
Multi-attribute Bayesian optimization with interactive preference learning

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Abstract

We consider black-box global optimization of time-consuming-to-evaluate functions on behalf of a decision-maker (DM) whose preferences must be learned. Each feasible design is associated with a time-consuming-to-evaluate vector of attributes and each vector of attributes is assigned a utility by the DM’s utility function, which may be learned approximately using preferences expressed over pairs of attribute vectors. Past work has used a point estimate of this utility function as if it were error-free within single-objective optimization. However, utility estimation errors may yield a poor suggested design. Furthermore, this approach produces a single suggested “best” design, whereas DMs often prefer to choose from a menu. We propose a novel *multi-attribute Bayesian optimization with preference learning* approach. Our approach acknowledges the uncertainty in preference estimation and implicitly chooses designs to evaluate that are good not just for a single estimated utility function but a range of likely ones. The outcome of our approach is a menu of designs and evaluated attributes from which the DM makes a final selection. We demonstrate the value and flexibility of our approach in a variety of experiments.

1 INTRODUCTION

We begin with a motivating example: helping a cancer patient (the “decision-maker” or “DM”) find the best treatment. Cancer treatments exhibit a range of efficacies, side effects and financial costs (Aning

et al., 2012; Wong et al., 2013; Marshall et al., 2016), referred to here as “attributes”. Suppose a patient considers k real-valued attributes when selecting a cancer treatment. Also suppose a time-consuming-to-evaluate black-box computational simulator can use the patient’s medical history to compute the attributes, $f(x) \in \mathbb{R}^k$, of treatment x . The patient has an implicit preference over these attributes and our goal is to help her find her most preferred treatment by querying our simulator.

One existing approach, pursued within preference-based reinforcement learning (Wirth et al., 2017), is to first learn a point estimate of the patient’s preferences (Dewancker et al., 2016; Abbas, 2018) and then optimize assuming this point estimate is correct. We call this the “point-estimate approach”. This approach asks the patient for her preference between attribute vectors $f(x)$ and $f(x')$ corresponding to pairs of treatments x and x' , and uses this information to learn a utility function $\hat{U} : \mathbb{R}^k \rightarrow \mathbb{R}$, e.g., using preference learning with Gaussian processes (Chu and Ghahramani, 2005), such that the judgments are as consistent as possible with the estimated utility differences $\hat{U}(f(x)) - \hat{U}(f(x'))$. It then solves $\max_x \hat{U}(f(x))$ using a method for optimizing time-consuming-to-evaluate black-box functions, such as Bayesian optimization (BayesOpt) (Frazier, 2018), assuming that the estimated utility function is correct. This approach, however, is not robust to residual uncertainty in preference estimates.

To better illustrate that becoming robust to uncertainty in preferences can improve performance, suppose that preference learning suggests that the patient’s true utility function is close to one of L possible functions $\{U_\ell\}_{\ell=1}^L$. Then, a better approach would be to offer the patient a set of treatments $\{x_\ell^*\}_{\ell=1}^L$, where $x_\ell^* \in \operatorname{argmax}_x U_\ell(f(x))$, and let her choose among them. This will provide near-optimal utility to the patient, while optimizing for a single point estimate of the utility function will not. While this approach improves over the standard approach in the utility it provides, it requires solving L optimiza-

tion problems with a time-consuming-to-evaluate objective, which becomes computationally infeasible as L grows. Our approach (described below) delivers similar utility gains using fewer queries to the objective function.

Another approach, which can be used when each attribute is a quantity that the patient wants to be as large (or small) as possible, is to use multi-objective Bayesian optimization (Knowles, 2006; Abdolshah et al., 2019) to estimate the Pareto frontier. This approach, however, typically does not use interaction with the patient to focus optimization on the parts of the Pareto frontier most likely to contain the patient’s preferred solution. Intuitively, such information could accelerate optimization, especially when moderate or large numbers of attributes (> 3) create high-dimensional Pareto frontiers and lead to many Pareto optimal solutions.

Motivated by the shortcomings of existing approaches, we propose *optimization with preference learning*, which learns preferences from the DM’s feedback and acknowledges uncertainty in these learned preferences. In contrast with the point-estimate approach, our approach is significantly more robust to residual preference uncertainty because its optimization actions are appropriate for a range of plausible utility functions. In contrast with multi-objective optimization approaches, learned preferences allow our approach to use fewer objective function queries by focusing optimization on portions of the attribute space most likely to be preferred by the DM. Our approach, therefore, fills an important gap between today’s single-objective optimization approaches, which assume perfect knowledge of preferences, and multi-objective optimization approaches, which do not provide a principled way to accommodate partial preference information.

