translate it to a numeric preference signal over the observed outcomes. In this section, we describe the core steps of LILO. Algorithm 1 presents the main pseudo-code, while the exact prompt formats used by the subroutines can be found in Appendix B.2.

Our BO procedure consists of T sequential trials indexed by $n \in \{1, 2, \ldots, T\}$. 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 a proxy GP model $M_n : \mathcal{X} \to \mathcal{P}(\mathbb{R})$, approximating the composite function $g \circ f$, enabling principled candidate generation in the subsequent trial.

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 ($D_0^{\text{exp}} = \varnothing$), so the LILO agent generates B^{pf} gen-

eral 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. As illustrated in Figure 1, each trial consists of three stages: (i) Candidate Generation & Experimentation, (ii) Feedback Acquisition, and (iii) Utility Estimation via LLM Labeling + GP Modeling.

Algorithm 1: `LILO`

Require: Max number of iterations T, experiment batch size B^{exp}, feedback batch size B^{pf}. **Optional:** Prior knowledge prompt P_{prior}

$D_0^{\text{exp}} \leftarrow \varnothing$;
$\{q_j\}_{j=1}^{B^{\text{pf}}} \leftarrow$ `LILO.get_init_questions()`;
$\{a_j\} \leftarrow$ `DM.get_answers`$(\{q_j\}_{j=1}^{B^{\text{pf}}})$;
$D_0^{\text{pf}} \leftarrow \{(q_i, a_i)\}_{i=1}^{B^{\text{pf}}}$;
for $n = 1$ **to** T **do**
  if $n = 1$ **then**
    if $P_{prior} \neq \varnothing$ **then**
      $\{x_i\}_{i=1}^{B^{\text{exp}}} \sim$ `LILO.get_init_x`$\big(D_0^{\text{pf}}, P_{\text{prior}}\big)$;
    else
      $\{x_i\}_{i=1}^{B^{\text{exp}}} \sim \text{Uniform}(\mathcal{X})$;
  else
    $\{x_i\}_{i=1}^{B^{\text{exp}}} \sim \text{acqf}\big(\mathcal{X}; M_{n-1}\big)$;
  $D_n^{\text{exp}} \leftarrow D_{n-1}^{\text{exp}} \cup \{(x_i, y_i) : y_i = f(x_i)\}_{i=1}^{B^{\text{exp}}}$;
  $\{q_j\}_{j=1}^{B^{\text{pf}}} \leftarrow$ `LILO.get_questions`$\big(D_n^{\text{exp}}, D_{n-1}^{\text{pf}}\big)$;
  $\{a_j\}_{j=1}^{B^{\text{pf}}} \leftarrow$ `DM.get_answers`$\big(\{q_j\}_{j=1}^{B^{\text{pf}}}\big)$;
  $D_n^{\text{pf}} \leftarrow D_{n-1}^{\text{pf}} \cup \{(q_j, a_j)\}_{j=1}^{B^{\text{pf}}}$;
  $M_n \leftarrow$ `label_data_and_fit_proxy`$\big(D_n^{\text{exp}}, D_n^{\text{pf}}\big)$;

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 proxy model M_{n-1}, a BO acquisition function (e.g. Expected Improvement) over the search space $\mathcal{X}$ is used to select a batch of B^{exp} candidate inputs $\{x_i\}_{i=1}^{B^{\text{exp}}}$. Each candidate input x_i is then evaluated on the (black-box) function f, producing observable outcomes $y_i = f(x_i)$. After this step, the experimental dataset is updated as $D_n^{\text{exp}} = D_{n-1}^{\text{exp}} \cup \{(x_i, y_i)\}_{i=1}^{B^{\text{exp}}}$.

Feedback Acquisition. After obtaining new experimental outcomes, the `LILO` agent generates B^{pf} questions for the domain expert to answer. These queries can include, for instance, high-level questions regarding overall optimization goals or 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^{pf} questions q_j, and the DM provides corresponding answers a_j. The preference feedback dataset is updated as $D_n^{\text{pf}} = D_{n-1}^{\text{pf}} \cup \{(q_j, a_j)\}_{j=1}^{B^{\text{pf}}}$.

Algorithm 2: `label_data_and_fit_proxy`

Input: Experimental dataset D^{exp}, Feedback dataset D^{pf}, labeling budget K, chunk size S.

$N_{\text{iter}} \leftarrow \lceil \frac{K}{S} \rceil$;
$D^{GP} \leftarrow \varnothing$;
for $i = 1$ **to** N_{iter} **do**
  if $i = 1$ **then**
    $\mathcal{P} \leftarrow$ `get_all_pairs`$(\{y : y \in D^{\text{exp}}\})$;
    $\{(y_\ell, y'_\ell)\}_{\ell=1}^{S} \leftarrow$ `random_sample`$(\mathcal{P}, S)$;
  else
    $q \leftarrow \lceil \sqrt{2S} \rceil$;
    $\{x_i\}_{i=1}^{q} \sim \text{qEUBO}(\{x : x \in D^{\text{exp}}\}, M)$;
    $\{y_i\}_{i=1}^{q} \leftarrow \{y_j : (x_j, y_j) \in D^{\text{exp}}, x_j : \{x_i\}_{i=1}^{q}\}$;
    $\{(y_\ell, y'_\ell)\}_{\ell=1}^{S} \leftarrow$ `get_all_pairs`$(\{y_i\}_{i=1}^{q})[: S]$;
  $\mathcal{L} \leftarrow \{(y_\ell, y'_\ell)\}_{\ell=1}^{S}$;
  $\{s_\ell\}_{\ell=1}^{S} \leftarrow$ `LILO.get_pair_labels`$(\mathcal{L}, D^{\text{exp}}, D^{\text{pf}})$;
  $D^{\text{GP}} \leftarrow D^{\text{GP}} \cup \{(y_\ell, y'_\ell, s_\ell)\}_{\ell=1}^{S}$;
  $M \leftarrow$ `fit_pairwise_GP`(D^{GP});
return M

Utility Estimation via LLM Labeling + GP Modeling. To convert natural language feedback from the DM into a usable optimization signal, we construct pairwise comparisons between experimental outcomes in D^{exp}, which are labeled with binary preference labels by the `LILO` agent using preferential information in D^{pf}. Because the number of possible outcome pairs grows quadratically with the size of D^{exp}, we restrict labeling to a budget of K comparisons. In cases where LLM-labeling costs are a concern, we propose a sequential proxy fitting procedure that acquires labels in batches of size $S \ll K$ selected via qEUBO (Astudillo et al., 2023) (see Algorithm 2). Otherwise, for sufficiently large values of K, we can simply sample K pairs uniformly at random. An ablation on the effect of sequential labeling with qEUBO vs random labeling is in Appendix 5.3.4.

The procedure runs for $N_{\text{iter}} = \lceil K/S \rceil$ iterations. At each iteration, a subset of experimental datapoints is selected using the qEUBO acquisition function under the current pairwise GP proxy model. The corresponding outcomes are retrieved, and a batch of S distinct outcome pairs are constructed from this subset. These outcome pairs are then labeled by the `LILO` agent to produce binary preference labels. All labeled pairs are accumulated across iterations, and after each batch the pairwise GP proxy model is refit to the full set of labeled comparisons. After the labeling budget is exhausted, the final proxy model is returned and used in the subsequent trial to guide candidate generation.

Figure 12 in the Appendix shows that `LILO` agent is able to provide accurate pairwise comparisons and the accuracy continues improving as we observe more natural language feedback. Despite this high accuracy, we do not assume noise-free label from `LILO` agent's and leverage the pairwise GP likelihood to absorbs the comparison noise.

4.1. 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 and the optimization loop (e.g., through specialized kernels, custom mean functions, problem-specific acquisition 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 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 replace the uniform sampling at $n = 1$ with LLM-based sampling. Given D_0^{pf} and prior information represented in a textual form as P_{prior}, we generate B^{pf} candidate points x_i via LLM prompting (see Prompt 6, Appendix B.2). Incorporation of prior knowledge is optional in LILO; in our experiments in Section 5.3.2 we demonstrate how leveraging a good prior can significantly enhance optimization performance.