We develop optimization with preference learning within the specific context of Bayesian optimization. We use pairwise judgments from the DM to form a Bayesian posterior distribution over her utility function and model the attributes f with a multi-output Gaussian process. We then use one of two novel acquisition functions, the *expected improvement under utility uncertainty* (EI-UU) or *Thompson sampling under utility uncertainty* (TS-UU), to iteratively choose designs x at which to evaluate f . Optionally, during optimization, additional DM’s judgments on the evaluated designs may be incorporated into our posterior distribution on the utility. At the conclusion of optimization, a menu of designs is shown to the DM, who makes a final selection.

Our proposed acquisition functions, EI-UU and TS-UU, generalize existing Bayesian optimization acqui-

sition functions to the optimization with preference learning setting. EI-UU is more challenging to maximize than its classical counterpart. However, we provide a simulation-based method for computing an unbiased estimator of its gradient, which we use within a multi-start stochastic gradient optimization method.

The remainder of this paper is organized as follows. We first formalize our problem setting in §2, before defining the EI-UU acquisition function in §3, and reviewing other related work in §4. §5 presents numerical experiments, and §6 concludes.

2 PROBLEM SETTING

We now formally describe our problem setting.

2.1 Designs and Attributes

We assume that both designs and attributes can be represented as vectors. More concretely, we assume that the space of designs can be represented as a compact set $\mathbb{X} \subset \mathbb{R}^d$, and attributes are given by a derivative-free time-consuming-to-evaluate black-box continuous function, $f : \mathbb{X} \rightarrow \mathbb{R}^k$. As is common in BayesOpt, we assume that \mathbb{X} is a simple set such as a hyperrectangle or a polytope, and that d is not too large (< 20).

2.2 Decision-Maker’s Preferences

We assume that there is a DM whose preference over designs is characterized by the the designs’ attributes through a *Von Neumann-Morgenstern utility function* (von Neumann and Morgenstern, 2007), $U : \mathbb{R}^k \rightarrow \mathbb{R}$. This implies that the DM (strictly) prefers a design x over x' if and only if $U(f(x)) > U(f(x'))$. Thus, of all the designs, the DM most prefers one in the set $\operatorname{argmax}_{x \in \mathbb{X}} U(f(x))$. As is standard in preference learning (Fürnkranz and Hüllermeier, 2011), we assume that the DM can provide ordinal preferences between two designs x and x' when shown previously evaluated attribute vectors $f(x)$ and $f(x')$.

2.3 Interaction With the Decision-Maker and Computational Model

In our approach, an algorithm interacts sequentially with a human DM and a time-consuming-to-evaluate objective function (typically a computer model). The algorithm interacts with the computational model simply by selecting a design x and evaluating $f(x)$. We let x_n indicate the n^{th} point at which we evaluate f . As is standard in BayesOpt, the first set of evaluations of f is chosen uniformly at random or according to a space-filling design over the feasible domain (Parker,

2016), and subsequent evaluations are guided by an acquisition function described below in §3.

The algorithm interacts with the DM by receiving ordinal preferences between pairs of attribute vectors. We index interactions with the DM by m , letting y_m and y'_m refer to the attribute vectors queried in this interaction, and $a_m \in \{-1, 0, 1\}$ indicating the DM's response, where $a_m = -1$ indicates a preference for y'_m , $a_m = 0$ indicates indifference, and $a_m = 1$ indicates preference for y_m . We let m_n be the number of design pairs evaluated by the DM by the completion of the n^{th} run of the computational model. We envision that the y_m and y'_m would typically be the attribute vectors for previously evaluated designs, $f(x_n)$ and $f(x_{n'})$, where $m \geq \max(m_n, m_{n'})$.

For concreteness, our numerical experiments assume that, before each evaluation of f , the DM provides feedback on one pair of designs chosen uniformly at random from among those previously evaluated. Our framework easily supports other patterns of interaction. For example, it supports a setting where the DM provides feedback in a single batch after the first-stage evaluations of the computational model are complete, either over random previously evaluated attribute vectors or using a more sophisticated and query-efficient selection of attribute vectors (see, e.g., Lepird et al. 2015). It also supports a setting in which the DM provides feedback at a random series of time points on pairs of previously evaluated attribute vectors of her choosing.

2.4 Statistical Model Over f

As is standard in BayesOpt, we place a (multi-output) Gaussian process (GP) prior on f (Álvarez et al., 2011), $\mathcal{GP}(\mu, K)$, characterized by a mean function, $\mu : \mathbb{X} \rightarrow \mathbb{R}^k$, and a positive definite covariance function, $K : \mathbb{X} \times \mathbb{X} \rightarrow \mathbb{S}_{++}^k$ ¹. Thus, after observing n noise-free evaluations of f at points x_1, \dots, x_n , the estimates of the designs' attributes are given by the posterior distribution on f , which is again a multi-output GP, $\mathcal{GP}(\mu_n, K_n)$, where μ_n and K_n can be computed in closed form in terms of μ and K (Liu et al., 2018).

2.5 Statistical Model Over U

We use Bayesian preference learning (Chu and Ghahramani, 2005; Lepird et al., 2015) to infer a posterior probability distribution over the utility function, U , given preferences expressed by the DM. Although this method is standard in the literature, we describe it here for completeness.

We use a parametric family of utility functions

¹ \mathbb{S}_{++}^k denotes the cone of $k \times k$ positive definite matrices.

$\{U(\cdot; \theta) : \theta \in \Theta\}$, (following, for example, Akrouer et al. 2014; Wirth et al. 2016); a prior probability distribution over θ , p^θ ; and a likelihood function, L , giving the conditional probability $L(a_m; U(y_m; \theta) - U(y'_m; \theta))$ of the DM expressing preference a_m in response to an offered pair of attribute vectors y_m, y'_m with utility difference $U(y_m; \theta) - U(y'_m; \theta)$. The posterior distribution over θ after feedback on m pairwise comparisons, written $p_m^\theta(\theta)$, is then given by Bayes' rule:

$$p_m^\theta(\theta) \propto p^\theta(\theta) \prod_m L(a_m; U(y_m; \theta) - U(y'_m; \theta)).$$

In our approach, we rely only on the ability to sample from this posterior distribution.

The most widely used parametric family of utility functions is linear functions, $U(y; \theta) = \theta^\top y$ (Wirth et al., 2017), with other examples including linear functions over kernel-based feature spaces (Wirth et al., 2016; Kupcsik et al., 2018) and deep neural networks (Christiano et al., 2017). Commonly used likelihood functions include probit and logit (Wirth et al., 2017). In our numerical experiments, for simplicity, we assume fully accurate preference responses, i.e., $L(a; \Delta) = 1\{a = \text{sign}(\Delta)\}$, with parametric families and priors described below. Although we assume parametric utility functions, conceptually, our approach generalizes to handle nonparametric Bayesian preference learning (see, e.g., Chu and Ghahramani 2005). However, this poses additional computational challenges as our approach internally performs optimization given samples of the utility function, which can be slow for nonparametric models.

2.6 Measure of Performance

We suppose that, after N evaluations of the computational model (and m_N judgments on attribute vector pairs), the DM selects her most preferred design among all evaluated designs. Thus, the utility generated, given θ , is

$$\max_{i=1, \dots, N} U(f(x_i); \theta), \quad (1)$$

and we wish to adaptively choose designs to evaluate, x_1, \dots, x_N , to maximize the expected value of (1),

$$\mathbb{E} \left[\max_{i=1, \dots, N} U(f(x_i); \theta) \right], \quad (2)$$

where the expectation is taken over the prior on θ and the randomness in x_1, \dots, x_N (induced by the random first stage of samples and randomness in the DM's responses).

The full BayesOpt with preference learning loop is summarized in Algorithm 1.

Algorithm 1 BayesOpt with preference learning

Require: Prior over θ ; GP prior over f .

- 1: Evaluate a few designs uniformly at random.
 - 2: **for** $n = 0, \dots, N - 1$ **do**
 - 3: Choose y_{n+1}, y'_{n+1} uniformly at random between attributes of previously evaluated designs.
 - 4: Observe preference information, a_{n+1} , and update posterior distribution on θ .
 - 5: $x_{n+1} \leftarrow \arg \max_{x \in \mathbb{X}} \text{EI-UU}_n(x)$.
 - 6: Observe evaluation of f at x_{n+1} , and update posterior GP distribution on f .
 - 7: **end for**
 - 8: **return** Pareto front of $\{f(x_1), \dots, f(x_N)\}$.
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3 ACQUISITION FUNCTIONS

We propose two novel acquisition functions, the Expected Improvement under Utility Uncertainty (EI-UU), and Thompson Sampling under Utility Uncertainty (TS-UU), for selecting points at which to query f . The bulk of our development and analysis focuses on EI-UU, since this is the more difficult of the two to optimize, and this acquisition function performs best in numerical experiments. The description of TS-UU is deferred to the supplementary material.