5. Experiments

5.1. Benchmarking Setup

Test problems. We evaluate LILO on several outcome functions $f : \mathcal{X} \to \mathcal{Y}$, subject to various utility functions $g : \mathcal{Y} \to \mathbb{R}$. In our test problems, we let $\mathcal{X} \subseteq [0, 1]^d$ and $\mathcal{Y} \subseteq \mathbb{R}^k$. Our main benchmark considers the following synthetic and real-world outcome functions f:

- *DTLZ2* (Deb et al. (2002), $d = 8, k = 4$) 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 dimensions of a vehicle, which affect the vehicle's mass and safety.
- *Car Cab Design* (Liao et al. (2008), $d = 7, k = 11$), 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 the following utility functions g 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 D. All utility functions are designed to take values in $[0, 1]$.

Baselines. We compare LILO against two families of baselines: a) LLM-based baselines relying on the same NL feedback as LILO; b) baselines with conventional, quantitative feedback (implementation details provided in Appendix D).

NL feedback: ▶ LLM (direct): a method relying fully on the LLM's in-context learning abilities to propose the next batch of candidates for experimentation. Given the NL feedback collected in D_n^{pf} and a table of paired inputs and outputs (x_i, y_i) from D_n^{exp}), the LLM is prompted to suggest a new batch of points $\{x_i\}_{i=1}^{B^{\text{exp}}}$. No utility-estimation step is present. **▶ LLM (2-step)**: an ablation of LILO in which the acquisition function is replaced by LLM-based candidate generation. In each iteration, the utilities of previously observed outcomes in D_n^{exp} are estimated via the LLM pairwise labeling and GP model fitting as in LILO. Given the data from D_n^{exp} with the estimated utilities of outcomes and the feedback in D_n^{pf}, the LLM is prompted to suggest a new batch of points $\{x_i\}_{i=1}^{B^{\text{exp}}}$.

Both approaches rely on LLMs as in-context Bayesian acquisition functions as in the LLAMBO method of Liu et al. (2024). However, in LLAMBO, the ground-truth utilities of individual candidates x_i are directly observable. In our setup, they must be deduced from the DM's feedback in natural language, making the setup more challenging.

Quantitative feedback: ▶ true utility BO: a GP-based BO that directly observes ground-truth utilities $u_i = g(y_i)$ for a subset of B^{pf} outcomes y_i. **▶ preference BO**: a setup with binary comparison feedback provided to a subset of B^{pf} paired outcomes. Pairwise comparisons between two

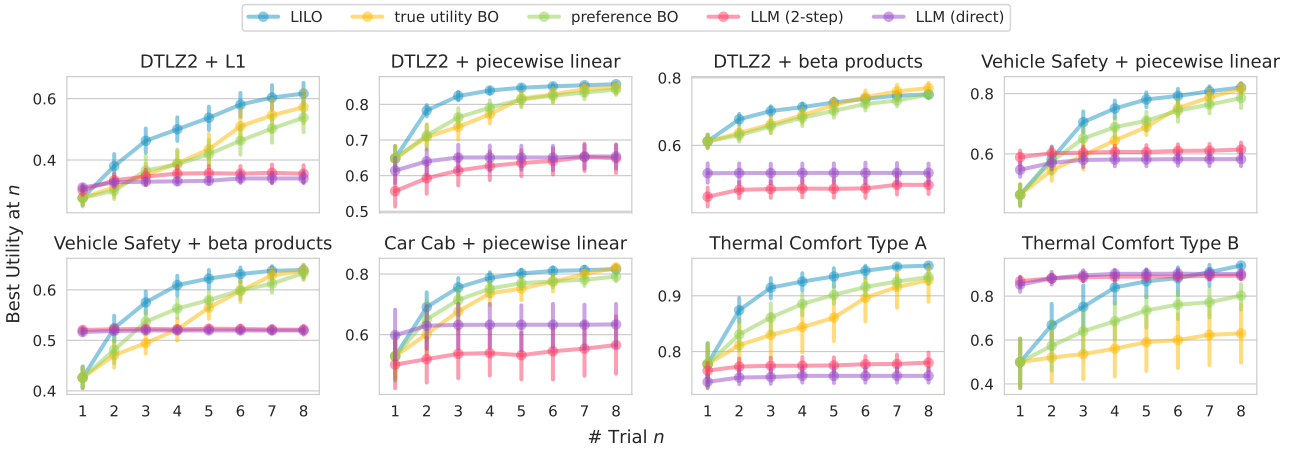

Figure 3. **Main benchmark.** Each panel plots the best *ground-truth* utility found so far, $\max_{x \in D_n^{\text{exp}}} g(f(x))$ over BO trial n of batched experiments. LILO improves rapidly and consistently outperforms preference BO, true-utility BO, and LLM-only optimizers, especially in early trials; error bars are 95% confidence intervals over 32 replications.

outcomes y, y' are derived from the ground-truth utility differences $g(y) - g(y')$.

The subset of B^{pf} feedback points / pairwise preferences, is selected, as in LILO using the qEUBO acquisition function (see Appendix E.3 for an ablation on the choice of the feedback acquisition function). We also note that, in the real world, ground-truth utility values are never directly observable due to the noisy and inconsistent nature of human decision-makers. Thus, the above noise-less quantitative baselines should be seen as "gold standard".

Benchmarking setup. For LILO, our acquisition function of choice is the batch version of *Log Noisy Expected Improvement* (Ament et al., 2023). It is well-suited here because our proxy model is trained on noisy, LLM-derived utility estimates rather than exact evaluations of the ground-truth utility function. For fairness of comparison, for the quantitative baselines we employ the Expected Improvement acquisition function, as the observed feedback is noise-free. Alternative options for the choice of the acquisition functions are also viable (see Appendix E.6 for a comparison with UCB and Thompson Sampling). We run the BO loop for $T = 8$ batched iterations with $B^{\text{exp}} = d$ (the dimension of the search space), simulating real-world scenarios where each evaluation of the outcome f is often expensive yet parallelizable (Frazier, 2018) (See Appendix E.5 for investigation on longer-horizon experiments). For the main experiments we use a feedback batch size of $B^{\text{pf}} = 2$ (see Appendix E.1 for an ablation across varying values of B^{pf}). For methods involving natural language feedback, answers to questions posed by LILO are simulated with an independent LLM feedback simulator (the DM agent) that is provided with a textual description of the ground-truth utility function to ensure consistency between the NL feedback and the ground-truth utility (see Appendix D.3 for details). The simulated DM agent allows us to perform extensive and replicable experiments ablating various aspects of the proposed algorithm. 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 LLMs are presented in Appendix E.7.

5.2. Key Results

We first present the results across all 8 environments, where no prior knowledge about the problem is provided ($P_{\text{prior}} = \varnothing$), 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 5.3.2.

Figure 3 shows the maximum ground-truth utility achieved after n trials of experimentation and feedback collection, that is, $\max_{x \in D_n^{\text{exp}}} g(f(x))$. 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 preference-based 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** as illustrated in Figure 2. The DM may provide auxiliary feedback not only on the performance of specific outcomes, but also on the overall shape of the underlying utility function (e.g., the directionality of the utility function with respect to different metrics, their relative im-

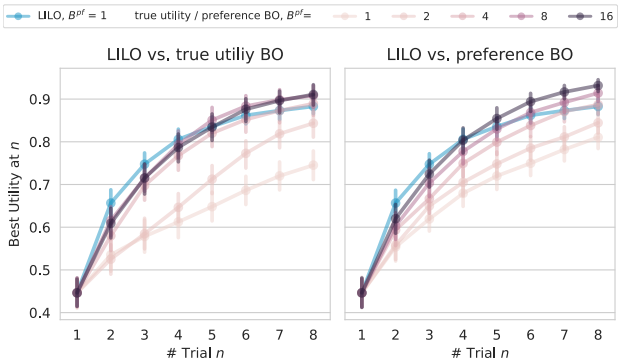

Figure 4. **Natural language is information-dense.** With one DM message per trial (B^{pf}=1), LILO matches or exceeds quantitative-feedback baselines that receive B^{pf} labels.[1]

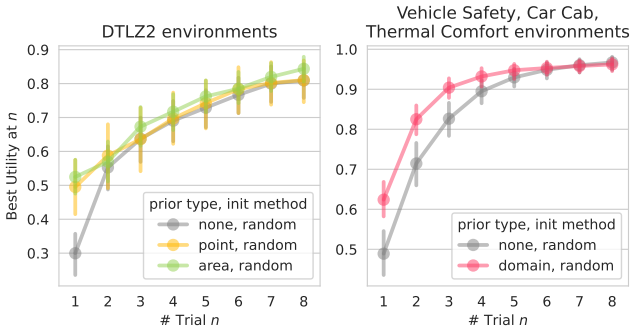

Figure 5. **Textual priors improve initialization.** A prior message provided only at initialization (n=1) warm-starts LILO: "point/area" priors specify a promising candidate or region, "domain" priors describe the semantics of a task. LLM-based initialization yields improved early-trial performance versus random.[1]

portance, etc.). See Appendix F 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. This effect is even more evident when running the experiments for even more iterations (see Appendix E.5).