3.1 Expected Improvement Under Utility Uncertainty (EI-UU)

Expected improvement is arguably the most popular acquisition function in BayesOpt. It has been successfully generalized for multi-objective and constrained optimization (Emmerich et al., 2006; Gardner et al., 2014), and we next show that it can be naturally generalized to our setting as well by extending expected improvement’s one-step optimality analysis (Jones et al., 1998; Frazier, 2018).

After evaluating designs x_1, \dots, x_n , the utility obtained by the DM when she selects her most preferred design among this set is

$$U_n^*(f; \theta) := \max_{i=1, \dots, n} U(f(x_i); \theta).$$

On the other hand, if we evaluate one more design, x , the utility obtained by the DM increases by

$$\begin{aligned} & \max \{U(f(x); \theta), U_n^*(f; \theta)\} - U_n^*(f; \theta) \\ &= \{U(f(x); \theta) - U_n^*(f; \theta)\}^+. \end{aligned}$$

This difference measures improvement from sampling x . Thus, a natural sampling policy is to evaluate the design that maximizes the expected improvement

$$\text{EI-UU}_n(x) := \mathbb{E}_n \left[\{U(f(x); \theta) - U_n^*(f; \theta)\}^+ \right], \quad (3)$$

where the expectation is over both $f(x)$ and θ , and \mathbb{E}_n indicates that the expectation is computed with respect to their corresponding posterior distributions given the previous computational evaluations, $f(x_1), \dots, f(x_n)$, and DM’s responses, a_1, \dots, a_{m_n} .

We call EI-UU the *expected improvement under utility uncertainty* and refer to the above policy as the EI-UU policy. By construction, this sampling policy is one-step Bayes optimal.

3.2 Computation and Maximization of EI-UU

In contrast with the standard expected improvement, EI-UU cannot be computed in closed form. However, as we show next, it can still be efficiently maximized. First, we introduce some notation. Making a slight abuse of notation, we denote $K_n(x, x)$ by $K_n(x)$. We also let $C_n(x)$ be the lower Cholesky factor of $K_n(x)$.

We note that, for any fixed $x \in \mathbb{X}$, the time- n posterior distribution of $f(x)$ is normal with mean $\mu_n(x)$ and covariance matrix $K_n(x)$. Therefore, we can express $f(x) = \mu_n(x) + C_n(x)Z$, where Z is a k -variate standard normal random vector, and thus

$$\text{EI-UU}_n(x) = \mathbb{E}_n \left[\{U(\mu_n(x) + C_n(x)Z; \theta) - U_n^*(f; \theta)\}^+ \right].$$

This implies that we can compute $\text{EI-UU}_n(x)$ using Monte Carlo as summarized in Algorithm 2.

Algorithm 2 Computation of EI-UU

Require: Point to be evaluated, x ; number of Monte Carlo samples, I .

- 1: **for** $i = 1, \dots, I$ **do**
 - 2: Draw samples $\theta^{(i)}$ and $Z^{(i)}$, and compute $\alpha^{(i)} := \{U(\mu_n(x) + C_n(x)Z^{(i)}; \theta^{(i)}) - U_n^*(f; \theta^{(i)})\}^+$.
 - 3: **end for**
 - 4: Estimate $\text{EI-UU}_n(x)$ by $\frac{1}{I} \sum_{i=1}^I \alpha^{(i)}$.
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In principle, the above is enough to maximize EI-UU using a derivative-free global optimization algorithm (for non-expensive functions). However, we could optimize EI-UU more efficiently if we were able to leverage derivative information; this is the case using the derivative information we construct in the following proposition.

Proposition 1. *Under mild regularity conditions, EI-UU_n is differentiable almost everywhere, and its gradient, when it exists, is given by*

$$\nabla \text{EI-UU}_n(x) = \mathbb{E}_n [\gamma_n(x, Z; \theta)],$$

where the expectation is over θ and Z , and

$$\gamma_n(x, Z; \theta) = \begin{cases} 0, & \text{if } U(\mu_n(x) + C_n(x)Z; \theta) \leq U_n^*(f; \theta) \\ \nabla U(\mu_n(x) + C_n(x)Z; \theta), & \text{otherwise,} \end{cases}$$

where the gradient $\nabla U(\mu_n(x) + C_n(x)Z; \theta)$ is with respect to x .

Thus, γ provides an unbiased estimator of $\nabla \text{EI-UU}$, which can be used within a gradient-based stochastic optimization algorithm, such as stochastic gradient ascent, to find stationary points of EI-UU. We may then start stochastic gradient ascent from multiple starting points and use simulation to evaluate the EI-UU for each and select the best. By increasing the number of starting points, we may find a high-quality local optimum and asymptotically find a global optimum.

A formal statement and proof of Proposition 1, along with the statements and proofs of all other theoretical results, can be found in the supplementary material.

3.3 Computation of EI-UU When U Is Linear

While the above approach can be used for efficiently maximizing EI-UU for general utility functions, we can make maximization even more efficient for linear utility functions, the most widely used class in practice.

Proposition 2. *Suppose that $\Theta \subset \mathbb{R}^k$ and $U(y; \theta) = \theta^\top y$ for all $\theta \in \Theta$ and $y \in \mathbb{R}^k$. Then,*

$$\text{EI-UU}_n(x) = \mathbb{E}_n [\Delta_n(x; \theta) \Phi(\zeta) + \sigma_n(x; \theta) \varphi(\zeta)],$$

where the expectation is over θ , $\Delta_n(x; \theta) = \theta^\top \mu_n(x) - U_n^*(f; \theta)$, $\sigma_n(x; \theta) = \sqrt{\theta^\top K_n(x) \theta}$, $\zeta = \frac{\Delta_n(x; \theta)}{\sigma_n(x; \theta)}$, and φ and Φ are the standard normal density function and cumulative distribution function, respectively.

The result above shows that, when each $U(\cdot; \theta)$ is linear, the computation of EI-UU essentially reduces to that of the standard expected improvement, modulo integrating the uncertainty over θ . In particular, the uncertainty with respect to Z can be integrated out. Moreover, in this case one can also derive an analogous result to Proposition 1 for computing the gradient of EI-UU in which the explicit dependence on Z is eliminated as well.

4 ADDITIONAL RELATED WORK

The introduction discusses the two lines of most closely related work: the point-estimate approach pursued within preference-based reinforcement learning (PbRL); and multi-objective BayesOpt.

The most closely related work in PbRL is utility-based PbRL using trajectory utilities (Wirth et al., 2017). This variant of PbRL seeks to design a control policy to maximize the utility of a human subject using features computed from trajectories. Work in this area includes Akrouer et al. (2014) and Wirth et al. (2016). Unlike

our work, the uncertainty in utility function estimates is not considered when performing optimization.

Multi-objective BayesOpt includes Knowles (2006); Bautista (2009); Binois et al. (2015); Shah and Ghahramani (2016); Feliot et al. (2017); Garrido-Merchán and Hernández-Lobato (2019). Multi-objective optimization cannot easily incorporate prior information about the DM’s preferences, though several attempts have been made, mostly through modified Pareto-dominance criteria or weighted-sum approaches (Cvetković and Coello, 2005; Zitzler and Künzli, 2004; Rachmawati and Srinivasan, 2006). Most of this work is outside the BayesOpt framework, with only three exceptions, which we describe below, known to us.

Feliot et al. (2019) proposes a weighted version of the expected Pareto hypervolume improvement approach (Emmerich et al., 2006) to focus the search on certain regions of the Pareto front. However, no method is provided for choosing weights from data, in contrast with our approach’s ability to learn from interactions with the DM. Moreover, this method suffers the same computational limitations of the standard expected Pareto hypervolume improvement approach, limiting its applicability to at most three objectives (Garrido-Merchán and Hernández-Lobato, 2019). Abdolshah et al. (2019) also proposes a weighted version of the expected Pareto hypervolume improvement approach to explore the region of the Pareto frontier satisfying a preference-order constraint over the objectives. Finally, Paria et al. (2019) proposes an approach based on random scalarizations. In contrast with our approach, no method is available for estimating the distribution of these scalarizations from data.

Another related literature is preferential BayesOpt. Preferential BayesOpt (Gonzalez et al., 2017) has been applied to realistic material design in computer graphics (Brochu et al., 2010) and optimization of a parameterized control policy for robotic object handover in (Kupcsik et al., 2018). To apply preferential BayesOpt in our setting, we would choose pairs of treatments x and x' , evaluate our computational model $f(x)$ and $f(x')$ for each, and obtain feedback from the DM on which treatment is preferred. Pairs of treatments would then be chosen to best support the goal of finding the DM’s preferred design. Critically, these methods do not use the attributes, $f(x)$, except to present them to the DM, but instead learn preferences directly as a function of x . Thus, these methods tend to require many queries of the DM (Wirth, 2017; Pinsler et al., 2018). Our approach leverages attribute observations to be more query efficient.

Our work is also related to a line of research on adap-

tive utility elicitation (Chajewska and Getoor, 1998; Chajewska et al., 2000; Boutilier, 2002; Boutilier et al., 2006). Unlike in classical utility elicitation (Farquhar, 1984; Abbas, 2018), which has accurate estimation as its final goal, this work elicits the DM’s utility function with the final goal of finding a good decision, even if this leaves residual uncertainty about the utility function (Braziunas, 2006). However, this work assumes that attributes are inexpensive to evaluate, and that the space of designs is finite, preventing its use in our setting.