5.3. Additional Studies

5.3.1. The value of natural language feedback.

A crucial advantage of LILO is its use of natural language feedback, which can be more information-dense from conventional alternatives. It is not straightforward to compare the DM's workload necessary to answer a natural language questions vs. the mental effort required to provide ratings or pairwise comparisons. The DM's burden depends on the specific questions being asked, and for conventional feedback formats it depends on the complexity of the underlying latent utility function and the dimensionality of the outcomes being judged. Experiments presented in this subsection are aimed at understanding how many pairwise comparisons or queries to the ground-truth utility are roughly equivalent to a single message of the DM in natural language. In Figure 4, we compare the performance of LILO with $B^{\text{pf}} = 1$ and the quantitative baselines with $B^{\text{pf}} \in \{1, 2, 4, 8, 16\}$. Results demonstrate that even one natural language statement can outperform as many as 8-16 pairwise comparisons or point-wise evaluations of the ground-truth utility. The competitive performance of LILO is most pronounced at the very initial stages of experimentation. This underscores the sample efficiency and information density of natural language feedback, when used effectively.

5.3.2. Incorporating prior knowledge.

As described in Section 4.1, 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}: ▶ **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. ▶ **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. ▶ **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 D.4. For the DTLZ2 outcome function, we apply the point and area priors with $q = 10$ and $N = 5000$. 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 E.2. 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.

[1] Average results over all 8 environments. 32 (Figure 14) or 16 (all other figures) replications per environment, values min-max standardized within each environment before aggregation.

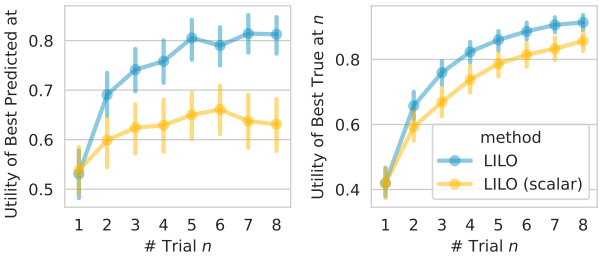

Figure 6. **Pairwise labeling beats direct scalar scoring.** Compared to prompting the LLM for numerical values (LILO (scalar)), LLM-based pairwise comparisons yield a more reliable proxy. Left shows the true utility of the proxy-selected best point, and right shows the best achieved utility. Pairwise supervision produces better "best-point selection" and stronger optimization progress.[1]

5.3.3. Pairwise vs. direct 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 $D_n^{\text{GP}} = \{(x_i, \hat{u}_i)\}$. This dataset is then used to fit the proxy model M_n as a standard (non-pairwise) GP. All other parts of the pipeline remain unchanged. The prompt used for this method and the modified algorithm are presented in Appendix B.

Results. Figure 6 reports average results over 16 replications per each environment from our benchmark. 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, i.e. $g(\hat{x}_n^*)$, where $\hat{x}_n^* = \arg\max_{x \in D_n^{\text{exp}}} M_n(x)$. In practice, it may be preferable or even necessary to use the proxy model to perform "best point selection'. Especially with many observations, it may 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).

5.3.4. Pair Selection with qEUBO

For maximal performance, experiments presented in the previous sections used a large budget ($K = 64$) to generate the LLM pairwise comparisons. In this experiment, we show LILO's performance for $K \in \{8, 16, 32\}$. We also compare our labeling method based on the qEUBO acquisition function, as presented in Algorithm 2 against the performance of a baseline with random pair selection. Across all experiments we keep the same labeling chunk size ($S = 4$).

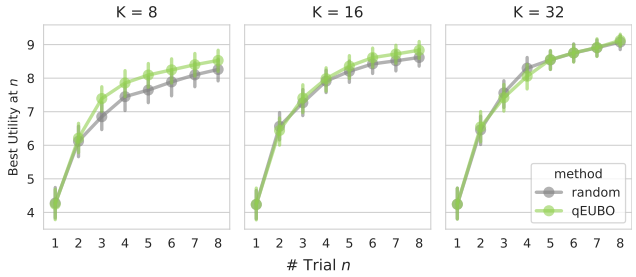

Figure 7. **Which pairs to label matters when labels are scarce.** Under a fixed budget of K LLM comparisons per trial, selecting outcome pairs via qEUBO yields higher best utility than labeling at random. The advantage grows as the labeling budget decreases.[1]

Results. Figure 7 shows that as the labeling budget decreases, the advantage of qEUBO labeling increases, justifying the choice of our approach.

5.3.5. Additional Ablation Studies

Appendix E contains additional results and detailed ablation studies, including analyses of feedback batch size (E.1), prior knowledge (E.2), feedback acquisition strategies (E.3), LILO's pairwise comparison accuracy (E.4), longer-horizon trials (E.5), candidate acquisition function ablations (E.6), and the use of alternative LLMs within LILO (E.7).

6. Discussion and Conclusion

We presented LILO, a framework for black-box optimization that enables decision makers to express goals and preferences in natural language rather than requiring large numbers of pairwise comparisons or scalar ratings. Across benchmark problems, LILO achieves strong performance and we believe it is well suited to real-world optimization settings with complex multi-metric tradeoffs (e.g., online experimentation), where explicit objectives are often unavailable. LILO's performance gains arise from combining information-dense natural language feedback with probabilistic modeling and principled acquisition from BO. While LLM-only optimization methods can process language feedback via in-context learning, their performance often plateaus, whereas LILO sustains improvement through calibrated uncertainty and exploration.

Several directions remain for future work. Utility estimation ultimately depends on the LLM's ability to interpret nuanced feedback, suggesting potential gains from improved prompting or fine-tuning on past experimental data. While our experiments rely on simulated DM responses to enable controlled evaluation, studies with human decision makers could provide deeper insight into real-world interaction dynamics. Hybrid approaches that combine unstructured natural language with structured quantitative feedback may also help mitigate limitations of in-context learning during utility estimation. Finally, extending LILO to settings with high-dimensional outcomes, such as text or images, remains an exciting direction.

Impact Statement

This paper presents work whose goal is to advance the field of machine learning. There are many potential societal consequences of our work, none of which we feel must be specifically highlighted here.

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Appendix Contents

A. Reproducibility

The code to reproduce the results of our experiments is made available as part of this submission in the supplementary materials.

B. `LILO`: Implementation Details

B.1. Pseudo Code

Algorithm 1 presents the pseudo code of `LILO`. The `fit_proxy_models` subroutine is presented in Algorithm 2.

The algorithm for `LILO` with scalar utility estimation (experiment 5.3.3) 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 the Algorithm 3. All prompts used in the `LILO.xxx` subroutines are presented in section B.2.

Algorithm 1: `LILO`: Language-in-the-Loop Optimization

Require: Max number of iterations T, experiment batch size B^{exp}, feedback batch size B^{pf}. **Optional:** Prior knowledge prompt P_{prior}

$D_0^{\text{exp}} \leftarrow \varnothing$;
$\{q_j\}_{j=1}^{B^{\text{pf}}} \leftarrow$ `LILO.get_init_questions()`;
$\{a_j\} \leftarrow$ `DM.get_answers`$(\{q_j\}_{j=1}^{B^{\text{pf}}})$;
$D_0^{\text{pf}} \leftarrow \{(q_i, a_i)\}_{i=1}^{B^{\text{pf}}}$;
for $n = 1$ **to** T **do**
  if $n = 1$ **then**
    if $P_{prior} \neq \varnothing$ **then**
      $\{x_i\}_{i=1}^{B^{\text{exp}}} \sim$ `LILO.get_init_x`$\big(D_0^{\text{pf}}, P_{\text{prior}}\big)$;
    else
      $\{x_i\}_{i=1}^{B^{\text{exp}}} \sim \text{Uniform}(\mathcal{X})$;
  else
    $\{x_i\}_{i=1}^{B^{\text{exp}}} \sim \text{acqf}\big(\mathcal{X}; M_{n-1}\big)$;
  $D_n^{\text{exp}} \leftarrow D_{n-1}^{\text{exp}} \cup \{(x_i, y_i) : y_i = f(x_i)\}_{i=1}^{B^{\text{exp}}}$;
  $\{q_j\}_{j=1}^{B^{\text{pf}}} \leftarrow$ `LILO.get_questions`$\big(D_n^{\text{exp}}, D_{n-1}^{\text{pf}}\big)$;
  $\{a_j\}_{j=1}^{B^{\text{pf}}} \leftarrow$ `DM.get_answers`$\big(\{q_j\}_{j=1}^{B^{\text{pf}}}\big)$;
  $D_n^{\text{pf}} \leftarrow D_{n-1}^{\text{pf}} \cup \{(q_j, a_j)\}_{j=1}^{B^{\text{pf}}}$;
  $M_n \leftarrow$ `label_data_and_fit_proxy`$\big(D_n^{\text{exp}}, D_n^{\text{pf}}\big)$;

Algorithm 2: LILO `label_data_and_fit_proxy`

Input: Experimental dataset D^{exp}, Feedback dataset D^{pf}, labeling budget K, chunk size S.
$N_{\text{iter}} \leftarrow \lceil \frac{K}{S} \rceil$;
$D^{GP} \leftarrow \varnothing$;
for $i = 1$ **to** N_{iter} **do**
  if $i = 1$ **then**
    $\mathcal{P} \leftarrow$ `get_all_pairs`$(\{y : y \in D^{\text{exp}}\})$;
    $\{(y_\ell, y'_\ell)\}_{\ell=1}^{S} \leftarrow$ `random_sample`$(\mathcal{P}, S)$;
  else
    $q \leftarrow \left\lceil \sqrt{2S} \right\rceil$;
    $\{x_i\}_{i=1}^{q} \sim \text{qEUBO}(\{x : x \in D^{\text{exp}}\}, M)$;
    $\{y_i\}_{i=1}^{q} \leftarrow \{y_j : (x_j, y_j) \in D^{\text{exp}}, x_j : \{x_i\}_{i=1}^{q}\}$;
    $\{(y_\ell, y'_\ell)\}_{\ell=1}^{S} \leftarrow$ `get_all_pairs`$(\{y_i\}_{i=1}^{q})[:S]$;
  $\mathcal{L} \leftarrow \{(y_\ell, y'_\ell)\}_{\ell=1}^{S}$;
  $\{s_\ell\}_{\ell=1}^{S} \leftarrow$ `LILO.get_pair_labels`$(\mathcal{L}, D^{\text{exp}}, D^{\text{pf}})$;
  $D^{\text{GP}} \leftarrow D^{\text{GP}} \cup \{(y_\ell, y'_\ell, s_\ell)\}_{\ell=1}^{S}$;
  $M \leftarrow$ `fit_pairwise_GP`(D^{GP});
return M

Algorithm 3: LILO (scalar) `label_data_and_fit_proxy`

Input: Experimental dataset D^{exp}, Feebdback dataset D^{pf}.
$N \leftarrow |D^{\text{exp}}|$
$\{\hat{u}_i\}_{i=1}^{N} \leftarrow$ `LILO.estimate_utilities`$(\{y_i\}_{i=1}^{N}; D^{\text{exp}}, D^{\text{pf}})$
$D^{\text{GP}} \leftarrow \{(x_i, \hat{u}_i)\}_{i=1}^{N}$ `$x_i$'s are the inputs corresponding to $y_i$'s`
$M \leftarrow$ `fit_simple_gp`(D^{GP})
return M

B.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 prompts 3, 4, `human_feedback_summary` is a summary of the feedback stored in D_n^{pf}, self-generated by `LILO` using the prompt 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`.

Initial question generation with `LILO.get_init_questions`

```
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.

Question generation with `LILO.get_questions`

```
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.

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.
```

Pairwise comparisons with `LILO.get_pair_labels`

```
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.

Scalar utility estimation with with `LILO.estimate_utilities`

```
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 <probability>
should be your best estimate for the probability between 0 and 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.

Human Feedback Summarization

```
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.

Candidate Generation at $n = 1$ when $P_{\text{prior}} \neq \varnothing$, `LILO.get_init_x`

```
You are performing optimization of a utility function u(x) = g(y) = g(f(x)), where x
is a vector of parameters: x = {x_names} and y = f(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.

## 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 [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 6. The prompt used for candidate generation by `LILO` at $n = 1$ when prior knowledge is available (`LILO.sample_init_candidates` subroutine).

B.3. GP models and acquisition functions

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.

Main experiments are presented for the LogNEI acquisition function for candidate generation and qEUBO acquisition function for feedback datapoint selection. Both functions are used in their batched-versions, which jointly evaluate the utility of an entire batch of candidates via Monte Carlo sampling—rather than selecting points greedily. Specifically, we employ the `qLogNoisyExpectedImprovement` method from BoTorch, which follows the work of Ament et al. (2023) and the `qExpectedUtilityOfBestOption` (Lin et al., 2022).

C. Baselines: Implementation Details

C.1. Natural Language Feedback Baselines

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

LLM (2-step) follows the same algorithm 1 as `LILO` with the following 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 7.

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 8

Candidate Generation, LLM (2-step)

```
You are performing optimization of a utility function u(x) = g(y) = g(f(x)), where x
is a vector of parameters: x = {x_names} and y = f(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 xˆ* = {x_star} with utility u(xˆ*) = {u_star}.

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 [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 7. 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 $M(x_i)$. `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) = g(y) = g(f(x)), where x
is a vector of parameters: x = {x_names} and y = f(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 8. 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}^{pf}.

C.2. Quantitative Feedback 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 (preference BO). This feedback is obtained on B^{pf} outcomes y_i or paired outcomes (y_i, y_i') sampled with the qEUBO acquisition function (see Appendix E.3 for a justification of this choice). In `LILO`, the LLM extends the natural feedback to the observation in D_n^{exp} via pairwise labeling. For our quantitative baselines, to extend the quantitative feedback within D^{pf} to the entirety of D_n^{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 the M_n^y model.

We present the exact implementation of these methods in algorithms 4 and 5.

Algorithm 4: True utility BO

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

Algorithm 5: Preference BO

Input: Max number of iterations T, Experiment batch size B^{exp}, Feedback batch size B^{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**

    $\{x_i\}_{i=1}^{B^{\text{exp}}} \sim \text{Uniform}(\mathcal{X})$

  else

    $\{x_i\}_{i=1}^{B^{\text{exp}}} \sim \text{LogNEI}(\mathcal{X}; M_{n-1}^x)$

  `# Run the experiments and update the experimental dataset`

  $D_n^{\text{exp}} \leftarrow D_{n-1}^{\text{exp}} \cup \{(x_i, y_i) : y_i = f(x_i)\}_{i=1}^{B^{\text{exp}}}$

  `# Sample a batch of paired outcomes for feedback`

  if $n = 1$ **then**

    $\{(y_i, y_i')\}_{i=1}^{B^{\text{pf}}} \sim$ `random_sample`(D^{exp})

  else

    $\{(y_i, y_i')\}_{i=1}^{B^{\text{pf}}} \sim \text{qEUBO}(D_n^{\text{exp}}, M_{n-1}^y)$

  `# 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`

  $M_n^y \leftarrow$ `fit_pairwise_gp`(D_n^{pf})

  `# Label all experimental datapoints`

  $D_n^{\text{GP}} \leftarrow \{(x_i, y_i, \hat{u}_i) : (x_i, y_i) \in D_n^{\text{exp}}\}$ `// ` $\hat{u}_i$`'s are the mean predictions with respect to` $M_n^y : \mathcal{Y} \to \mathcal{P}(\mathbb{R})$

  `# Fit the proxy model`

  $D_n^{\text{GP},x} \leftarrow \{(x_i, \hat{u}_i) : (x_i, y_i, \hat{u}_i) \in D_n^{\text{GP}}\}$

  $M_n^x \leftarrow$ `fit_simple_gp`$(D_n^{GP,x})$

D. Simulation Environments

We benchmark LILO on synthetic and real-world outcome functions as well as several utility functions. In all our test problems we have $\mathcal{X} = [0, 1]^d$ and $\mathcal{Y} = \mathbb{R}^k$. The main benchmark considers four outcome functions: *DTLZ2* ($d = 4, k = 8$, Deb et al. (2002)), *Vehicle Safety* ($d = 5, k = 3$, Tanabe & Ishibuchi (2020)), and *Car Cab Design* ($d = 7, k = 11$, 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 iterations, setting $B^{\text{exp}} = d$ (the dimension of the search space). We seed the conversation between the DM and LILO by hard-coding the first message of the DM agent. Details of each outcome and utility funcitons alongside the seeding messages are presented below.