Our work builds on BayesOpt (Frazier, 2018), a framework for optimization of time-consuming-to-evaluate black-box functions. Our proposed EI-UU acquisition function is a natural generalization of the classical *expected improvement* acquisition function in standard BayesOpt (Moćkus, 1975; Jones et al., 1998). EI-UU also generalizes the *expected improvement for composite functions* (Astudillo and Frazier, 2019), which can be obtained as a special case when U is known.

Our work is also related to Frazier and Kazachkov (2011), which pursued a similar approach for the pure exploration multi-attribute multi-armed bandit problem with linear utility functions and without iterative interaction with the DM. Finally, an earlier version of this work, which considered linear utility functions only and no iterative interaction with the DM, appeared at Astudillo and Frazier (2017).

5 EXPERIMENTS

We compare the performance of our sampling policies (EI-UU and TS-UU) against the policy that chooses the points to sample uniformly at random (Random), and ParEGO (Knowles, 2006), a popular for multi-objective BayesOpt algorithm. To understand the benefit obtained from preference information within our proposed sampling policies, we also report their performance without preference learning, i.e., where the distribution of θ remains equal to its prior distribution throughout all evaluations of f . In the plots, we distinguish from our sampling policies with preference learning by appending the subindex npl (which stands for “no preference learning”).

In all problems, an initial stage of evaluations is performed using $2(d+1)$ points chosen uniformly at random over \mathbb{X} . A second stage (pictured in plots) is then performed using the given sampling policy. For our algorithms, the outputs of f are modeled using independent GP prior distributions. All GP models in our experiments have a constant mean function and ARD Matérn covariance function with smoothness parameter equal to $5/2$; the associated hyperparameters are estimated under a Bayesian approach. As proposed in

Snoek et al. (2012), for all algorithms, except TS-UU, we use an averaged version of the acquisition function obtained by first drawing 10 samples of the GP hyperparameters, computing the acquisition function conditioned on each of these hyperparameters, and then averaging the results; for TS-UU, a single sample of the GP hyperparameters is used.

In all problems and for each replication, we draw one sample θ_{true} from the prior distribution to obtain a true underlying utility function, $U(\cdot; \theta_{\text{true}})$, which is used to obtain the preference information from the DM. The performance of the algorithms is reported with respect to this true underlying utility function.

Our code and experiments are available at <https://github.com/RaulAstudillo06/BOPL>.

5.1 Synthetic Test Functions

The first three problems use well known test functions drawn from the evolutionary multi-objective optimization literature (Van Veldhuizen and Lamont, 1999; Deb et al., 2005; Knowles, 2006). We define these functions in detail in the supplementary material.

Results of these experiments are shown on a logarithmic scale in Figures 1, 2, and 3. In these three test problems, EI-UU and TS-UU substantially outperform Random and ParEGO. In the first and third problems, EI-UU outperforms TS-UU, whereas in the second problem the opposite occurs. Throughout these problems, EI-UU greatly benefits from preference information. TS-UU also benefits from preference information, especially in the first two problems

5.1.1 DTLZ1a With a Linear Utility

A general form of this test function was first introduced in Deb et al. (2005). The version we use was defined in Knowles (2006). This function has $k = 2$ attributes and is defined over $\mathbb{X} = [0, 1]^6$. In this experiment, we use a linear utility function $U(y; \theta) = \theta y_1 + (1 - \theta)y_2$, and let the prior distribution on θ be uniform over $[0, 1]$.

5.1.2 DTLZ2 With a Quadratic Utility

This function was first introduced in a general form in Deb et al. (2005). We use a concrete version of this function with $k = 4$ attributes defined over $\mathbb{X} = [0, 1]^5$. Here, we use a quadratic utility function $U(y; \theta) = -\|y - \theta\|_2^2$, where θ is uniform over Θ , and Θ consists of 8 points lying in the Pareto front of f , obtained as

$$\Theta = \left\{ f(x) : x_i \in \left\{ \frac{i-1}{3}, \frac{i}{3} \right\}, i \leq 3, x_4, x_5 = 0.5 \right\}.$$

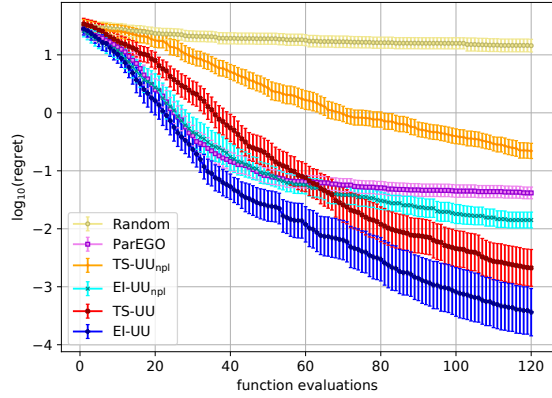


Figure 1: Average performance over 50 replications on the test problem described in §5.1.1.

We envision that, in practice, such utility function could be used for finding designs with attributes as close as possible to an uncertain vector of “ideal” attributes, which could take a range of values depending on the type of DM in question.

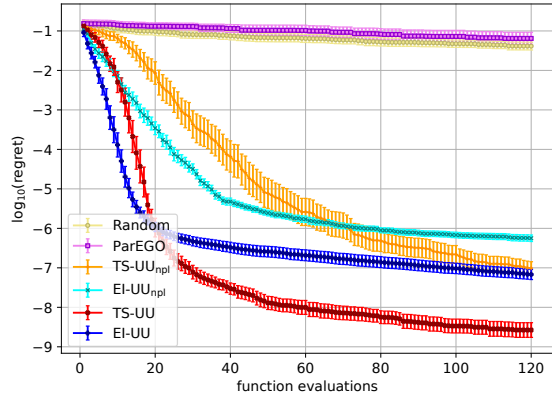


Figure 2: Average performance over 50 replications on the test problem described in §5.1.2.

5.1.3 VLMOP3 With an Exponential Utility

This test function first appeared in Van Veldhuizen and Lamont (1999). It has $k = 3$ attributes and is defined over $\mathbb{X} = [-3, 3]^2$. Here, we use an exponential utility function

$$U(y; \theta) = \frac{1}{3} \sum_{j=1}^3 \frac{1 - \exp(-\theta y_j)}{\theta},$$

and let the prior on θ be uniform over $[0.1, 0.5]$.

We note that, when $\theta \rightarrow 0$ from the right, the solution that maximizes $U(f(\cdot); \theta)$ converges to the solution that maximizes $\frac{1}{3} \sum_{j=1}^3 f_j$ (neutral risk), whereas when $\theta \rightarrow \infty$, it converges to the one that maximizes $\min_{j=1,2,3} f_j$ (worst-case risk). Therefore, if $f_1(x), \dots, f_k(x)$ denote the outcome of an event under k plausible scenarios with known likelihoods, p_1, \dots, p_k (in the above example ($p_j = 1/k$, $j = 1, \dots, k$)), this utility function provides a natural way to optimize the (expected) utility of a DM with uncertain (constant absolute) risk aversion with respect to this outcome.

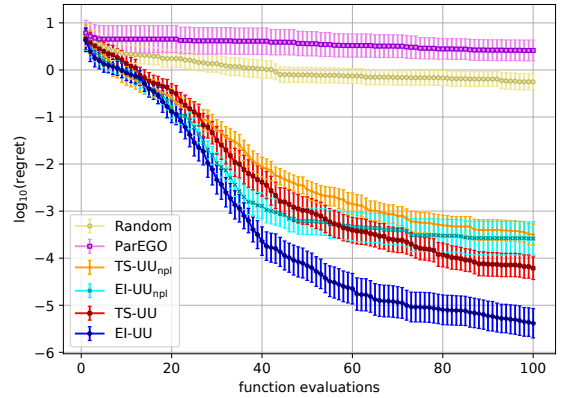


Figure 3: Average performance over 50 replications on the test problem described in §5.1.3.

5.2 Portfolio Simulation Optimization

In this test problem, we use our algorithm to tune the hyperparameters of a trading strategy so as to maximize the return of a DM with an unknown risk aversion tolerance. We envision this as modeling a financial advisor that has many clients, each of which requires customized financial planning based on their own portfolio, and has a different risk tolerance. Using choices made by past clients about which financial product they prefer, the financial advisor may form a probability distribution over utility functions to use when using a computationally expensive simulation to develop a menu of options to show a new client.

We use CVXPortfolio (Boyd, 2017) to simulate and optimize the evolution of a portfolio over a period of four years, from Jan. 2012 through Dec. 2015, using open-source market data; the details of the simulation can be found in §7.1 of Boyd (2017). Here, f has two outputs, the mean and (*minus* the) standard deviation of the daily returns. We use a non-standard utility function that sets $U(y; \theta)$ to y_1 if $\theta \leq y_2$ and ∞ otherwise. This recovers the constrained optimization problem that maximizes $f_1(x)$ subject to the con-

straint that $\theta \leq f_2(x)$. Analogous to the case of linear utility functions, discussed in Proposition 2, it can be shown that for this class of utility functions, EI-UU admits an expression similar to that of the *constrained expected improvement* (Gardner et al., 2014).