D.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.

D.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 {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

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

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

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

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 $Y = [\text{PPD},\ \text{DR},\ dT_{\text{vert}},\ dT_{\text{pr}},\ T_{\text{floor}}]$ 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

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

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

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

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

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

.

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.

$$l_{\text{PPD}} = 0.0,\ h_{\text{PPD}} = 30.0,$$
$$l_{\text{DR}} = 10.0,\ h_{\text{DR}} = 35.0,$$
$$l_{\text{dT}_{\text{vert}}} = 3.0,\ h_{\text{dT}_{\text{vert}}} = 9.0,$$
$$l_{\text{dT}_{\text{pr}}} = 5.0,\ h_{\text{dT}_{\text{pr}}} = 22.0,$$
$$l_{\text{min,T}_{\text{floor}}} = 16.0,\ l_{\text{T}_{\text{floor}}} = 19.0,\ h_{\text{T}_{\text{floor}}} = 26.0,\ h_{\text{min,T}_{\text{floor}}} = 30.0.$$

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.

$$
\begin{gathered}
l_{\text{PPD}} = 0.0,\ h_{\text{PPD}} = 24.0, \\
l_{\text{DR}} = 30.0,\ h_{\text{DR}} = 45.0, \\
l_{\text{dT}_{\text{vert}}} = 2.5,\ h_{\text{dT}_{\text{vert}}} = 6.0, \\
l_{\text{dT}_{\text{pr}}} = 4.0,\ h_{\text{dT}_{\text{pr}}} = 12.0, \\
l_{\text{min,T}_{\text{floor}}} = 19.0,\ l_{\text{T}_{\text{floor}}} = 20.0,\ h_{\text{T}_{\text{floor}}} = 23.0,\ h_{\text{min,T}_{\text{floor}}} = 25.0.
\end{gathered}
$$

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.
```

D.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 9. `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.

D.4. Prior Knowledge Messages P_{prior}

Below we present the prior messages P_{prior} used in our experiments from section 5.3.2.

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 * 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, ..., y_11, corresponding to lowering
the vehicle's weight and minimizing the impact on the dummy and the car.
```