Thus, in this setting we wish to maximize average return subject to an unknown constraint on the DM’s risk tolerance level, θ , which we assume is uniform over $[-2, -10]$ (recall that f_2 is *minus* the standard deviation). The hyperparameters to be tuned are the trade, hold, and risk aversion parameters over the domains $[0.1, 1000]$, $[5.5, 8.]$, and $[0.1, 100]$, respectively. Results are shown in Figure 4. Here, the optimal solution is unknown so we report the utility value instead. As before, EI-UU substantially outperforms Random and ParEGO, and is followed in performance by TS-UU. Both EI-UU and TS-UU benefit from preference information.

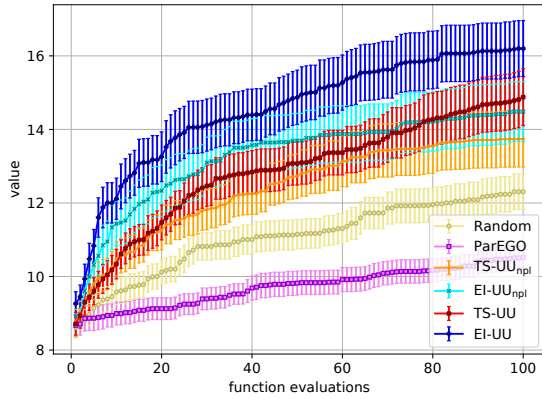


Figure 4: Average performance over 100 replications on the test problem described in §5.2.

5.3 Optimization of Ambulance Bases

In this test problem, we optimize the location of three ambulance bases according to the distribution of the response times. We consider $k = 5$ attributes, representing the number of response times falling within some given intervals of time, and assume a DM considers these attributes to choose the *ideal* locations of the ambulance bases. We let f_j be the number of response times falling within $(5(j-1) \text{ minutes}, 5j \text{ minutes}]$, $j = 1, \dots, 4$, and f_5 be the number of those falling within the interval $(20 \text{ minutes}, \infty)$. Due to the nature of these attributes, which are positive, we model their logarithms as GPs instead of the attributes directly. We then use the utility function

$$U(y; \theta) = \sum_{j=1}^5 \theta_j \frac{\exp y_j}{\sum_{i=1}^5 \exp y_i},$$

which corresponds to a linear utility function over the fraction of response times within the various intervals. Here, θ is taken to be uniform over the set $\Theta = \{\theta : \theta_1 \geq \dots \geq \theta_5 \geq 0 \text{ and } \sum_{j=1}^5 \theta_j = 1\}$.

Results of this experiment are shown in Figure 5. As before, EI-UU substantially outperforms Random and ParEGO, and is followed by TS-UU. In contrast with all other test problems, however, here neither EI-UU nor TS-UU seem to benefit from preference information. A closer inspection to the data obtained from this experiment shows that there is highly concentrated region of designs that poses a high utility value for a wide range of values of θ , which explains this behavior. This also suggests that our sampling policies are able to find *robust* designs if they exist.

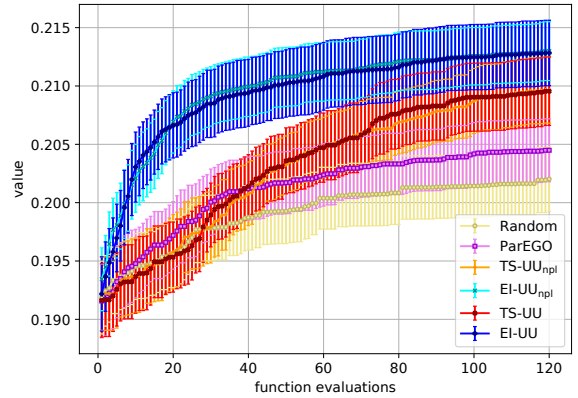


Figure 5: Average performance over 75 replications on the test problem described in §5.3.

6 CONCLUSION

We introduced multi-attribute Bayesian optimization with preference learning, a novel approach for black-box global optimization of time-consuming-to-evaluate physical or computational experiments with multiple attributes that allows us to accommodate partial preference information in a principled way. By leveraging preference information, our approach is more efficient than multi-objective optimization approaches. By acknowledging uncertainty in the DM’s preferences, our approach is more flexible and robust than single-objective optimization approaches that use a point estimate of the DM’s utility function. Relevant directions for future work include developing more sophisticated policies for selecting the pairs of attributes to be shown to the DM, and using nonparametric models for estimating the DM’s utility function.

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