DM's answer generation for `DM.get_answers`

```
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 9. The prompt used for answer generation in the `DM.get_answers` subroutine.

E. Additional Experimental Results

E.1. Preference Feedback Batch Size Ablation

It is not straightforward to compare the DM's workload necessary to answer natural language questions vs. providing e.g. pairwise comparisons. The DM's workload would depend heavily on the specific questions being asked, and in the case of pairwise comparisons, it would depend on the complexity of the utility function and the kind of outcomes being presented. Experiments presented in this subsection are aimed at understanding how many pairwise comparisons or queries to the ground-truth utility are roughly equivalent to a single message of the DM in natural language. In Figures 8, 9, and 10, we compare the performance of `LILO` with $B^{\text{pf}} = 1$ with the quantitative baselines (true utility BO and preference BO) with $B^{\text{pf}} \in \{1, 2, 4, 8, 16\}$. The results demonstrate that even one natural language statement can outperform as many as 8-16 pairwise comparisons or point-wise evaluations of the ground-truth utility. As expected, the competitive performance of `LILO` is most pronounced at the very initial stages of experimentation, which is crucial in feedback-limited regimes.

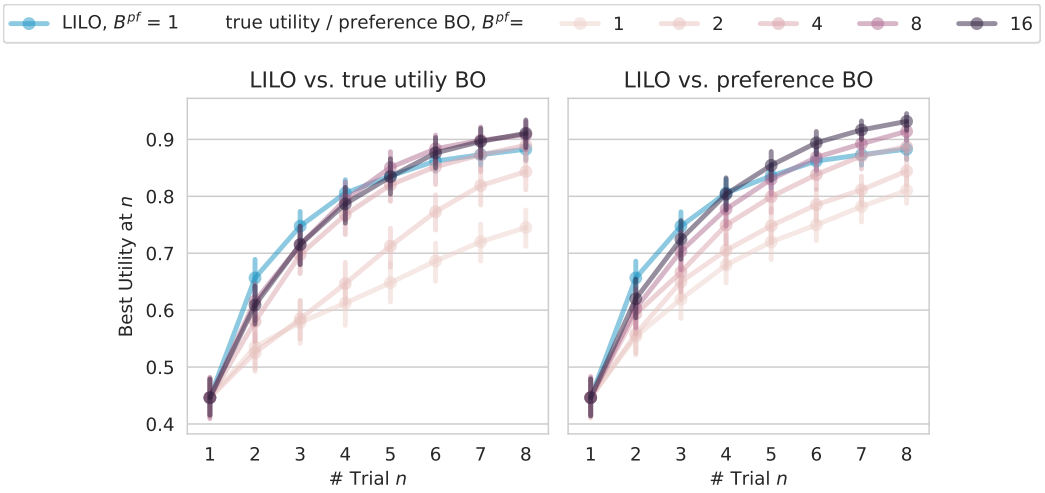


Figure 8. LILO vs. preference BO and true utility BO with varying feedback batch size. Results averaged across all environments, with min-max normalization applied within each environment prior to aggregation.

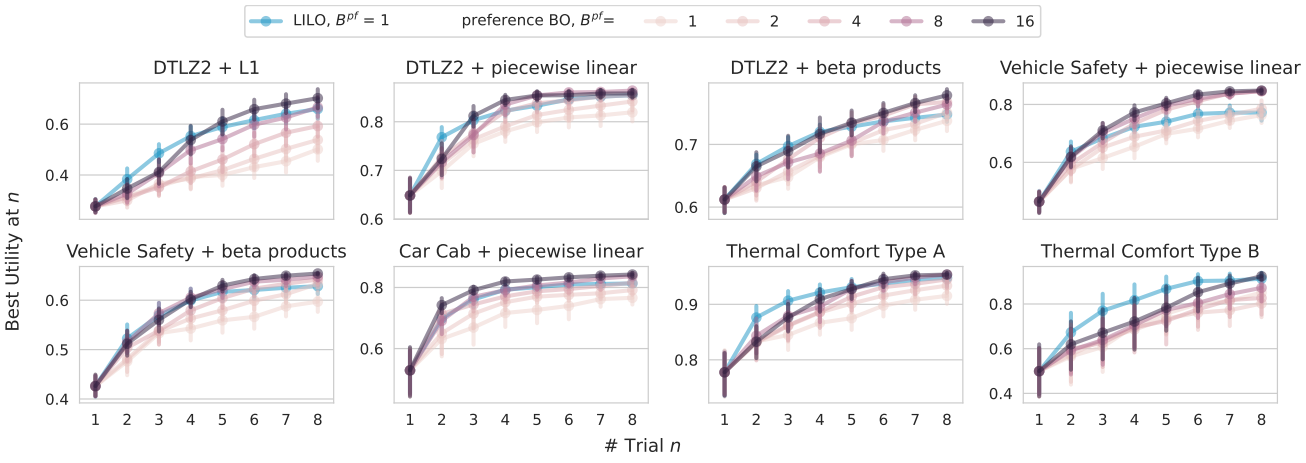


Figure 9. LILO vs. preference BO with varying feedback batch size. Results by environment.

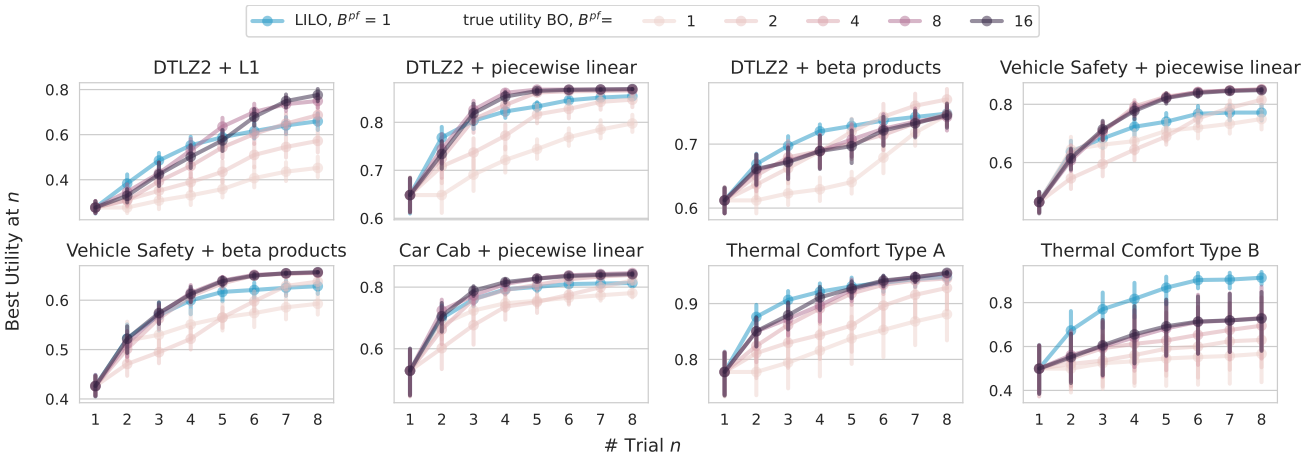


Figure 10. LILO vs. true utility BO with varying feedback batch size. Results by environment.

E.2. Incorporating Prior Knowledge

In addition to the summarized results on prior knowledge incorporation from Section 5.3.2, in Figure 11 we present an environment-by-environment view of these results.

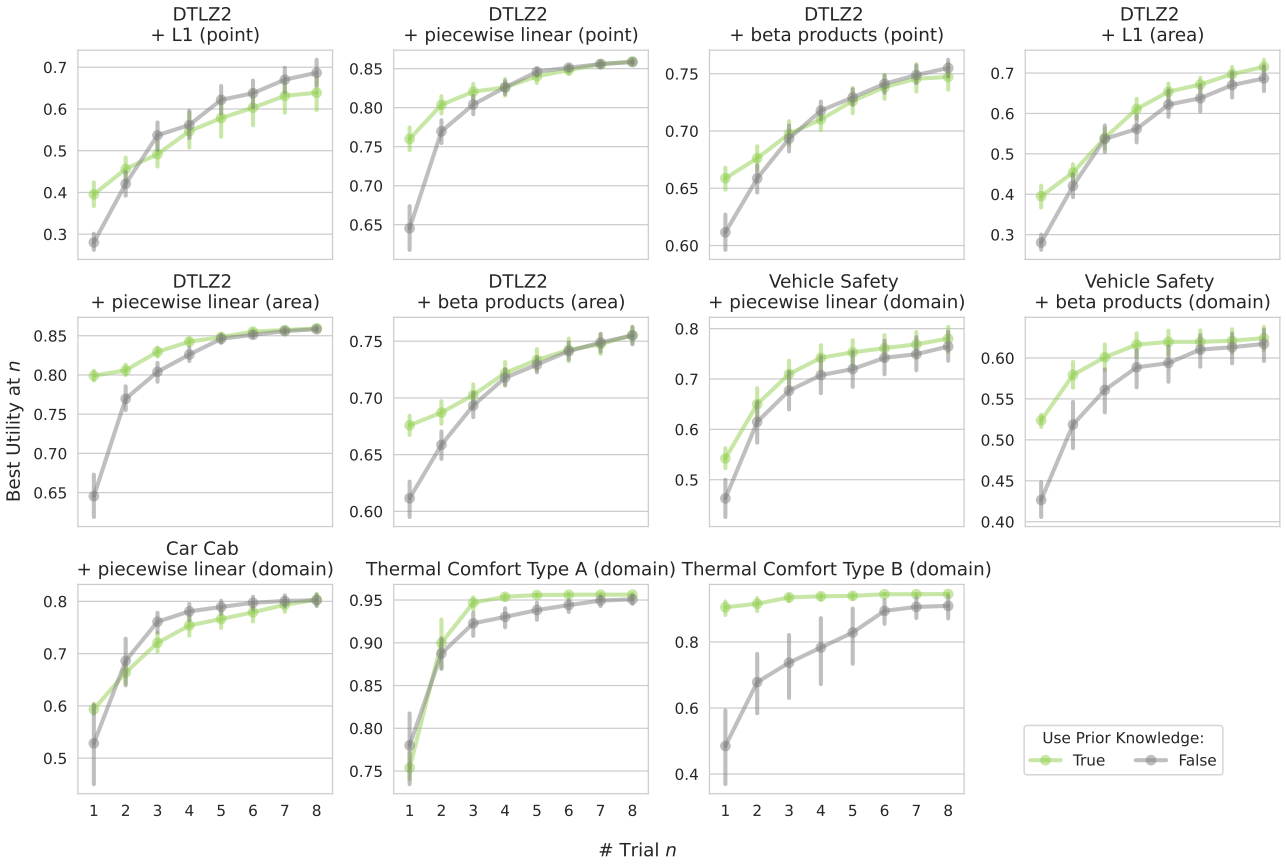


Figure 11. Performance of LILO with and without prior knowledge. Results across environments and knowledge types.

E.3. Baselines – feedback acquisition ablation

This section is aimed to justify the choice of the qEUBO feedback acquisition function by the quantitative baselines.

For true utility BO, we consider the following batch acquisition functions: EUBO, Max Value Entropy Search (Moss et al., 2021), Predictive Entropy Search (Seo et al., 2000) and a random acquisition function. For preference-based BO, we compare acquisition functions designed for preference learning: two versions of the EUBO (batched and greedy) acquisition functions and the pairwise BALD (Houlsby et al., 2011) acquisition function. Batched EUBO is implemented by selecting q points from D_n^{exp} and creating all possible pairs among them. The number q is set to the smallest integer so that $\frac{q(q-1)}{2} > B^{\text{pf}}$ and a subset of B^{pf} is used. The greedy EUBO is implemented by firstly computing the value of EUBO for all pairs (at $q = 2$ the EUBO admits an analytics expression) and selecting the top B^{pf} pairs.

Results. We compute the results across all environments, 32 replications and extend the optimization horizon to $T = 16$ iterations for the results to stabilize. As in the main results, we let $B^{\text{exp}} = d$ and $B^{\text{pf}} = 2$. Table 1 shows the average utility of the best candidate at iteration n. While the differences in performance across different feedback acquisition methods are not substantial, we observe a slight advantage of qEUBO against the alternatives. This observation is in line with the prior work on preference-based BO (Lin et al., 2022). These results justify our choice of baseline implementation.

Table 1. 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

trial n	qEUBO	qMaxES	qPredES	random
1	0.449 (0.016)	0.449 (0.016)	0.449 (0.016)	0.449 (0.016)
2	0.532 (0.017)	0.529 (0.017)	0.532 (0.017)	0.53 (0.017)
3	0.599 (0.017)	0.604 (0.016)	0.609 (0.017)	0.602 (0.017)
4	0.667 (0.016)	0.673 (0.016)	0.672 (0.016)	0.659 (0.017)
5	0.724 (0.016)	0.735 (0.016)	0.73 (0.016)	0.718 (0.016)
6	0.776 (0.016)	0.781 (0.016)	0.782 (0.016)	0.764 (0.017)
7	0.809 (0.016)	0.819 (0.015)	0.819 (0.016)	0.793 (0.016)
8	0.838 (0.015)	0.845 (0.015)	0.848 (0.015)	0.814 (0.016)
9	0.862 (0.014)	0.867 (0.014)	0.866 (0.014)	0.839 (0.015)
10	0.879 (0.014)	0.88 (0.014)	0.877 (0.014)	0.854 (0.015)
11	0.89 (0.014)	0.889 (0.013)	0.885 (0.013)	0.863 (0.015)
12	0.905 (0.013)	0.898 (0.013)	0.89 (0.013)	0.871 (0.014)
13	0.913 (0.012)	0.903 (0.013)	0.894 (0.013)	0.879 (0.014)
14	0.917 (0.012)	0.908 (0.013)	0.899 (0.013)	0.885 (0.014)
15	0.923 (0.012)	0.911 (0.013)	0.903 (0.013)	0.892 (0.013)
16	0.928 (0.011)	0.916 (0.012)	0.906 (0.013)	0.897 (0.013)

(b) Preference BO

trial n	qEUBO	qEUBO (greedy)	BALD	random
1	0.45 (0.016)	0.45 (0.016)	0.45 (0.016)	0.45 (0.016)
2	0.567 (0.016)	0.567 (0.017)	0.568 (0.017)	0.566 (0.017)
3	0.641 (0.016)	0.649 (0.016)	0.636 (0.016)	0.627 (0.016)
4	0.7 (0.015)	0.696 (0.015)	0.699 (0.016)	0.691 (0.016)
5	0.746 (0.015)	0.748 (0.014)	0.741 (0.015)	0.739 (0.015)
6	0.795 (0.013)	0.79 (0.012)	0.774 (0.014)	0.77 (0.014)
7	0.822 (0.012)	0.814 (0.012)	0.809 (0.013)	0.803 (0.013)
8	0.844 (0.012)	0.843 (0.011)	0.836 (0.012)	0.828 (0.013)
9	0.865 (0.011)	0.864 (0.011)	0.854 (0.011)	0.842 (0.012)
10	0.879 (0.01)	0.879 (0.01)	0.871 (0.011)	0.861 (0.011)
11	0.893 (0.01)	0.893 (0.01)	0.885 (0.01)	0.875 (0.011)
12	0.907 (0.008)	0.902 (0.009)	0.9 (0.008)	0.885 (0.01)
13	0.917 (0.008)	0.912 (0.009)	0.912 (0.008)	0.9 (0.009)
14	0.927 (0.007)	0.918 (0.009)	0.923 (0.007)	0.909 (0.009)
15	0.934 (0.006)	0.922 (0.008)	0.933 (0.007)	0.913 (0.009)
16	0.939 (0.006)	0.928 (0.008)	0.939 (0.006)	0.919 (0.009)

E.4. LLM's Accuracy

In this section, we look at the accuracy of LILO in generating pairwise preference labels. Figure 12 shows the average accuracy at each trial, computed across 16 seeds and the 3 DTLZ2 environments. We find that already at the first iteration, LILO yields high-fidelity predictions, with an average accuracy of 85%. As more information about the optimization objective is gathered, its accuracy reaches values above 90%. The relatively high accuracy contrasted with low labeling costs (in comparison to the cost of human labor) justify the validity of our approach – human feedback in natural language can be effectively translated into a numerical signal suitable for optimization via LLM pairwise labeling followed by GP model fitting.

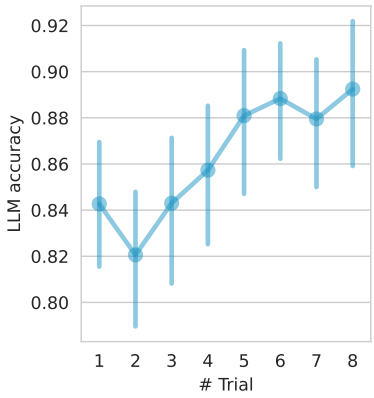


Figure 12. The accuracy of LILO in generating pairwise preference choices in step 3. of the BO loop.

E.5. Longer Trials

We note that this paper primarily concerns settings where configurations are very costly to evaluate, and therefore in practice the number of trials is very limited. Our overarching goal is to minimize human effort during optimization, which is why the main experiments focus on the impact of queries after only a few batched rounds. Nevertheless, in this section, we present additional results evaluating the performance of LILO over longer horizons, with up to 16 batched experimental trials. Figure 13 compares LILO to both preferential and true utility BO (excluding the two LLM baselines, as they do not show meaningful progression across iterations). We observe that LILO maintains competitive performance even in this extended setting. As noted in the main results, the advantage of LILO tends to diminish as the number of experimental trials increases, with quantitative baselines eventually catching up and, in some cases, surpassing LILO in the long run. This behavior is expected – the in-context learning capabilities of LLMs are inherently limited and do not offer the convergence guarantees provided by conventional baselines operating on quantitative feedback.

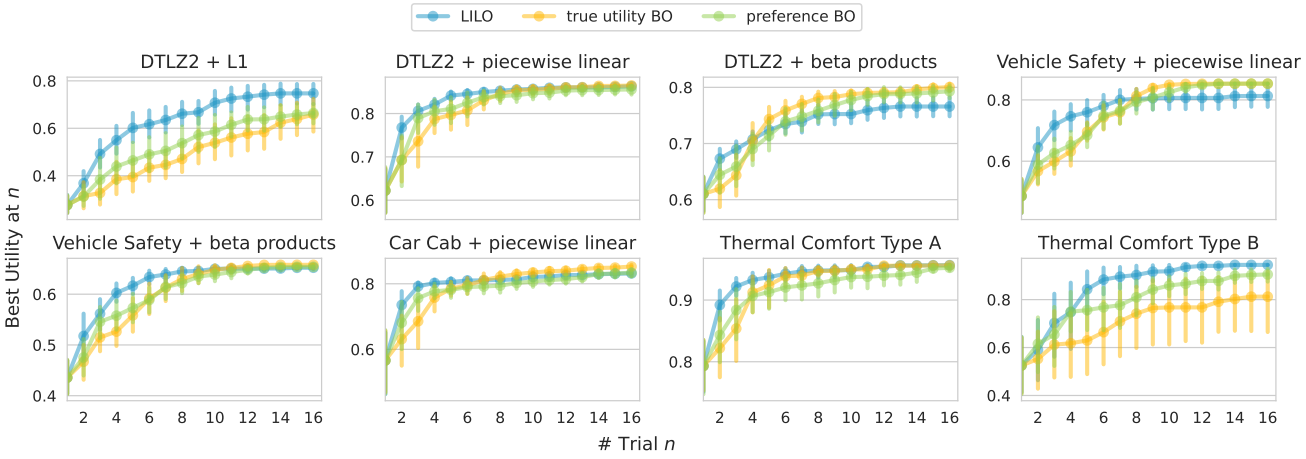


Figure 13. LILO vs. true utility and preference BO on longer horizons. Results aggregated across 16 replications per environment.

E.6. Acquisition Function Ablation

In our main experiments, we demonstrate the performance of LILO against baselines with all methods using the (Noisy) Expected Improvement as the acquisition function for candidate generation. However, this choice can be replaced with other alternatives. In this section, we demonstrate that LILO maintains competitive performance irrespective of this choice.

In Figures 14 and 15 we demonstrate the performance of LILO and the quantitative baselines with three different choices of acquisition functions for candidate generation: (Noisy) Expected Improvement (as in the main text), Upper Confidence Bound (UCB) with the parameter β controlling the trade-off between exploration and exploitation set to 0.5, and Thompson Sampling. All other elements of LILO and the baselines stay fixed. Figure 14 shows results summarized across all environments considered and Figure 15 shows a detailed view of the results. We observe that the Expected Improvement and the UCB acquisition functions, overall, perform better than Thompson Sampling on our selected set of test problems. The advantage of LILO against the baselines is most competitive in these two settings. With Thompson Sampling, LILO performs similarly to the true utility BO baseline, slightly outperforming it at the very first iterations.

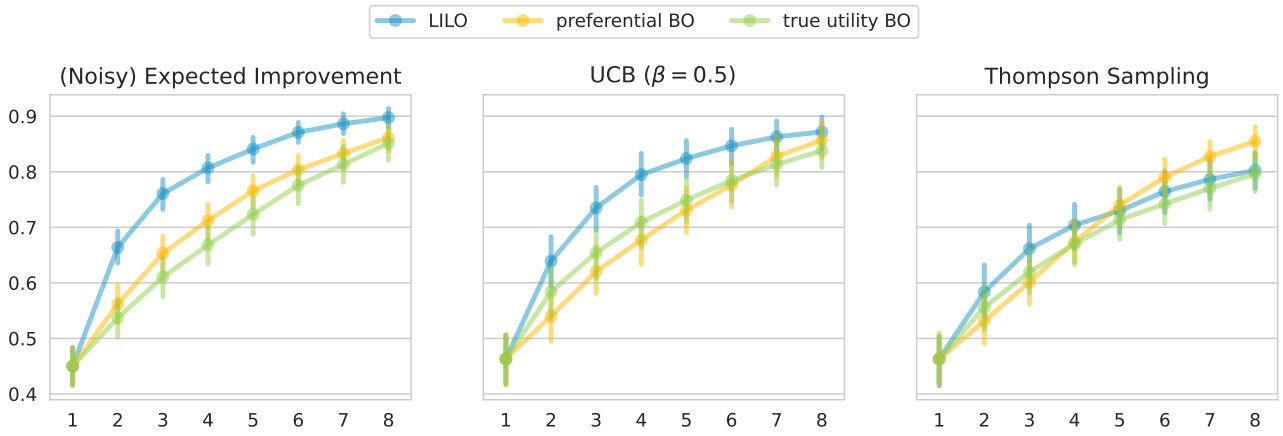
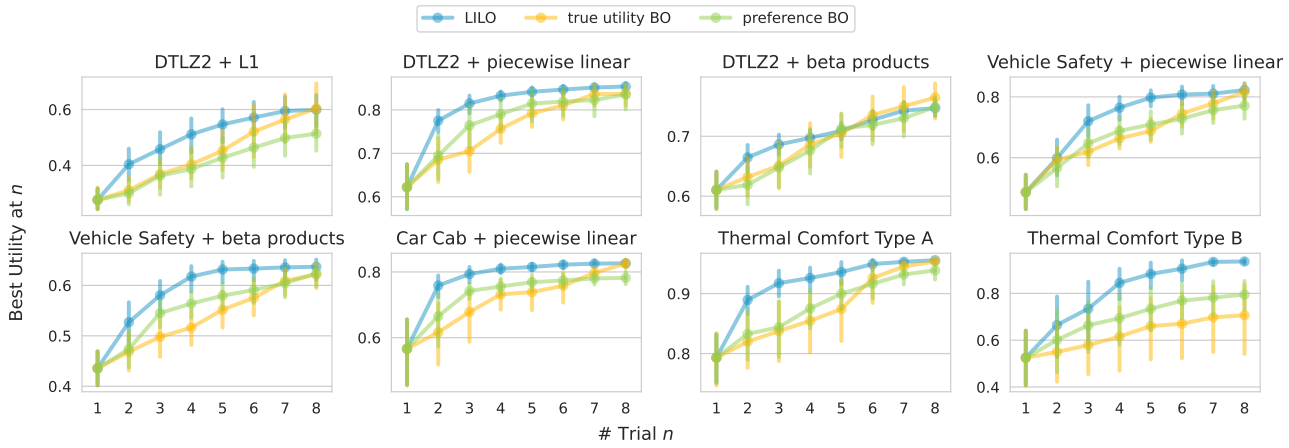
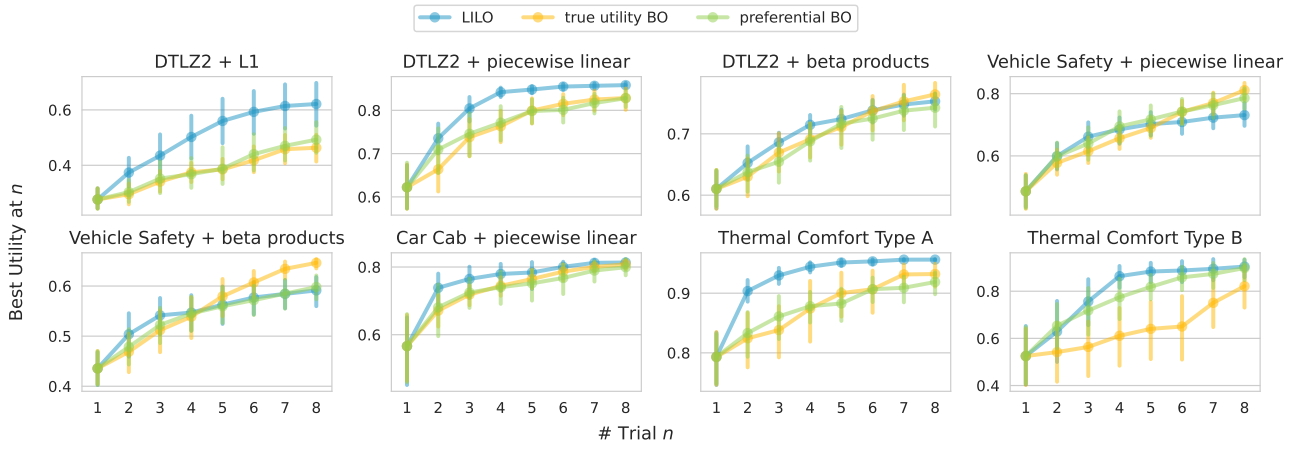


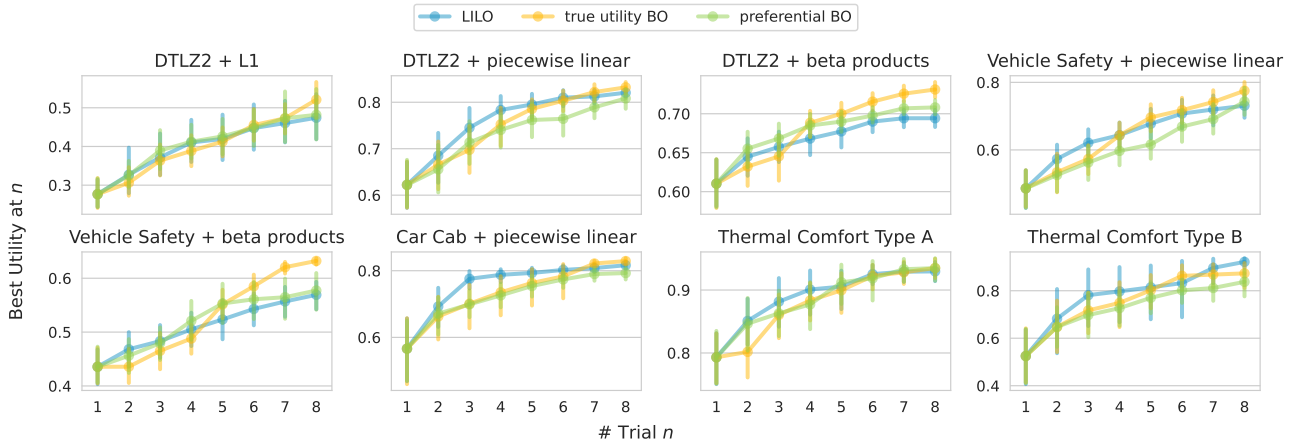
Figure 14. LILO vs. quantitative baselines using different acquisition functions for candidate generation. Results averaged across all 8 environments with 16 replications per environment.



(a) (Noisy) Expected Improvement



(b) UCB ($\beta = 0.5$)



(c) Thompson Sampling

Figure 15. LILO vs. quantitative baselines using different acquisition functions for candidate generation. Detailed results across all 8 environments with 16 replications per environment.

E.7. 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 $B^{\text{pf}} = 2$ and $B^{\text{exp}} = d = 8$.

Results. Table 2 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.

Table 2. 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) DTLZ2 + L1

method # trial	LILO (Llama-3.3-70b)	LILO (Llama-4-scout)	LILO (Qwen3-14B)	preference BO	true utility BO
1	0.28 ± 0.01	0.28 ± 0.01	0.28 ± 0.01	0.28 ± 0.01	0.28 ± 0.01
2	0.42 ± 0.02	0.43 ± 0.02	0.42 ± 0.02	0.31 ± 0.02	0.33 ± 0.02
3	0.54 ± 0.03	0.53 ± 0.02	0.54 ± 0.03	0.35 ± 0.02	0.37 ± 0.02
4	0.56 ± 0.03	0.59 ± 0.02	0.59 ± 0.03	0.37 ± 0.02	0.4 ± 0.02
5	0.62 ± 0.02	0.64 ± 0.02	0.63 ± 0.03	0.41 ± 0.02	0.43 ± 0.02
6	0.64 ± 0.02	0.67 ± 0.02	0.66 ± 0.03	0.44 ± 0.02	0.46 ± 0.02
7	0.67 ± 0.02	0.7 ± 0.02	0.69 ± 0.02	0.46 ± 0.02	0.5 ± 0.02
8	0.69 ± 0.02	0.71 ± 0.02	0.71 ± 0.02	0.5 ± 0.02	0.54 ± 0.03

(b) DTLZ2 + beta products

method # trial	LILO (Llama-3.3-70b)	LILO (Llama-4-scout)	LILO (Qwen3-14B)	preference BO	true utility BO
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)	preference 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

F. 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 1. Example fragments of conversation of 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 2. Example fragments of conversation of LILO with the DM on the Thermal Comfort + Type A environment.